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**PREDICTION OF MASS TRANSFER COEFFICIENTS OF AIR
STRIPPING PACKED TOWERS FOR VOLATILE ORGANIC
COMPOUND REMOVAL**

by

YASSINE DJEBBAR

**A Thesis Submitted to the University of Ottawa in Partial Fulfillment of the
Requirements for the Degree of Doctor of Philosophy in Civil Engineering**

**Under the supervision of
Dr. Roberto M. Narbaitz**

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ABSTRACT

Removal of volatile organic carbons (VOCs) from contaminated ground water using air stripping towers is a best available technology. The design of packed towers necessitates an estimate of the overall mass transfer coefficient, $K_{L,a}$, which is usually computed using parametric models. These models have been found to have several drawbacks and limitations. The main thrusts of this thesis are a critical analysis of the literature and existing data, the compilation of a very large, high quality database, and the development of an alternative methods for predicting $K_{L,a}$.

The thesis describes packed tower air stripping technology, including design considerations, design procedures, and potential operation problems. It presents methods that are used to develop mass transfer coefficient; including theoretical, empirical, and statistical methods. Also, it investigates the collection and use of experimental data utilized for the estimation of mass transfer characteristics.

For the purpose of investigating existing methods and proposing a new one, a new database that is both comprehensive and representative of current air stripping applications has been assembled. The database originates from 12 different studies, tested 19 modern packing types, and investigated the removal of 22 compounds of interest to ground water remediation. The thesis gives an overview of the data selection procedure and the data characteristics including the methods used to estimate experimental mass transfer coefficient, physical characteristics of water, air, VOCs and packings.

An evaluation of the well-accepted Onda correlations concluded that the latter systematically overestimates $K_{L,a}$ for packings that are typically used in full-scale applications. Also, the effect of measurement errors of the variables involved in the calculation of both the experimental and the predicted $K_{L,a}$ values revealed that a large part of the observed difference between the experimental and Onda predictions is due to a lack of fit of the Onda model. Thus, the prediction quality of the correlations still can be improved. Also, experimental $K_{L,a}$ values obtained in this study varied with packing depth in contradiction with a basic assumption of mass transfer theory, which states that $K_{L,a}$ is spatially constant.

Based on the above and using the Onda model form, a new and improved Onda model was developed. The new correlations addressed several of the shortcomings of the Onda model. The

predictions by the improved correlations were superior to those of the Onda model. For the validation database, the average absolute error of the improved correlations' predictions was less than 23% while it was 29% for the Onda model. The improved correlations also estimated well the mass transfer characteristics of structured packings. However, the improved correlations did not simulate well a few observed characteristics of mass transfer, namely the effect of gas flow rate at high gas loading rates, and the effect of packing diameter. In fact, the analysis showed that the predictions cannot be improved further without changing the form of the correlations.

To overcome the chronic limitations of the existing methodology, this thesis proposes a new approach based on neural network (NN) technology. The NN solution can be divided in three steps: (i) architecture selection, (ii) weights optimization, or training, and (iii) validation of the solution. The K_{La} predictions by the NN were superior to those of both the Onda and the improved Onda models. In the validation step, the NN model had an error of 19% which represents more than 40% improvement over the Onda model predictions and more than 20% improvement over the improved Onda model. The NN model addressed many of the shortcomings of both the Onda and improved Onda models. The average absolute error for the validation, as well as for the development data, is less than 19% with 68% of the data being within a factor of 1.27 from the best fit line. The same parameters are 24% and 1.3 for the improved Onda model and 29% and 1.39 for the Onda model.

The main achievement of the neural network model is not only the lower error of its estimates through a better fit of the experimental data, but it is also its ability to describe better the relationships between mass transfer and the operating variables. The NN model successfully simulated the sharp increase in K_{La} at high gas loading rates that both the Onda and improved Onda models were unable to simulate. Moreover, the NN model was able to simulate the high non-linearity of the process, particularly the effect of packing depth, and liquid and gas loading rates. Both parametric and nonparametric methods could not capture the impact of the packing particles geometry via the packing diameter.

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*To my mother and father
for their love and patience
for all they gave me
for all they taught me
for all what I am*

*For my brothers Tayeb and Mohammed
For my beloved sisters
Dzair, Nadia, Houda, Nawel, Souzen, and Samira*

*For the people of Algeria
for those who worked
those who continue to work for a better tomorrow
their sacrifices will not be in vein.*

For all those who struggle for a better and just world

*Yassine Djebbar
Burnaby, October 16, 1998*

.....

The applied scientist needs to cope increasingly with the nonlinear world and the extra mathematical sophistication that this requires. For that is where the rewards are. Linear models are honest and a bit sad and depressing: proportional efforts and results. It is in the nonlinear world that infinitesimal inputs may result in macroscopic outputs (or vice versa). To appreciate what I am hinting at: if electronics were linear we would have no fun with transistors and computers; we would have no TV; in fact you would not be reading these lines.

.....

Michiel Hazewinkel

TABLE OF CONTENTS

ABSTRACT	ii
ACKNOWLEDGMENTS	iv
TABLE OF CONTENTS.....	vii
LIST OF TABLES.....	x
LIST OF FIGURES.....	xi
GLOSSARY	xiii

CHAPTER 1

Introduction

1.1 MOTIVATION	1
1.2 SCOPE	3
1.3 OBJECTIVES.....	4
1.4 THESIS OVERVIEW	4
1.5 REFERENCES	6

CHAPTER 2

Air Stripping Technology

2.1 TREATMENT OF VOC CONTAMINATED GROUND WATER	1
2.1.1 Comparative Advantages of Air Stripping Technology.....	3
2.2 DESCRIPTION OF TOWER AIR STRIPPING SYSTEM	4
2.2.1 Tower shells	6
2.2.2 Packing	7
2.2.3 Liquid distribution.....	9
2.2.4 Packing support.....	10
2.2.5 Mist eliminator	10
2.2.6 Column Hydraulics.....	10
2.2.6.1 Flow Regions	10
2.2.6.2 Pressure Drop.....	11
2.3 OPERATIONAL CONCERNS.....	12
2.3.1 Off-gas treatment.....	12
2.3.2 Fouling and scale formation.....	12
2.3.3 Flow Maldistribution.....	14
2.3.3.1 Axial mixing.....	14
2.3.3.2 Channeling	15
2.4 AIR STRIPPING FUNDAMENTALS.....	15
2.4.1 Henry's Law	15
2.4.2 Design Equations and Procedure.....	19
2.4.3 Air Stripping Tower Design Parameters	21
2.4.4 Estimation of Mass Transfer Coefficient	24
2.5 CONCLUSION.....	25
2.6 REFERENCES	26

CHAPTER 3

Literature Review: Methods for Predicting Mass Transfer Coefficients in Packed Towers

3.1. INTRODUCTION.....	1
------------------------	---

3.2. DIMENSIONAL ANALYSIS AND ITS APPLICATION IN MASS TRANSFER	2
3.3. THEORETICAL BASED APPROACHES	5
3.3.1. MODEL FOR LAMINAR MASS TRANSFER	6
3.3.2. Models for Turbulent Mass Transfer	7
3.3.2.1. Film model	8
3.3.2.2. Penetration model.....	9
3.3.2.3. Film renewal model.....	10
3.3.2.4. Film-penetration model	10
3.3.3. Statistical Models of the Random Packing	11
3.3.4. Mass Transfer from Theory to Practice	12
3.4. REGRESSION BASED APPROACHES	14
3.4.1. Experimental Data	14
3.4.2. Interfacial Area	16
3.4.3. How Mass Transfer Correlations Have Been Developed.....	19
3.4.3.1. Novella et al. (1992)	20
3.4.3.2. Vivian and Peceman (1956)	21
3.4.3.3. Onda et al. (1968)	21
3.4.3.4. Bravo and Fair (1982)	22
3.4.4. Discussion.....	22
3.5. REVIEW OF CURRENT APPLICATION OF MASS TRANSFER CORRELATIONS	25
3.5.1. Current Application of the Onda Model	26
3.5.2. Investigation of the Onda Model.....	28
3.6. NONPARAMETRIC APPROACHES	34
3.6.1. Nonparametric Kernel Regression	34
3.6.2. Neural Network	35
3.7. CONCLUSIONS.....	37
3.8. REFERENCES	39

CHAPTER 4

Data Selection and Parameters Estimation

4.1. DATA BASE DEVELOPMENT	1
4.2. ESTIMATION OF OVERALL MASS TRANSFER COEFFICIENT $K_{L,A}$	4
4.3. ESTIMATION OF END EFFECTS	5
4.4. ESTIMATION OF PACKING AND FLUIDS PARAMETERS	6
4.4.1 Henry's Law Constant.....	7
4.4.2 Diffusion Coefficient	7
4.4.3 Viscosity	8
4.4.4 Packing Critical Surface Tension.....	8
4.4.5 Water and Air Densities	8
4.5. DATA ANALYSIS AND USE	9
4.6. REFERENCES	10

CHAPTER 5

Evaluation of the Onda Mass Transfer Correlations

5.1. INTRODUCTION.....	3
5.2. MASS TRANSFER IN PACKED TOWERS.....	3
5.3. EVALUATION OF THE ONDA CORRELATIONS	7
5.3.1 The Onda model	7
5.3.2 Description of the data base	8
5.3.3 Results of the Onda correlations' evaluation.....	10

5.4	IMPACT OF PACKING DEPTH.....	13
5.5	GENERAL VARIABLES ERROR ANALYSIS.....	17
5.5.1	Error estimation.....	18
5.5.2	Results and Analysis.....	18
5.6	CONCLUSIONS.....	20
5.7	REFERENCES.....	21

CHAPTER 6

Improved Correlations for VOC Air Stripping in Packed Towers

6.1	INTRODUCTION.....	2
6.2	ONDA MODEL.....	3
6.3	RECENT EVALUATIONS OF THE ONDA MODEL.....	5
6.4	DATABASE.....	10
6.5	DEVELOPMENT OF IMPROVED MASS TRANSFER CORRELATIONS.....	13
6.6	CONCLUSIONS.....	25
6.7	REFERENCES.....	27

CHAPTER 7

Neural Predictions of Air Stripping K_{La}

7.1	INTRODUCTION.....	2
7.3	PARAMETRIC APPROACH TO K_{La} ESTIMATION.....	3
7.3	EXISTING PARAMETRIC ESTIMATION METHODS.....	5
7.4	NONPARAMETRIC APPROACH.....	7
7.4.1	SCALING OF THE DATA.....	9
7.4.2	ARCHITECTURE AND TRAINING SELECTION.....	10
7.5	DESCRIPTION OF THE DATA BASE.....	12
7.6	METHOD OF ANALYSIS.....	15
7.7	RESULTS AND ANALYSIS.....	16
7.8	CONCLUSION.....	27
7.9	REFERENCES.....	29

CHAPTER 8

Conclusions and Recommendations

8.1	MAJOR CONCLUSIONS.....	1
8.2	RECOMMENDATIONS FOR FURTHER INVESTIGATIONS.....	3

APPENDICES

APPENDIX A1: Packing Characteristics.

APPENDIX A2: Chemical Characteristics of Volatile Compounds of Interest.

APPENDIX A3: Non Parametric Modeling of Mass Transfer Coefficients for Air Stripping Towers.

APPENDIX A41: Neural Network Estimation of Air Stripping Mass Transfer Coefficients.

APPENDIX A42: Network Selection Approach and Training.

APPENDIX A5: Summary of the Database.

APPENDIX A6: Neural Network FORTRAN Program.

LIST OF TABLES

	Page
Chapter 1	
Table 1.1	Main results of the Ground Water Supply Survey. 1
Chapter 2	
Table 2.1	Conversion of Henrys Law constant from one system of units to another using Equation 2.1. 17
Table 2.2	Safety factor for air stripping tower design. 23
Chapter 3	
Table 3.1	Discrepancy between the exponents of important liquid variables in different correlations (from Manger and Ponter, 1980a). 24
Table 3.2	Average error in the Onda and corrected Onda for data that did not produce better results. 28
Chapter 4	
Table 4.1	Summary of pilot-scale studies selected for the data base. 2
Table 4.2	Names and main characteristics of packings in the database. 3
Table 4.3	List of VOCs used in this study (Haarhoff and Cleasby, 1990). 3
Table 4.4	Critical surface tension for different material. 8
Chapter 5	
Table 5.1	Discrepancy between the exponents of important liquid variables in different correlations (from Manger and Ponter, 1980). 6
Table 5.2	Results of previous investigations on Onda correlation. 8
Table 5.3	Characteristics of the packing materials used in the Narbaitz et al. data base. 9
Table 5.4	Characteristics of the chemical compounds in the data base. 9
Table 5.5	Assessment of the correction (Equation 14) of the Onda predictions. 13
Table 5.6	Commonly reported errors in air stripping variables. 18
Chapter 6	
Table 6.1	Summary of pilot-scale studies selected for the test database. 12
Table 6.2	Names and main characteristics of packings. 12
Table 6.3	List of VOCs used in this study (Haarhoff and Cleasby, 1990). 13
Table 6.4	Average absolute error for different packing diameter definitions. 17
Chapter 7	
Table 7.1	Summary of pilot-scale studies selected for the test database. 13
Table 7.2	Names and main characteristics of packings. 13
Table 7.3	List of VOCs used in this study (Haarhoff and Cleasby, 1990). 14
Table 7.4	Dimensionless numbers mean and standard deviation values used in the neural network data transformation. 17
Appendices	
Table A1	Packing characteristics.
Table A2	Chemical characteristics of volatile compounds of interest.
Table A3	Summary of data.

LIST OF FIGURES

		Page
Chapter 2		
Figure 2.1	Countercurrent packed tower.	5
Figure 2.2	Packed tower air stripping.	6
Figure 2.3	Schematics of some random packings.	7
Figure 2.4	Flooding and pressure drop in random-packed towers (Eckert, 1961).	11
Figure 2.5	Equilibrium distribution at the air-water interface.	16
Figure 2.6	Applicability of Henry's Law and Raoult's Law.	16
Figure 2.7	Definition of tower parameters used in the analysis.	19
Figure 2.8	Optimal design air-to-water ratio for stripping VOCs at typical groundwater temperature of 13°C (Staudinger, 1986).	24
Chapter 3		
Figure 3.1	Boundary layer over a flat plate.	6
Figure 3.2	Laminar liquid film falling over a plate.	7
Figure 3.3	Film theory model.	8
Figure 3.4	Penetration model.	9
Figure 3.5	Film-surface renewal model.	10
Figure 3.6	Film-surface renewal model.	11
Figure 3.7	Flow over surface of a plate.	17
Figure 3.8	Droplet and rivulet flow pattern.	17
Figure 3.9	Mixing at the packing junction.	17
Figure 3.10	Change of the average error in the Onda prediction as a function of the data source.	29
Figure 3.11	Concept of neighborhood in nonparametric regression.	35
Figure 3.12	Concept of neural network.	36
Chapter 4		
Figure 4.1	Definition of Tower parameters used in the analysis.	5
Chapter 5		
Figure 5.1	Definition of tower parameters used in the analysis.	5
Figure 5.2	Experimental vs. predicted mass transfer coefficient for the Narbaitz et al. data base (538 data points).	11
Figure 5.3	Onda simulation results for individual packing.	12
Figure 5.4	Average error of the Onda correlations versus packing diameter.	12
Figure 5.5	Depth segments with decreasing mean concentration gradient (order from 1 to 10).	14
Figure 5.6	$K_L a$ versus segment depth for the case where the initial liquid distribution coincides with the packing's natural distribution frequency (Type I).	15
Figure 5.7	$K_L a$ versus segment depth for the case where the initial liquid distribution has a distribution capacity higher than the packing's natural distribution frequency (Type II).	16
Figure 5.8	$K_L a$ versus segment depth for the case where the initial liquid distribution has a distribution capacity lower than the packing's natural distribution frequency (Type III).	16

Figure 5.9.	Comparison between the expected error in the Onda predictions, the expected error in the experimental K_La and the difference between the Onda and the experimental K_La .	19
-------------	--	----

Chapter 6

Figure 6.1	Average error of the Onda predictions for data from various sources.	6
Figure 6.2	Definition of tower parameters used in the analysis.	14
Figure 6.3	Regressed versus observed liquid phase Sherwood number.	16
Figure 6.4	Results of the improved correlations using the developmental data set.	18
Figure 6.5	Average errors and F factor for the validation data set.	19
Figure 6.6	Average absolute error for individual data sources of the validation data set.	19
Figure 6.7	Average absolute error of the Onda and improved model as a function of the liquid loading for the validation data set.	20
Figure 6.8	Average absolute error of the Onda and improved model as a function of the packing diameter for the validation data set.	21
Figure 6.9	Effect of packing depth on simulated K_La .	22
Figure 6.10	Effect of liquid flow on K_La .	23
Figure 6.11	Effect of gas loading rate on simulated K_La .	24
Figure 6.12	Average absolute error and F factor for structured packings data.	25

Chapter 7

Figure 7.1	Example of the variation of the slope of K_La as a function of the gas loading rate.	7
Figure 7.2	Fully connected network with an input and an output layers and several hidden layers..	8
Figure 7.3	Architecture of a neuron.	9
Figure 7.4	Neural network development steps.	9
Figure 7.5	Definition of tower parameters used in the analysis.	15
Figure 7.6	Architecture of the selected network.	18
Figure 7.7	Results of the neural network using the developmental data base.	19
Figure 7.8	Average errors and F factor for the validation data set.	20
Figure 7.9	Average absolute error for individual data sources of the validation data set.	21
Figure 7.10	Average absolute error of the Onda and improved model as a function of the liquid loading for the validation data set.	21
Figure 7.11	Average absolute error of the Onda and improved model as a function of the packing diameter for the validation data set.	22
Figure 7.12	Effect of packing depth on simulated K_La .	23
Figure 7.13	Effect of liquid flow on K_La .	24
Figure 7.14	Effect of gas loading rate on simulated K_La .	26
Figure 7.15	Simulation results using small and structured packing data.	27

GLOSSARY

∇ and ∂	denote the gradient and the partial/total derivative, respectively.
$\prod X_i$	represents the multiplication of all X_i terms.
ρ	density of the liquid or gas phase, kg/m^3 .
σ_c	surface tension of packing material, kg/s^2 .
σ_L	surface tension of liquid, kg/s^2 .
μ	liquid or gas dynamic viscosity, kg/ms .
ν	liquid or gas kinetic viscosity, s/m^2 .
v	velocity, m/s .
μ_a	the diffusion in the air at temperature T Celsius, Ns/m^2 .
μ_L, μ_G	dynamic viscosities in kg/ms for water and air, respectively.
ρ_G	gas density, kg/m^3 .
ρ_L	liquid density, kg/m^3 .
δ	the liquid film depth, m .
θ	exposure time, s .
%E	percentage difference between Onda-predicted $K_L a$ and measured $K_L a$,
AAE	average absolute error, %.
AGE	average algebraic error, %.
A	Henry's Law temperature dependence coefficient.
a	effective interfacial surface area, m^2/m^3 .
a_w	wetted specific surface area of the packing, m^2/m^3 .
a_s	total specific surface area of packing, m^2/m^3 .
a' and b'	modification factors for the Onda individual liquid-phase and gas-phase mass transfer coefficients, respectively.
b_i	parameters of a regression equation.
c^*	the VOC concentration in liquid phase that is in equilibrium with the VOC concentration in the gas phase, kg/m^3 .
c	Gas phase Onda correlation constant = 2 if $d_p < 15$ mm, otherwise $c = 5.23$.
c_i and c_{i+1}	the VOC concentrations in kg/m^3 the liquid at depths z_i and z_{i+1}
c_e	the liquid effluent VOCs concentration which corresponds to depth Z, the bottom of the packing media, kg/m^3 .
c_o	the liquid influent concentrations at $z = 0$, kg/m^3
C_f	packing friction factor.
C_L	the bulk liquid phase concentration, kg/m^3 .
d	packing characteristic diameter, m .
d_p	nominal packing diameter, m .
D	liquid or air diffusion coefficient, m^2/s .
D_L	diffusion coefficient of the contaminant in the liquid phase, m^2/s .
D_G	diffusion coefficient of the contaminant in the gas phase, m^2/s .
$D_{L,T}$	diffusion in water at specified temperature, m^2/s .
$D_{G,T}$	diffusion in air at specified temperature, m^2/s .
F	linear transform of the log based standard error of estimates.
f, f_1	functional relationships.
g	gravitational constant m/s^2 .
G	the gas volumetric flow rate per unit cross sectional area, $\text{m}^3/\text{m}^2\text{s}$.
G_f	gas mass flux, $\text{kg/m}^2\text{s}$.

H_T and H_{20}	Henry's Law constants at temperature T and 20 degree Celsius, respectively.
H	the Henry's Law coefficient on a volume to volume basis, atm.
H_i	Henry's law constant for component i.
H_D, H_u, H, H_m, H^*	Henry's Law coefficient for different system of units.
HTU, H_L	the height of the transfer unit, m
k	mass transfer coefficients, m/s.
k_L	chemical-specific liquid phase mass transfer coefficient L/T.
k_G	chemical-specific gas phase mass transfer coefficient L/T.
K_L	overall liquid phase mass transfer coefficient, m/s.
K_{La} ,	overall mass transfer coefficient (volumetrically based), 1/s.
K_{La}'	the Onda and the corrected Onda mass transfer coefficient, 1/s.
$K_{La_{obs}}$ or $K_{La_{exp}}$ and $K_{La_{pre}}$	experimental and predicted mass transfer coefficients, respectively, 1/s.
L	the liquid volumetric flow rate per unit cross sectional area $m^3/m^2 s$.
L_r	liquid mass flux, $kg/m^2 s$.
$m(x)$	expected value of the dependent variable y at x.
MW	molecular weight of the VOC.
NTUT	observed total number of transfer units.
NTUE	number of transfer units due to end effects.
NTU	net number of transfer units due to the packing only.
n	number of data points.
p	pressure, N/m^2 .
p_i	partial pressure of component i in the air.
P_t	total operating pressure, atm.
R	stripping factor, dimensionless.
R_u	universal gas constant = 0.0821 L.atm/mol. $^{\circ}$ K.
R_G	percent gas-phase control as predicted by the Onda correlations = $k_{La}/H k_g a$
Sol	water solubility in mmol/L,
T	temperature in degree Celsius.
VP	vapor pressure in mm Hg.
X_i	independent variables that affect the regressed quantity Y.
x_i	concentration of component i in water.
Y	dependent variable.
y_i	observation at x_i .
z	depth of packing media, m.
w_i	weight factor associated to the independent variable i.

Dimensionless numbers

Er	packing efficiency number, dimensionless.
$N_1^k, N_2^{\sigma}, N_3^{\mu}, N_4^g$	are dimensionless numbers that depend on k, σ , μ and g respectively.
Mc	= σ_c/σ_L .
Re_G	gas phase Reynolds number, dimensionless.
Re_L	liquid phase Reynolds number, dimensionless.
Fr_L	liquid phase Froude number, dimensionless.
We_L	liquid phase Weber number, dimensionless.
Sh_L	liquid-based Sherwood number, dimensionless.
Ge	geometry number, the dimensionless.
Sc_G	gas phase Schmidt number, dimensionless.
Sc_L	liquid phase Schmidt number, dimensionless.

CHAPTER 1

INTRODUCTION

1.1 MOTIVATION

Ground water contamination by trace levels of volatile organic compounds (VOCs) has emerged as a major water quality issue in the last two decades. Interest in VOCs in drinking water began escalating in the mid-70s when it became possible to measure these compounds concentrations at $\mu\text{g/L}$ levels. Since then, it has been recognized that volatile compounds are finding their ways into ground water, which is often used as the main source for drinking water.

The United States Environmental Protection Agency (USEPA) conducted a number of surveillance programs such as the National Organics Monitoring Survey (EPA, 1983), the Community Water Supply Survey (EPA, 1981), and the Ground Water Supply Survey (Westrick, 1982). The Ground Water Supply Survey (GWSS) included 945 community water supply sources, and found that ground water contamination by VOCs is a common problem. Table 1.1 summarizes the main findings of the GWSS.

Table 1.1. Main results of the Ground Water Supply Survey.

	random wells	non-random wells
Number of wells	466	475
Contaminated wells	99	131
% wells with more than one contaminant	45	60

VOCs are organic compounds with a tendency to migrate or diffuse from the aqueous phase (water) to the gaseous phase (air), or vice-versa. They are generally "highly" volatile, with

"low" molecular weight. VOCs are a widely used class of compounds employed in many types of industrial, commercial, agricultural, and household activities. There are over nine billion kilograms of this class of substance produced annually (DeMarco, 1983). These compounds find their way into the environment through industrial and municipal wastewater discharges, leachate from deficient, old waste disposal sites that received hazardous chemicals, illegal discharges, and leaks from above or underground storage tanks and pipes. Contamination of drinking water supplies may occur from any combination of these sources. In a given contaminated site, one or two compounds will predominate at relatively high concentrations, and several other compounds will be present at lower concentrations (Dyksen et al., 1982). Trichloroethylene (TCE) is detected most frequently and at the highest concentrations (Staudinger, 1986).

VOCs are considered as a serious public health hazard although evidences of the effects of some VOCs on human health are lacking. In recognition of this problem, the USEPA proposed maximum concentration levels for many VOCs that are frequently found in ground water used for drinking water supply. The USEPA estimated that 3800 community water supplies would have to install treatment processes at a total cost of about US\$1.3 billion to remove VOCs (Westrick, 1982). Hence seeking an engineered cost effective solution and design are more critical than ever before.

In the amendment to the Safe Drinking Water Act in 1986, the USEPA recognized air stripping as a best available technology for VOC treatment. The designer of a stripping tower determines the necessary packing depth Z that yields a pre-specified removal rate. The most critical variable in this calculation is the overall liquid (or gas) phase mass transfer coefficient, K_{La} (or K_{Ga}). To date, parametric correlations are the main approach used to estimate the value of K_{La} , because they are easy to use and avoid costly pilot-scale tests. Existing correlations are not precise; yet, existing designs generally perform well (Bolles and Fair, 1982). This is due to the fact that designers include many different safety factors, some of which may be hidden from view. Bolles and Fair (1982) indicated that the prevalent practice of compounding some safety factors and hiding others has led to the common, but erroneous, impression that existing packed column correlations are reliable when, in fact, they are not. Over the last fifty years, tens of empirically-derived mathematical parametric correlations have been developed to predict K_{La} for packed towers primarily due to the absence of a proven theoretical relationship.

There is agreement in the literature that the Onda model (Onda et al., 1968) is the best model for $K_L a$ estimation in air stripping applications (Staudinger et al., 1990; Roberts et al., 1985 and Lamarche and Droste, 1989). The literature shows also that this model yields satisfactory results for lab data. However, recent research reported 30 to 40 percent deviations from predictions in full-scale and modern applications (Lenzo et al., 1990, Staudinger et al., 1990 and Djebbar and Narbaitz, 1995). Narbaitz and Djebbar (1998) enumerated several factors that contributed to the deviations. These are: (a) the extrapolative nature of the predictions; (b) the limited operating conditions in the databases used to develop the correlations; (c) the parametric regression techniques used to generate these correlations; and (d) the changing nature of mass transfer relationships from one set of operating conditions to another, which are not well understood and are poorly mimicked by current parametric models (Djebbar and Narbaitz, 1995; Bravo et al., 1992). Therefore, several authors expressed the need to improve the predictions through ameliorating existing estimation methods, or by developing new estimation techniques.

Recent developments in statistical theory have provided new modeling approaches using nonparametric methods such as the nonparametric kernel regression and neural network technique. Nonparametric approaches have produced excellent results in other domains such as geology, hydrology, process control, and in market forecasting, especially for pattern recognition and function estimation (Wen and Kung, 1993; French et al., 1992; Härdle, 1989; Adamowski, 1985; Djebbar and Narbaitz, 1995). The author proposes a new approach based on neural network technique to improve the prediction of mass transfer coefficient and to ameliorate the understanding of mass transfer characteristics in air stripping towers.

1.2 SCOPE

While there has been vigorous research activities to evaluate existing methods and to develop new ones using the traditional parametric modeling approach, there has been little, if any, innovation in the approach itself. This thesis proposes a new approach for the estimation of mass transfer coefficients in air stripping towers. Data used in most previous research are typical of laboratory set ups and only a small part of it reflects current full scale applications of air stripping towers. In contrast, this thesis assembled a data base that is comprehensive and representative of modern application of air stripping towers. To the best of the author's

knowledge, this research is one of the first to examine mass transfer characteristics in air stripping towers while addressing its two critical and impeding points: the data and the modeling approach.

1.3 OBJECTIVES

The primary objective of the thesis is to develop a better estimation method for K_La for full-scale air stripping packed tower applications. The use of a new database that is more accurate and more representative of today's applications provides a tool that was lacking, or at least controversial, in previous studies. The use of a new approach to develop the estimation model is expected to overcome some of the limitations of traditional parametric regression methods. Specific objectives of the thesis are as follow:

1. Assemble a new database using full and pilot-scale studies that are representative of field applications of air stripping towers.
2. Evaluate existing methods currently used to estimate mass transfer coefficients.
3. Use the above database to develop a new K_La model based on the Onda correlations. The development approach uses the traditional parametric regression method and addresses the drawbacks of the Onda model.
4. Develop a K_La estimation method using neural network method

1.4 THESIS OVERVIEW

The thesis is divided into eight chapters. The first chapter is an introduction which defines the problem and the study needs, identifies the objectives, and provides a summary of the thesis content.

Chapter two presents air stripping technology for the treatment of VOCs. It presents a comparison between alternative treatment technologies for the removal of VOCs from contaminated ground water. It addresses VOCs characteristics as they relate to aeration technologies, and gives a special emphasis on the Henry's law constant. Then, it discusses air stripping technology along with its main advantages and drawbacks. Following that, it covers

state of the art in design procedures and operation of air stripping towers. Finally, it briefly reviews mass transfer estimation methods.

Chapter three presents a critical review of techniques that have been used to develop mass transfer coefficient prediction methods. It reviews dimensional analysis, which is frequently used in air stripping studies, and investigates basic mass transfer theories and their applications. Next, it covers the collection and use of experimental data, reviews empirical approach that is used to estimate mass transfer components. Then, it presents new approaches to K_La prediction based on nonparametric methods including neural network and nonparametric kernel regression. Finally, it presents a review of existing mass transfer correlations and their limitations.

Chapter four discusses the data used in this study. It describes the selection procedure, presents the characteristics of the database, and gives detailed explanation of the methods used to estimate physical characteristics of water, air, VOCs, and packings.

Chapter five evaluates the well-accepted Onda correlations using the Narbaitz et al. (1998) database. It investigates the Onda model's ability to estimate the mass transfer coefficient in modern air stripping towers. Also, it examines the effect of variables measurement errors on the calculation of both the experimental and the predicted K_La values. Finally, it analyzes the deviation between measured and estimated K_La values, and tries to evaluate the different sources that cause the deviation such as variable measurement errors, and lack of fit of the Onda model.

Chapter six presents an improved Onda correlation developed using the parametric approach and the database presented in Chapter four. It investigates alternative packing diameter definitions, and addresses some of the shortcomings of the Onda model identified in Chapter five.

Chapter seven uses an alternative approach, a nonparametric approach based on neural networks technology, to analyze and predict mass transfer characteristics. The predictive abilities of this technique are compared with those of the parametric approach developed in Chapter six. It investigates the neural network modeling of the effect of the main operating variables, such as liquid and gas flow rates, packing diameter, and packing depth. Also, it compares the predictions of the three models to established theory and observations. Finally, Chapter 8 presents the conclusions of this study and recommendations for further investigations.

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CHAPTER 2

AIR STRIPPING TECHNOLOGY

This chapter consists of a review of air stripping technology for the treatment of VOCs, including design considerations, design procedures and potential problems. First, a comparison between alternative VOC treatment technologies is presented. It is followed by an exposition on VOCs characteristics as they relate to aeration technologies, with an emphasis on Henry's Law constant. Then, packed tower air stripping technology is described along with a discussion of its main advantages and drawbacks. Following that, the state of the art in design procedures and operation of air stripping towers is discussed. Finally a review of mass transfer coefficient estimation methods is presented.

2.1 TREATMENT OF VOC CONTAMINATED GROUND WATER

There are several types of treatment technologies that can be used to remove $\mu\text{g/L}$ levels of VOCs from contaminated ground water. These are: (a) advanced oxidation technologies, (b) membrane separation technologies, (c) granular activated carbon adsorption, and (d) aeration.

Advanced oxidation technologies, like ozonation and UV/oxidation, are intended for the destruction of organic contaminants (VOCs among others). On the other hand, adsorption, air stripping, and membrane technologies are strictly separation processes that transfer the VOCs to another phase or process stream, thus they do not totally eliminate the problem.

Results of VOCs oxidation using ozone showed that aromatic compounds, alkenes, and certain pesticides are removed well, but alkanes are removed poorly (Clark et al., 1988). Chevront et

al. (1990) found that the UV peroxidation system is less expensive than air stripping when the exhaust air from the latter must be treated using vapor phase carbon. However, Topudurti et al. (1993) indicated that UV peroxidation has some drawbacks. These include: (i) the oxidation byproducts are not well identified, (ii) some organics are difficult to oxidize, (iii) oxidant is consumed by side reactions with alkalinity and compounds other than organics, (iv) regular maintenance of the system by trained personnel is required, (v) some compounds may be oxidized to more toxic forms, and (vi) some metals may be oxidized to less soluble forms and precipitate in the treatment unit. These potential disadvantages are common to all advanced oxidation processes. Due to these drawbacks this type of process has been applied to a limited number of sites.

Membrane based technologies, such as pervaporation, could be used to separate the influent liquid into two streams: a VOC highly concentrated stream and a VOC "free" stream. Another membrane process, membrane stripping, could potentially be used to strip VOC from contaminated water (Zander et al., 1989). Though membrane technology has shown promising results, more work is needed for its establishment and full characterization. The literature showed no citation of field scale pervaporation or membrane stripping units for the treatment of contaminated ground water. Membrane stripping showed promise for removing VOCs from low pH and low chlorine waters, but it is incompatible with ozonated waters or waters with high pH or high chlorine concentration. Also, membranes were found to be sensitive to temperature and particulate matter (Zander et al., 1989, Castro and Zander, 1995). Membrane stripping like other aeration processes produces a VOC laden off-gas stream; however, it has a much smaller flowrate.

Granular activated carbon (GAC) uses its adsorption capacity to transfer VOCs to its large internal surface area and produces a cleaner effluent. One of the main advantages of GAC columns adsorbers is their ability to remove 100% of contaminants for a given period of time, something that the other processes can not achieve. This is particularly important for very toxic contaminants. Due to the less than linear adsorption characteristics, GAC is more economical and competitive with decreasing contaminant levels. GAC adsorption has been widely applied for the treatment of VOC contaminated ground water because it can remove most organic contaminants, which are generally in the $\mu\text{g/L}$ levels. However, it should be noted that GAC removes some more efficiently than others, the removal of VOCs ranges from poor to good.

Aeration technologies exploit the natural tendency of VOCs to migrate from water into air. This natural process is accelerated by providing intimate and rough contact between the air and water phases. Different types of aeration equipment can accomplish the contact between air and water. They include bubbling air through a pool of water, spraying water into a stream of air, whirling air and water together in a mechanical device, and forcing air to flow through a packed bed wetted by a stream of water. Aeration equipment can be classified into three categories: (a) water fall aerators such as spray nozzles, cascades, multiple trays, and packed tower columns; (b) injection aerators, such as bubbles of compressed air through the water; and (c) mixing aerators.

In addition to the removal of VOCs, aeration improves, directly or indirectly, other chemical and physical characteristics of water for public and industrial usage. Improvements in water quality by aeration include: (a) removal of taste and odor producing substances such as hydrogen sulfide; (b) removal of corrosive substances such as carbon dioxide and hydrogen sulfide; and (c) removal of substances that consume or interfere with chemicals used in subsequent treatment, for instance, carbon dioxide before lime softening, and hydrogen sulfide before chlorination (Dyksen, 1998).

Important features of an efficient aeration system include a high surface area of contact between the air and water and a reasonable amount of turbulence to bring VOCs to the water surface where the transfer occurs. These factors are maximized in an air stripping tower setting (Treybal, 1980).

2.1.1 Comparative Advantages of Air Stripping Technology

The selection of a treatment option should be sanctioned by a cost effective analysis that is based upon the volume and concentration of contaminated material to be treated, treatment efficiency, discharge criteria and environmental impacts, total capital investment, and annual operating and maintenance cost (Bouwer et al., 1988; Nirmalakhandan et al., 1987). Compared to other aeration processes, counter current packed tower aeration has generally been proven to be the best suited for treatment of drinking water due to its ability to achieve high VOC removal efficiencies at low cost (Bishop and Cornwell, 1984, Lenzo et al., 1990).

The Safe Drinking Water Act (SDWA) acknowledges that air stripping and GAC are the best available technologies (BAT) for removal of most VOCs. However, only air stripping is recognized as BAT for the removal of two weakly adsorbing VOCs: vinyl chloride and ethylene chloride (Clark et al., 1988; Zander et al., 1989). The USEPA selection of air stripping as BAT was based on the degree of treatment that can be achieved with this technology when it is used for water contaminated with the most commonly occurring VOCs.

Flathman et al. (1992) performed modeling studies for GAC and air stripping processes. They concluded that air stripping is a better technology because of the low adsorption efficiency of GAC for methylene chloride and vinyl chloride. Also, they found that the additional cost of transporting and disposing off of the spent carbon, or its regeneration, as well as the additional cost of replacing the fresh carbon in the contactor cell makes activated carbon a more expensive technology. This conclusion was based on three important factors: (i) the documented ease of stripping of concerned VOCs from contaminated ground water in past emergency and remedial field operations, (ii) the regulatory agencies did not require the implementation of vapor-phase scrubbing units, and (iii) the use of air stripping is generally maintenance free unlike granular activated carbon, which requires regeneration and/or disposal off of contaminated media. Gross and TerMaath (1985) found that the removal of TCE using air stripping costs ten times less than using activated carbon.

Even with off-gas treatment, which is rarely necessary in order to comply with regulations, packed tower air stripping is still very attractive in terms of cost, efficiency and operation (Ball et Edwards, 1992, Chevront et al., 1990, Clark et al., 1988). Furthermore, air stripping is still necessary for the removal of compounds that are difficult to oxidize and poorly adsorbed by GAC.

2.2 DESCRIPTION OF TOWER AIR STRIPPING SYSTEM

A packed tower consists of a tower enclosure partially filled with a bed of small pieces of material (packing). In counter current flow systems, air is introduced to the tower below the packed bed and water is distributed over the top of the bed. Thus, the cleanest air contacts the cleanest water at the bottom of the packed bed, providing an opportunity for water to reach very low VOC levels. A schematic of a packed-tower air stripper is shown in Figure 2.1.

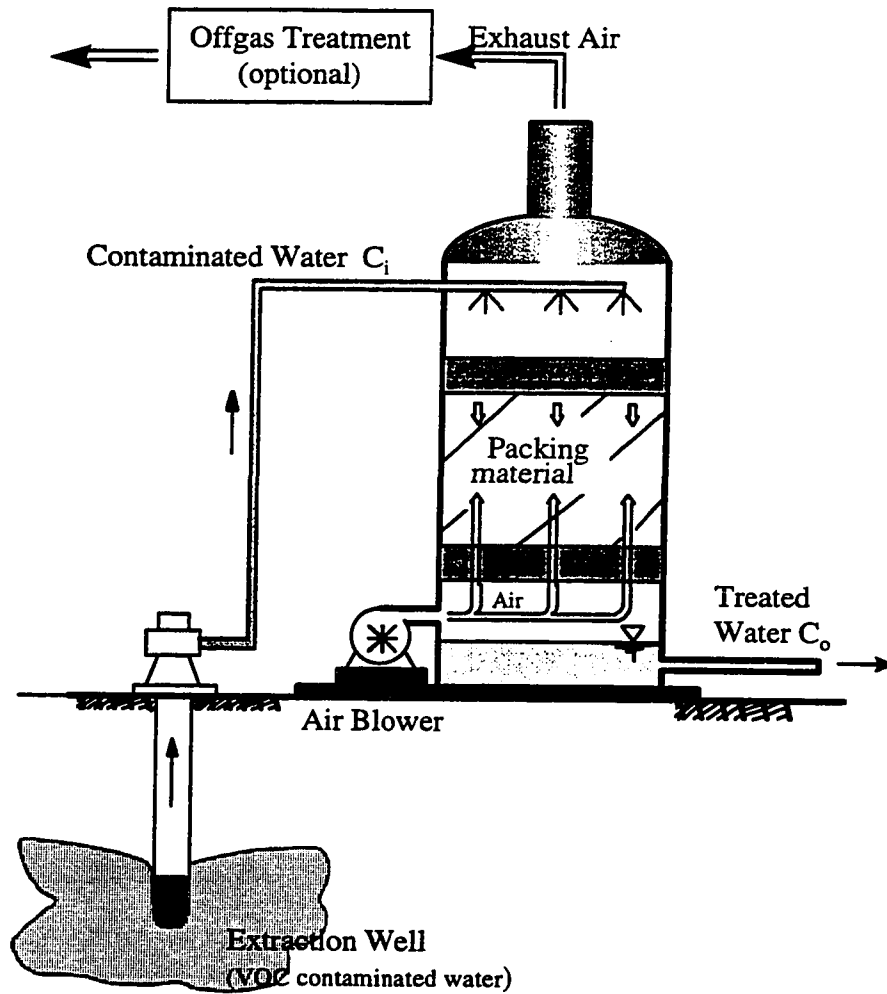


Figure 2.1. Countercurrent packed tower.

Simply stated, air stripping towers are vertical columns which have been filled with packing or devices of large surface areas. Figure 2.2 shows a cut-away view of a typical packed tower air stripper. A typical tower includes a tower shell, packing support, packing, bed limiter, liquid distributor, mist eliminator (optional), air blower, and water pump.

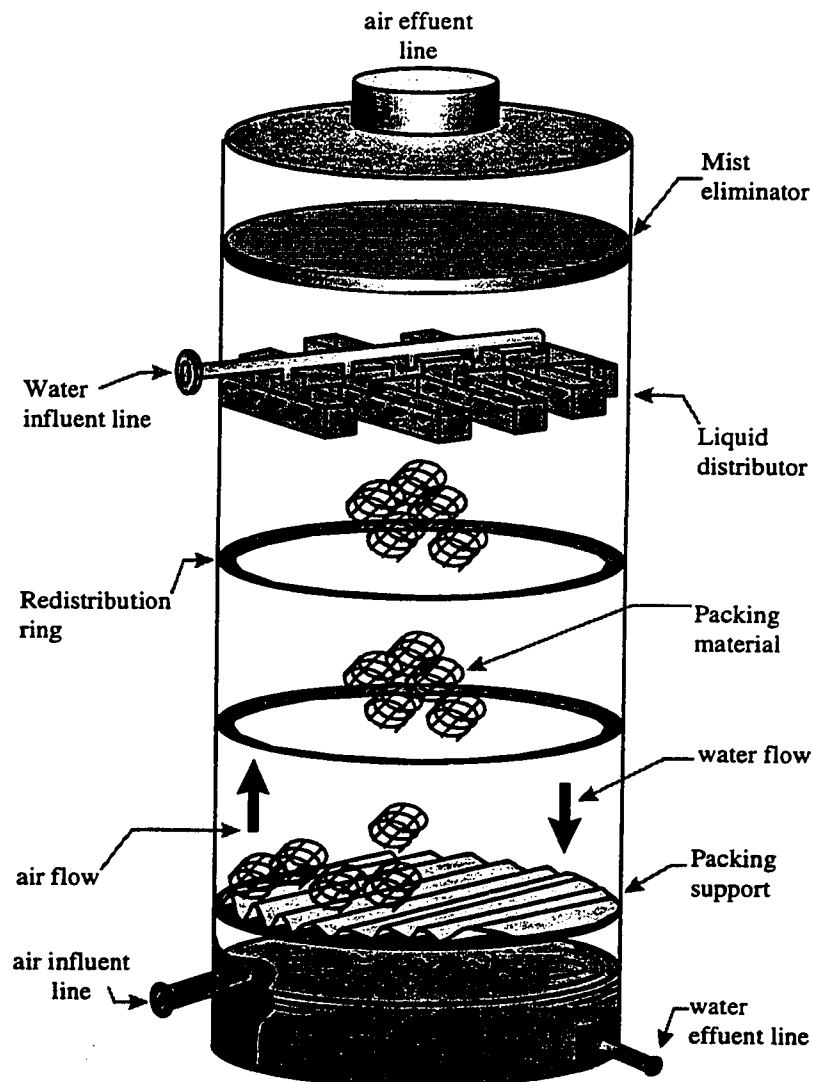


Figure 2.2. Packed tower air stripping.

2.2.1 Tower shells.

For ease of construction and strength, tower shells are usually circular in cross section. They can be made of wood, metal, acid proof brick, glass, plastic, fiberglass, or other material. The recommended ratio of tower diameter to tower height is larger than 1:8 to minimize channeling (Treybal, 1980). The tower shell provides a reservoir for water in the bottom of the tower and may be equipped with an internal seal, or an external trap in the outlet piping, to prevent the air from escaping through the water outlet line. The shell provides a space below the packing to

allow the inlet air even distribution throughout the tower cross section before moving upward through the packing.

2.2.2 Packing

Virtually any material that will promote intimate contact between air and water can be used for tower packing. Material as simple as redwood slats have been used. At the other end of the spectrum are a variety of highly engineered structured packings. The most common packings for VOC stripping have been the random dumped packings. These include such nonproprietary packings as pall-type rings and saddles available from a variety of suppliers, and proprietary packing such as Jaeger Tripacks™, Glitsch Cascade Minirings™, and Ceilcote Tellerettes™. The proprietary packings are claimed to be more efficient and offer lower pressure drop than the nonproprietary packings. However, they have a higher initial cost. Random packings are obtained by simply dumping the packing in an empty tower. To minimize damage to fragile packing, the later can be dumped into the tower which was already filled with water. Table 4.2 in Chapter 4 presents a list of typical packings and their characteristics. Figure 2.3 shows schematics of some random packings.

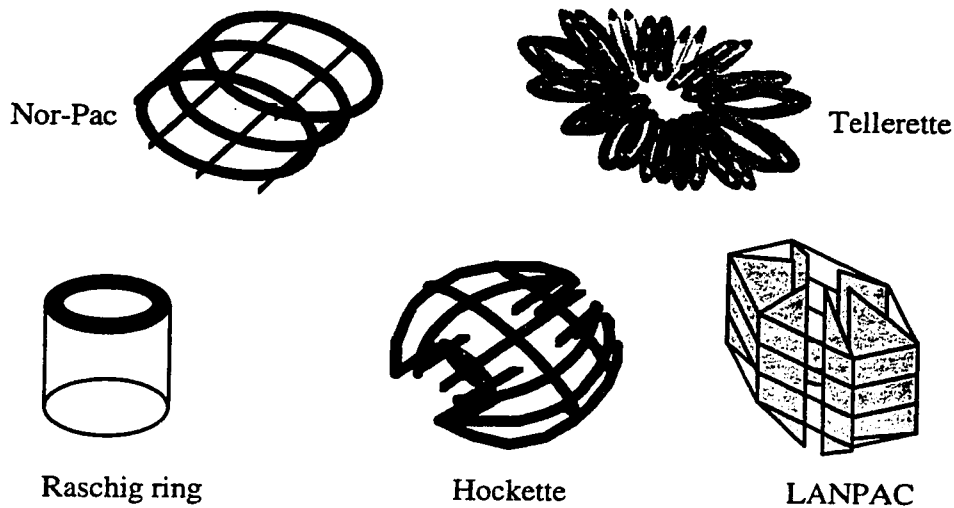


Figure 2.3. Schematics of some random packings.

Chemical engineering applications frequently use traditional packings, such as Raschig, pall and partition-rings, Berl and Intalox saddles, made of ceramics with diameters that are smaller than 5 cm (2 in). However, current air stripping applications generally use 5 cm or larger diameter modern and proprietary packings made of plastic. Packings with small diameters provide larger specific surface area compared to packings with larger diameter. However compared to the former, the later offer less resistance to gas movement. Compared to random packing, structured packing offers higher surface area, lower void ratio and, generally, lower pressure drop because of the defined uniform voids and higher surface area per unit volume (Billet and Bravo, 1989). However, they are more expensive than random packing.

Some packings show a tendency to be arranged in certain patterns, which results in predominant packing pattern in parallel, and/or in series. Patterns in packing promote channeling and reduce mixing resulting in lower transfer efficiency (Hoek et al., 1986). Some types of packing, such as Raschig rings, show neither in parallel nor in series patterns, while other packings, such as Intalox saddles show both in series and in parallel packing patterns. Irregular packing shape will permit a large number of mutual packing arrangement combinations. Hoek et al. (1986) observed differences in performance of up to 60% in two separate hand-placement of the same packing. They concluded that the reproducibility of results with packings that have virtually no tendency to pattern pack is very satisfactory, while packings that show a pattern in pack cause a significant variation in the transfer characteristics from one packing pattern to another.

Mass transfer in packed towers occurs at the interface between water and air, which is called the effective surface area. The effective surface area increases with the increasing geometric surface area. Most mathematical correlations for the prediction of the interfacial area consider the geometrical surface area of the packing as the upper limit of the effective (interfacial) surface area. However, recent work clearly show that for some packings the effective area may substantially exceed the geometrical surface area at high liquid flow rates (Bravo et al., 1992).

Surface characteristics of the packing material affect the flow behavior inside the column and the resulting effective surface area. It is conceivable that the solution will spread into films more rapidly over one material than over another. Because of the obvious importance of the interfacial surface area of contact, a , it has been suggested that anything that might affect the wetting of the packing by the liquid should affect the rate of mass transfer. The wetted area is

the packing surface area that is covered with water. The effective area is the interfacial area between air and water through which the VOC passes from one phase to the other phase. These two areas are intimately related, the greater the wetted surface area is the higher the effective surface area will be. Different packing materials yield different wetted area. For example, using two packings of equal specific surface area, the ceramic packing will lead to larger wetted areas than the plastic packing. However, because of the change in the surface of the packing with the age of the material, the importance of these factors tends to diminish (Billet and Bravo, 1989).

2.2.3 Liquid distribution

A liquid distributor assures adequate initial liquid distribution. After the packing, the liquid distributor may be the most important and controversial device in the tower. Many more instances of poor tower performance have been traced to poor liquid distribution than to improper sizing of the packed bed (Harriott, 1989). A good liquid distributor will apply streams of water to the top surface of the packing bed rather than fine droplets or sprays. Examples of good liquid distributor devices include weir-through distributors, orifice-riser distributors, and orifice-pipe distributors (Hoek et al., 1986). The liquid distribution quality and its effect on mass transfer in air stripping tower are not well characterized. Perry et al. (1990) reported the results of two identical experiments using two different distribution systems, a tubed drip pan with 104 holes per square meter, and a standard weir trough type with 32 distribution points per square meter. The tubed drip pan system showed 50% better efficiency than the standard weir trough system. Harriott (1989), Perry et al. (1990) and Djebbar and Narbaitz (1995) found that each packing has a natural frequency of distribution that will develop in any packed bed of sufficient height. One should not take frequency in its statistical meaning. It is a terminology used to describe the quality of the flow distribution of the flow distributor or the packings themselves. A good liquid distributor is not critical at high liquid loadings (Harriott, 1989). At loadings above 7 L/s/m^2 , a tower may tolerate some minor maldistribution without noticeable impact on performance. However, at loadings less than 3.5 L/s/m^2 , the need for liquid distribution is imperative. If just 2% of liquid runs down the wall of the tower without significant contact with the air, the removal will not exceed 98%, no matter how deep the bed may be (Harriott, 1989).

2.2.4 Packing support

The packing support, or the bed limiter, is a plastic or stainless steel netting mounted on a frame attached to the tower wall at both the top and bottom of the packing. The bed limiter has three functions (i) it prevents the entrainment of packing into the liquid distributor, (ii) it ensures good distribution of the gas and liquid into the packing, and (iii) it supports the packing atop. A packing support is necessary at the bottom of the packed bed, but not at the top. Packing support should have a large open area, with openings small enough to prevent the packing from slipping through.

2.2.5 Mist eliminator

A mist eliminator is an option in an air stripping tower. It can be used to reduce the amount of entrained mist that leaves the tower and form an unsightly plume at the air outlet. As moisture greatly impacts the performance of activated carbon off-gas treatment systems, mist eliminators are essential when such systems are utilized.

2.2.6 Column Hydraulics

Liquid in an operational column can be subdivided into moving liquid and static holdup liquid (Treybal, 1980). On stopping the gas and liquid flows, the moving liquid drains and the static holdup stays as pools in protected interstices in the packing. The latter is largely stagnant and only slowly replaced by fresh liquid. In the transfer operation, the static holdup comes to equilibrium with the adjacent gas. Therefore, interfacial surface area of static holdup does not contribute to mass transfer, except as it is slowly being replaced (Shulman et al., 1955). As the gas flow rate increases, the static holdup increases, and with it increases the pressure drop. The flow rates and the pressure drop are closely related as explained below.

2.2.6.1 Flow Regions. As the gas flow rate increases, one of the following flow regions is encountered successively (Treybal, 1980):

- **Region A.** The liquid contained in the packing bed (liquid hold-up) is reasonably constant with changing gas velocity.
- **Region B.** Both liquid hold-up and pressure drop increase rapidly with gas rate; this is known as loading.
- **Region C.** Also called the flooding region. As the gas rate increases beyond the loading region, one of the following will occur: (i) a layer of liquid forms, through

which the gas bubbles may start building up at the top of the packing; (ii) liquid may fill the tower starting at the bottom, or at any intermediate restriction, or (iii) slugs of foam may rise rapidly through the packing.

Most chemical engineering towers operate in the lower part of the loading region (region B) or just below it. Air stripping towers normally operate at lower pressure drops of less than 400 N/m²/m, because the energy costs associated with the air blower are major part of the overall cost. Eckert (1961) produced a set of generalized curves that relate pressure drop to liquid and gas flow rates (Figure 2.4).

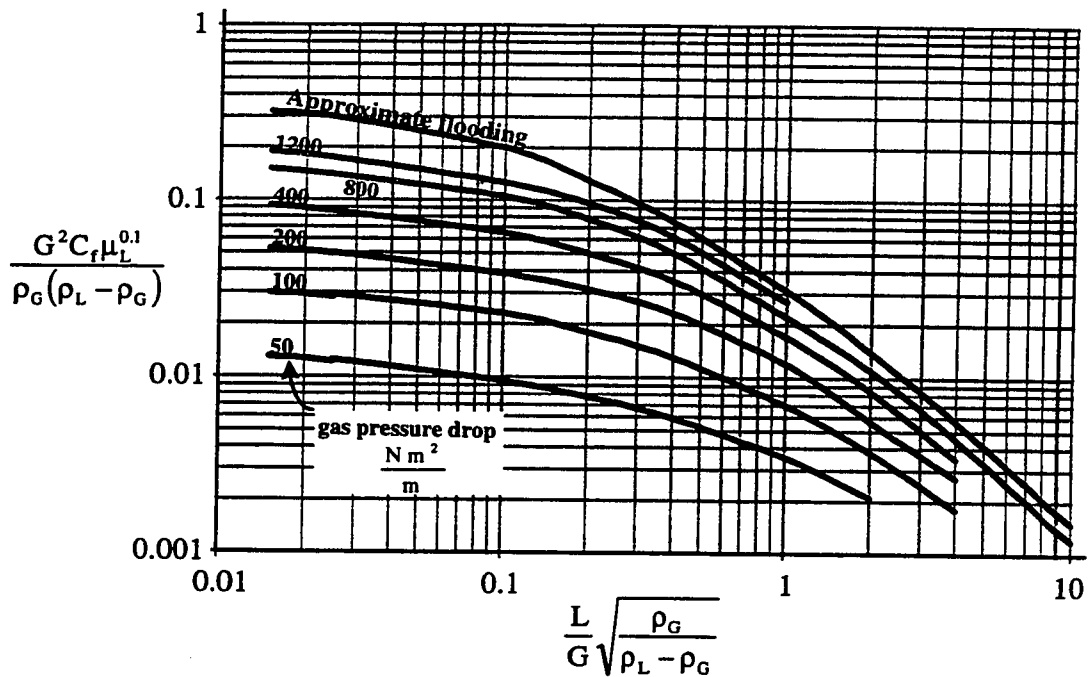


Figure 2.4. Flooding and pressure drop in random-packed towers (Eckert, 1961).

2.2.6.2 Pressure Drop.

Pressure drop is an indication of the difficulty encountered by the air in passing through the packing voids. Air friction in the column is frequently characterized by the packing-dependent dimensionless air friction factor, C_f , which expresses the air pressure gradient across the stripping tower. The lower the air friction factor, the lower the air pressure gradient and, hence, the lower the blower operation cost will be. The pressure drop of the air flowing through a

packed bed is one of the major costs of operating an air stripper (Hand et al., 1986). The set of general curves in Figure 2.4 (Eckert, 1961) relate the expected pressure drop that will result from a set of operating conditions. Tables of packing friction factors for a variety of packing shapes are available from the packing manufacturers, and some of these are listed in Appendix A1.

2.3 OPERATIONAL CONCERNS

Some drawbacks are usually associated with air stripping technology. Many are associated with poor design practice and they can be minimized through sound design practices. These drawbacks include scale formation, fouling and poor flow patterns. However, it appears that air contamination by air stripping off-gases is the main drawback.

2.3.1 Off-gas treatment

The exhaust air from a stripping tower carries the contaminants out of the stripper and into the atmosphere where the volatile organics are dissipated by the velocity of the air stream and any wind currents. Once in the atmosphere, these chemicals will gradually break down by natural UV degradation. VOCs are implicated in ground level ozone air pollution.

In most locations off-gas treatment has not been required due to the relatively small mass of VOCs emitted (Byers and Morton, 1985). Compliance with emission standards can be controlled by the process stack design using atmospheric dispersion models, where plume dispersion can be enhanced by increasing the stack height and the exit gas velocity. Another alternative consists of vapor-phase activated carbon adsorption. Because of the low levels of VOC emissions, a non-regenerable carbon system is usually sufficient (Byers and Morton, 1985). Byers and Morton (1985) indicated that vapor-phase activated carbon adsorbs about ten times as much VOC per pound of activated carbon as the aqueous-phase activated carbon. Other methods for VOC emission control are available, but are not competitive (Cheuvront et al., 1990). These include UV-oxidant destruction systems and catalytic incineration.

2.3.2 Fouling and scale formation

Two factors are typically responsible for fouling, these are precipitation of scale forming salts, and growth of iron-oxidizing bacteria (Ball and Edwards, 1992). Removal of CO₂ in air

stripping process results in a shift in carbonate equilibrium, leading to the consumption of hydrogen ion and an increase in pH. If pH is increased high enough, scale-forming salts, including calcium carbonate, can precipitate out of solution and deposit on the packing (Ball and Edwards, 1992). The saturation of water with oxygen during air stripping can also result in oxidation and precipitation of certain metals. Ground water frequently contains significant quantities of iron and manganese in soluble ferrous and manganous forms. Upon aeration, the insoluble oxidation products, ferric hydroxide and manganese dioxide, can form and deposit on the packing media.

In a survey that looked at 72 packed columns throughout the USA, Dyksen et al. (1995) found that only twelve columns experienced some type of deposition on the media. The build up is made of iron, calcium carbonate, biomass or a combination of these three (Dyksen et al., 1995). Hand et al. (1986) found that the precipitation does not seem to cause significant operational problems in most cases. Hand et al. (1986) conducted continuous experimental runs in 2.5 and 3 m tall air stripping towers for four and eighteen months, respectively. The concentrations of iron and manganese in the influent stream were about 1.5 and 2.5 mg/L, respectively. Only a small amount of precipitation occurred and it did not increase the gas pressure drop or affect the removal of VOCs. If scale formation is suspected, chemical analysis is necessary to evaluate its potential effect on the tower normal operation, as well as necessary pretreatment options to avoid deposition.

In South Florida there are many air strippers that operate without pretreatment (such as lime softening/sedimentation/filtration) and the local iron levels are in the order of 3 mg/L. In these units fouling is an important problem. In Pompano Beach, two towers are periodically filled with muriatic acid to dissolve the scale. Use of packing with larger size may reduce potential plugging problems.

The presence of iron can also lead to the growth of iron-oxidizing bacteria. A prototype air stripping column (Norton et al., 1991) used to treat water contaminated with BETX (benzene, ethylbenzene, toluene and xylene) experienced fouling after two months of operation. The removal efficiency did not suffer because of this, but, the head losses increased to above 10 cm from the initial 1.5 cm. The fouling material behaved like a biofilm containing encapsulated

hydrocarbon particles. The packing medium had to be cleaned by rinsing and agitating the plastic packing in a cleaning tank.

2.3.3 Flow Maldistribution

In theory, the flow pattern in packed columns is assumed to be plug flow. However, this is seldom the case due to several factors such as non uniform velocity profiles, short circuiting, bypassing, channeling, velocity fluctuations due to molecular and turbulent diffusion, uneven flow distribution, effect of contactor shape and tower internals, back flow of fluids due to velocity differences between phases, or recycling due to agitation (Buchanan, 1971).

2.3.3.1 Axial mixing. The conception of an air stripping column is based on the assumption that the gas and liquid flows follow a plug flow pattern. However, as described by the following sentences, there are number of situations where the flow deviates from plug flow. Non uniformity of packing and uneven distribution of liquid lead to channeling: regions where the liquid flow is abnormally great. The liquid in the static holdup moves forward much more slowly than the liquid in the moving holdup. Drops of liquid falling from a packing piece may be blown upward by the gas. The downward movement of the liquid induces downward movement of some of the gas. All these phenomena can be categorized as follows (Buchanan, 1971):

- **Axial dispersion:** is the spreading of the residence time in unidirectional flow due to the departure from purely piston-type flow. The fluid particles moves forward, but at different speeds. Axial dispersion is mainly due to molecular and eddy diffusion.
- **Back mixing:** is the backward flow in a direction opposite to that of the flow caused by frictional drag of one fluid upon the other and entrainment of the liquid. Back mixing may induce circulation of gas downward.
- **Axial mixing:** is the relative movement within each fluid, parallel to the axis of the tower. Axial mixing is mainly due to uneven distribution of the liquid, channeling, and it is further magnified by molecular or eddy diffusion.

Back mixing and axial dispersion create localized low values of the air to water ratio, which decreases the driving force for mass transfer and necessitates taller towers to achieve the same level of treatment. The effects of the above can be minimized by installing redistribution rings, and packing support nets which help redistribute the liquid flow.

2.3.3.2 Channeling. Liquid tends to move to preferred channels as it passes down the column, where local flow rates may be several times the average flow rate. Porter and Templeman (1968) estimated the wall flow to be 40-60% of the total flow for a column whose diameter is 20 times the packing size. These percentages decrease to 10-20% for columns whose diameter is 25 times the packing size. Channeling and wall flow change the local stripping factor by changing the local ratio of liquid to gas flow rates. In columns with small diameters, there is a marked tendency for the liquid to migrate toward the walls. This wall flow is considered almost totally bypassed. Wall flow tends to disappear in columns with large diameter. Even though the column to packing diameter was at least 8:1 and redistribution rings were placed at spaces equivalent to three column diameters, as suggested by Treybal (1980), channeling was significant in the Lenzo et al. (1990) experiments. Visual observation gave Lenzo et al. (1990) the impression that up to 25-50% of the flow was channeled for 12.7 mm Raschig rings. However, it was less important for 12.7 mm saddles and 6.35 mm Raschig rings (Lamarche and Droste, 1989). Wall flow tends to occur more frequently in packing that has a tendency to pattern pack (Harriott, 1989).

The drawbacks discussed earlier are common in air stripping towers because of poor design practices. These drawbacks can be minimized when proper design and operation practices are observed. The following section discusses some of these practices.

2.4 AIR STRIPPING FUNDAMENTALS

Stripping VOCs from contaminated water relies on the natural faculty of VOCs to migrate from one phase to the other. This faculty is measured by the Henry's Law constant of the VOC. The higher this constant, the higher will be the driving force behind the transfer of VOC from water to the air, and the more effective aeration will be as a treatment alternative. Byers and Morton (1985) indicated that Henry's Law constant and the diffusion of the compound in both water and air are the primary variables that determine the rapidity of movement of the compound from one phase to the other, and therefore, the mass transfer coefficient.

2.4.1 Henry's Law

When air and VOC contaminated water are in contact, the concentration of VOC in the air will eventually reach equilibrium with the concentration of VOC in the water phase. Aeration-based

treatment technologies basically provide an environment that accelerate this process. However, the concentrations of the two phases at the interfaces are expected to be in equilibrium all the time (Lewis and Whitman, 1924). The equilibrium at the interface causes a concentration gradient to take place between the interface and the bulk liquid or air phase as shown in Figure 2.5. The concentration gradient forces the VOC to migrate from the phase with higher concentration, vis-à-vis the equilibrium state, to the other phase.

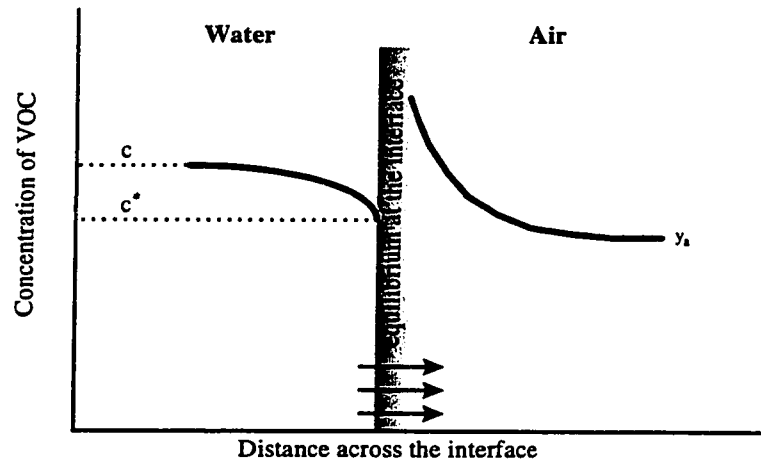


Figure 2.5. Equilibrium distribution at the air-water interface.

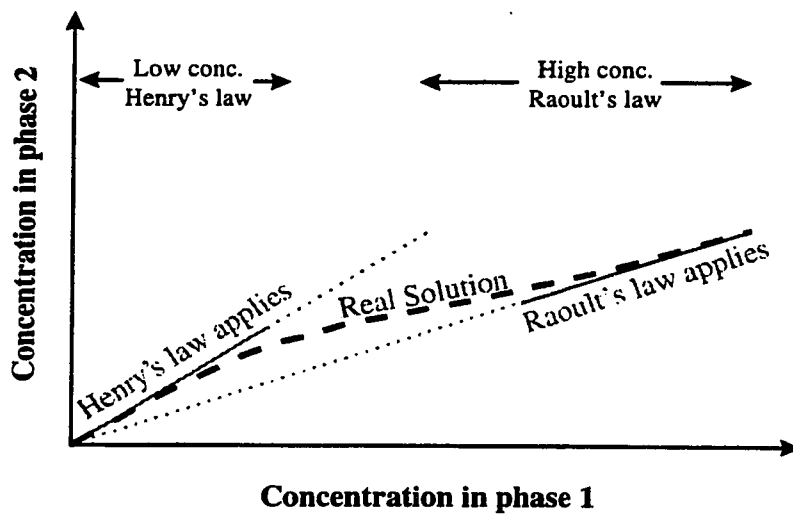


Figure 2.6. Applicability of Henry's Law and Raoult's Law.

Inspection of the partition of VOCs between air and water as a function of the VOC concentration in the liquid phase reveals two distinct trends at extreme VOC concentrations. At both very low and very high liquid VOC concentrations, the VOC vapor pressure is proportional to its mole fraction in the liquid phase, but with different proportionality constants (Figure 2.6).

At low concentration levels, the proportionality constant is called Henry's Law constant, while at high concentration level, the proportionality constant is called Raoult's law constant. VOCs in ground water are predominantly found at very low concentrations, e.g., in the parts per billion range, therefore Henry's Law describes equilibrium conditions for air stripping applications.

Henry's Law states that the mole fraction of any gas that will dissolve in any volume of water, at constant temperature, is directly proportional to the pressure that the gas exerts above water. Henry's Law can be expressed as,

$$p_i = H_i x_i \quad (2.1)$$

where p_i = partial pressure of component i in the air; H_i = Henry's Law constant for component i ; and x_i = concentration of component i in water. The partial pressure is typically expressed in atmospheres. Liquid-phase concentrations are expressed as mole fractions, moles per unit volume, or mass per unit volume. Chemists, chemical engineers and environmental engineers use different sets of units; accordingly, they have expressed Henry's Law in a number of different units.

Table 2.1 Conversion of Henrys Law constant from one system of units to another using equation (2.1).

Conversion equation	Unit of p	Unit of x	Unit of Henry's Law
H_u	$\frac{\text{mol gas}}{\text{mol air}}$	mg / L	mg/L
$H_c = 1/H_u$	$\frac{\text{mol gas}}{\text{mol air}}$	mg / L	$\frac{1}{\text{mg / L}}$
$H_D = H_u \cdot 55600 \text{ MW}$	$\frac{\text{mol gas}}{\text{mol air}}$	$\frac{\text{mol gas}}{\text{mol water}}$	$\frac{\text{mol gas / mol air}}{\text{mol gas / mol water}}$
$H_m = H_u \text{ MW}$	$\frac{\text{mol gas}}{\text{mol air}}$	mol gas / m ³	$\frac{\text{m}^3 \text{ water}}{\text{mol air}}$
$H = H_u \frac{55600 \text{ MW}}{4.56 (T + 273)}$	kg/m ³ , mol/L, mg/L	kg/m ³ , mol/L, mg/L	unitless

Table 2.1 shows some of these different units and how to convert from one system of units to another (Cornwell, 1990; Staudinger, 1986). In Table 2.1 MW = molecular weight of the VOC, and T = temperature in degree Celsius. This thesis uses the H form of Henry's constant with the unit of atm.

Factors governing gas solubility in water are temperature, pressure, and to a lesser extent, dissolved solids in the water and the chemical nature of the gas (Haarhoff and Cleasby, 1990). Because ambient conditions prevail in packed tower air stripping, the pressure can be assumed constant and its effect is disregarded (Roberts and Levy, 1985).

Temperature has a significant impact on Henry's Law constant. A 10°C temperature increase may double or even triple its value. With the assumption that the enthalpy changes are negligible over the expected temperature variation, and given Henry's Law constant at T = 20°C, (H_{20}), Henry's Law constant at T can be estimated by the following equation (Haarhoff and Cleasby, 1990):

$$H_T = H_{20} \left(\frac{293}{273 + T} \right)^{10^A \left(\frac{1}{293} - \frac{1}{273 + T} \right)} \quad (2.2)$$

where A is a constant. Values of H_{20} and A for different VOCs are given in Appendix A2. Haarhoff and Cleasby (1990) recommended the use of A = 4500 when the experimental value of A is not available.

Many studies (Gossett et al., 1985, Gossett, 1987, Munz and Roberts, 1987) have concluded that, practically, mutual effects on Henry's Law constants in aqueous organic mixtures is negligible. Lamarche and Droste (1991) and Gossett (1987) suggested that there is no mutual effect up to a total mixture concentration of 375 mg/l. Also, they indicated that the practical impact of ionic strength appears to be minimal.

Reliable values of Henry's Law constant are often not available for solutes of environmental concern. It should be noted that literature values for H may vary considerably for a given compound. Lamarche and Droste (1989) determined Henry's Law constant experimentally and their measurements had coefficients of variation that varied between 8 and 63% with an average value of 34%. In the absence of direct equilibrium measurements, Haarhoff and Cleasby (1990),

among others, recommended the use of water solubility and vapor pressure data using the following equation:

$$H = 1.32 \frac{VP}{Ru(T + 273) Sol} \quad (2.3)$$

where H = dimensionless Henry's Law constant, VP = vapor pressure in mm Hg, Sol = water solubility in mmol/L, Ru = universal gas constant = 0.0821 L.atm/mol.°K, and T = temperature in °C. Haarhoff and Cleasby (1990) indicated that whenever available, measured Henry's Law constants should be used instead of equation (2.3).

2.4.2 Design Equations and Procedure

Packed towers for air stripping are generally designed based on the change in liquid phase concentrations and $K_L a$. Using the Kavanaugh and Trussell (1980) and Treybal (1980) approach, the packing depth element z , i.e. from depth z_1 to z_2 (Figure 2.7), is given by:

$$z = \int_{z_i}^{z_{i+1}} dz = \frac{L}{K_L a} \int_{c_i}^{c_{i+1}} \frac{dc}{c - c^*} \quad (2.4)$$

where K_L = overall liquid phase mass transfer coefficient, m/s; a = effective interfacial surface area, m^2/m^3 ; c^* = the VOC concentration in liquid phase that is in equilibrium with the VOC concentration in the gas phase (Figure 2.5), kg/m^3 ; c_i and c_{i+1} = the VOC concentrations in the liquid at depths z_i and z_{i+1} , respectively, kg/m^3 ; and L = the liquid volumetric flow rate per unit cross sectional area ($m^3/m^2 s$).

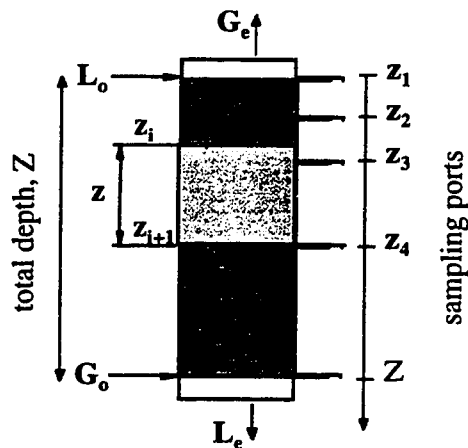


Figure 2.7. Definition of tower parameters used in the analysis

Air stripping applications are generally analyzed using the transfer unit model (Treybal, 1980; Kavanaugh and Trussell, 1980). This model assumes that: (i) the mass transfer coefficient is constant throughout the tower; (ii) plug flow conditions prevail; (iii) the volumetric air to water ratio, G/L , is constant, i.e., the volume of the VOCs removed from the water is too small to affect the volume of the air or water flows; (iv) Henry's Law applies; (v) the operation is isothermal, and steady-state conditions prevail. These assumptions are generally considered met in current air stripping applications. Using these assumptions, equation (2.4) can be solved analytically to yield:

$$z = \left[\frac{L}{K_L a} \right] * \left[\frac{R}{R-1} \text{Ln} \left\{ \frac{c_1 (1-1/R) + c_o / R}{c_2 (1+1/R) + c_o / R} \right\} \right] = [\text{HTU}] * [\text{NTU}] \quad (2.5)$$

where $R = \frac{H G}{P_i L}$ = the stripping factor, dimensionless; HTU = the height of a transfer unit, m;

NTU = the number of transfer units (dimensionless); c_o = the liquid effluent VOCs concentration which corresponds to depth Z , the bottom of the packing media in Figure 2.7, kg/m^3 ; H = the Henry's Law coefficient on a volume to volume basis, atm; P_i = the total operating pressure, atm; and G = the gas mass flow rate per unit cross sectional area, $\text{m}^3/\text{m}^2\text{s}$. The value of NTU indicates the difficulty in removing the solute from the liquid phase, while HTU characterizes the mass transfer efficiency from the liquid to the gas phase.

For the total packing height, Z , equation (2.5) becomes:

$$Z = \left[\frac{L}{K_L a} \right] * \left[\frac{R}{R-1} \text{Ln} \left\{ \frac{c_1/c_o (R-1) + 1}{R} \right\} \right] = [\text{HTU}] * [\text{NTU}] \quad (2.6)$$

where c_o is the liquid influent concentration at $z = 0$, kg/m^3 . This is the most frequently used equation. The mass transfer coefficient $K_L a$ can be obtained from either equations (2.5) or (2.6), as

$$K_L a = \frac{L}{z} \text{NTU} \quad (2.7)$$

In a column with multiple sampling ports, when the section of the column being analyzed does not include the bottom of the column, the gas phase concentration entering this section is not zero, and equation (2.5) must be used to calculate $K_L a$. Equation (2.6) is only valid for an inflow gas concentration equal to zero. Rearranging equation (2.7) gives:

$$NTU = K_L a \left\{ \frac{z}{L} \right\} \quad (2.8)$$

During experimental studies including pilot scale tests, the liquid phase VOC concentrations are measured at several packing depths. Based on these concentrations one can plot NTU versus $\left\{ \frac{z}{L} \right\}$, and if mass transfer is described by equation (2.8), it should yield a straight line with a slope equal to $K_L a$.

Many previous air stripping studies used estimates of $K_L a$ that are based just on an influent and an effluent samples from influent and effluent lines so they include end effects. The transfers that occur inside the column above and below the packing are called end effects. Spedding (1988) indicated that end effects accounts for 10 to 36% of the total transfer.

2.4.3 Air Stripping Tower Design Parameters

The design of an air stripping tower is based on the determination and choice of: (i) tower geometry, (ii) packing characteristics such as packing material, diameter, and specific surface area; (iii) air and water loading rates; and (iv) contaminant characteristics, such as Henry's Law constant and diffusion coefficients in water and air. These parameters can be determined either directly from data supplied by the manufacturer, experimental data, published data, or using existing equations.

Most packed towers operate just below, or in the lower part of, the loading region (Figure 2.4) with a packing pressure drop between 200 to 400 $N/m^2/m$ for traditional packing, and 50 to 250 $N/m^2/m$ for modern plastic packing. A packed column should not be operated above 1000 $N/m^2/m$ (1.25 in H_2O per foot of packing height). Above this pressure gradient, the downward flowing liquid becomes entrapped in the upward flowing air, resulting in poor removal efficiency, and may lead to flooding. Typical design values for liquid loading rate range between 0.4 and 2 m^3/m^2s (10 and 50 gpm/ft^2), and those for the volumetric air to water ratio range between 10:1 and 60:1 (Bishop and Cornwell, 1984). Various studies (Staudinger et al., 1990; Kavanaugh and Trussell, 1980) indicated that the optimal design region lies between stripping factor values of 3 and 7. Below a stripping factor of two, there will be a rapid increase in the tower height for marginal increase in the removal. Yet, with an R above 7, there will be little reduction in the tower height (Staudinger, 1986). The transfer appears to be less dependent

on gas flow rate as the air to water ratio approaches the design ranges. However, recent studies (Dvorak et al, 1996) showed that the transfer increase sharply at very high gas flow rates.

In practice, the tower diameter ranges between 0.5 and 3.0 m and the height ranges between 1 and 15 m. The tower cross section is usually determined based on the hydraulic loading.

As indicated in section 2.4.3, many instances of poor tower performance have been traced back to poor liquid distribution than to improper sizing of the packed bed. It is generally considered necessary to provide at least five points of introduction of liquid for each 0.1 m^2 of tower cross section (Ter Veer et al., 1980). The liquid re-distributors are placed at intervals varying from 3 to 8 tower diameters, but at least every 4 meters to minimize wall flow and channeling.

Selection of an appropriate packing includes selection of the packing shape, material of construction and a nominal packing size. Selection of shape and size involves a tradeoff between minimum head loss, and maximum overall rate of transfer. Selection of material of construction is influenced by the cost of packing material, its weight and the durability of the material under all possible operating conditions. In most water treatment applications, plastic packings are desirable because of low density, low cost and high durability. Larger packings are less expensive on a unit volume basis and allow high water application rates and, therefore, smaller tower diameters for a given water flow. Also larger size packing may be desirable because they would not foul as easily and they have lower pressure drop. On the other hand, smaller size packings provide larger mass transfer coefficients and smaller tower height. If a high degree of removal is required, smaller packing may be more economical.

Because of the uncertainties associated with the different design parameters, a safety factor is often used. The definition of an adequate safety factor is associated with the level of risk the designer is willing take. It depends on the degree of certainty in the values of the variables used in the design. The following table presents the findings of Lenzo et al. (1990) as to the necessary safety factors to produce safe designs when using the Onda correlation (Onda et al., 1968).

The design parameters indicated in the above paragraphs are just guidelines for optimum design and are an excellent starting point. Ball et al. (1984) found that the operating cost has a strong

influence on the optimum design conditions. Towers with larger diameters are preferable due to their lower headloss, an important operational and cost consideration. Also, air flow should be high enough to produce an optimum stripping factor.

Table 2.2 Safety factor for air stripping tower design.

to account for % of points	Safety factor
68%	1.30
99%	1.75

There are several approaches to design an air stripping tower (Kavanaugh and Trussell, 1980, Ball et al., 1984, Treybal, 1980). Ball et al. (1984) proposed the following steps:

1. Select packing, air to liquid ratio (G/L), stripping factor, and tower diameter
2. Select air pressure drop from the pressure drop curve (Figure 2.4) and determine blower requirements.
3. Estimate $K_L a$ from a correlation equation.
4. Apply equation (2.6) and determine the required height of the tower.

This procedure is repeated until a satisfactory, i.e., a cost-effective design is obtained.

A given removal efficiency can be achieved by different combinations of the design parameters, i.e., height of packing, air to water ratio, hydraulic loading rate and type of packing. Tower sizing is, therefore, a process of optimization, i.e., finding the combination of variables that will perform the desired function at the lowest cost. For site specific conditions, such as the cost of electricity and the cost of tower installation, there will be a combination of design parameters that minimize the treatment cost. Several studies (Nirmalakhanda et al., 1987) have been conducted, and numerous computer models have been developed to help determine the most cost effective design. Figure 2.8 (Staudinger, 1986) shows the optimal air to water ratio, shaded area, for different values of the Henry's Law constant.

Lenzo (1990) suggested that in situations where: (i) less common compounds are being treated, (ii) the water loading exceeds thousands liters per minute, (iii) and/or the required treatment efficiency exceeds 99%, it becomes cost-effective to conduct short-term, low-cost pilot tests to verify theoretical designs, and to minimize system size and full-scale energy requirements.

Design and optimization cannot be carried unless one has estimates of the mass transfer coefficient, K_{La} , for different operating conditions.

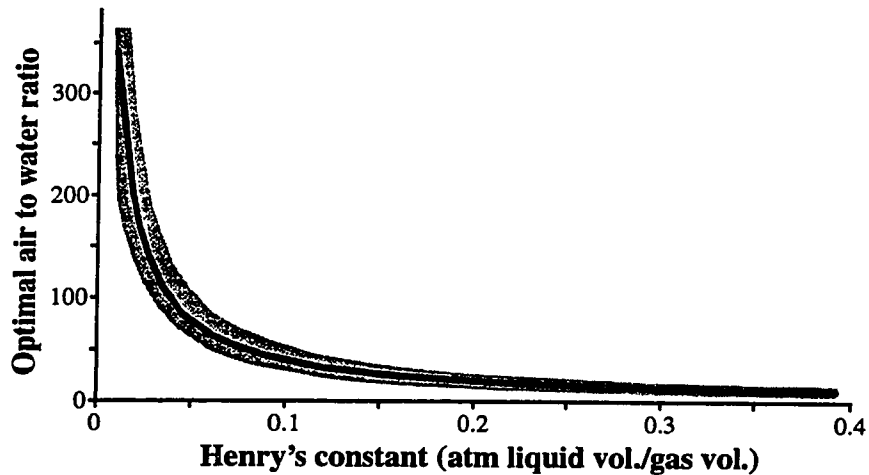


Figure 2.8. Optimal design air-to-water ratio for stripping VOCs at typical groundwater temperature of 13 °C (Staudinger, 1986).

2.4.4 Mass Transfer Coefficient: Estimation Methods

In designing a packed column for fixed operating conditions, the designer calculates the necessary packing depth, Z , that yields a pre-specified removal. The most critical variable in this calculation is the overall liquid (or gas) phase mass transfer coefficient, K_L (or K_G). The overall mass transfer coefficient takes into account the resistance to mass transfer in both phases, which permits design calculations to be based just on the change in concentration in a single phase. As it is nearly impossible to measure the interfacial area, a , the product of K_L and a , K_{La} , is generally used instead of K_L . K_{La} is sometimes called the volumetrically-based overall liquid phase mass transfer coefficient and its dimensions are T^{-1} .

The mass transfer coefficient, K_{La} , is a complex function of many design and operational variables. It can be determined either experimentally using a costly pilot scale, or using correlations and formulae. Most often engineers calculate K_{La} using a mass transfer correlation because they are easy to use and avoid the cost of pilot-scale tests and the time necessary to conduct them. The best mass transfer correlations produce an estimate of K_{La} with 30 to 50 percent deviation from predictions in full-scale applications (Lenzo et al., 1990, Staudinger et al., 1990 and Djebbar and Narbaiz, 1995). The lack of good predictive ability is due to: a) the

extrapolative nature of the predictions; b) the limited operating conditions in the databases used to develop the correlations; c) the limitations in parametric regression techniques used to generate these models; and d) the changing nature of mass transfer relationships from one set of operating conditions to another, that are not well understood and are poorly mimicked by current parametric models (Djebbar and Narbaitz, 1995; Bravo et al., 1992).

The following chapters discuss mass transfer coefficient development methods, evaluate existing methods, and propose a new approach to better estimate $K_L a$.

2.5 CONCLUSION

An air stripping tower is a best available technology for VOC removal from contaminated ground water. It compares well with alternative treatment options and it generally is the most economical. The main draw back of air stripping tower is the transfer of the contaminant from the water to the air, however, this can be overcome by installing an off-gas treatment unit if necessary. Other potential problems, such as channeling and maldistribution, are often associated with poor design practices. If well designed, the tower can perform as intended and drawbacks that are "associated" with tower operation can be minimized. Optimization can be used to find the combination of operating variables that yield the most efficient and economically viable tower.

The most critical parameter in the design of an air stripping tower is the mass transfer coefficient $K_L a$. Several methods are available for its estimation; but these methods have been shown to have several limitation and drawbacks, which will be discussed in the following chapter.

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CHAPTER 3

LITERATURE REVIEW: METHODS FOR PREDICTING MASS TRANSFER COEFFICIENT IN PACKED TOWERS

This chapter is a critical review of the methods for predicting mass transfer coefficients and their development. First, it reviews dimensional analysis which is frequently used in the analysis of mass transfer coefficients in packed towers. Then it covers basic mass transfer theories and their application. Next, it covers collection and use of experimental data, and empirical approaches for the estimation of the interfacial surface area and the mass transfer coefficient. This is followed by a review of current applications of mass transfer correlations with an emphasis on the Onda model and its drawbacks. Finally, it presents new approaches to $K_L a$ prediction based on nonparametric methods.

3.1 INTRODUCTION

Theory and practice of packed column operations have been extensively researched in the past 50 years (Kavanaugh and Trussell, 1980; Treybal, 1980; Sherwood and Pigford, 1952; Davidson, 1959a and b; among others). In practice, the estimation of mass transfer coefficient has been exclusively through parametric equations.

The parametric approach has produced tens of equations, which fall within one of three categories: (i) theoretical, (ii) statistical, and (iii) regression equations. The delineation between these methods is not always clearly defined. By far, regression equations constitute the bulk of existing equations and their development went through different methodologies. These regression equations are usually based on some results from the theoretical approach.

Several drawbacks have been attributed to the parametric approach (Djebbar and Narbaitz, 1995; Narbaitz and Djebbar, 1996) and several authors had indicated the need to improve them. Furthermore, two other important reasons revive the research to develop an alternative approach to parametric correlations. The first one are the current applications of air stripping tower to treat contaminated ground water, which are different from the conditions for which existing correlations have been developed. Second, new estimation techniques have been developed. In the last decade, there has been vigorous research activities to evaluate existing methods and, to a much lesser extent, to develop new ones using the traditional parametric modeling approach. However, there has been little, if any, innovation in the approach itself.

This chapter is a fundamental review of existing estimation methods in terms of basic theory and methodologies used to develop parametric correlations. An overview of actual application of mass transfer correlations is presented with a focus on the Onda model (Onda et al., 1968).

Alternative approaches based on nonparametric methods have been used recently in other domains. They include neural computing method and nonparametric kernel regression. These methods are briefly presented at the end of the chapter.

3.2 DIMENSIONAL ANALYSIS

Dimensional analysis has been extensively used in mass transfer analysis in air stripping towers. Dimensional analysis simplifies modeling and experimental work by combining variables into a smaller number of dimensionless groups. Therefore, it guarantees the dimensional consistency of the resulting relationships. The main feature of dimensional analysis is the transfer of certain aspects of similarity between model and prototype. Most dimensionless groups are expressed in terms of fundamental dimensions such as: mass (M), length (L), time (t) and temperature (T). The following equations present the dimensionless groups frequently used in the analysis of interfacial mass transfer in packed towers:

$$\text{Reynolds number; } Re = \frac{d L_M}{\mu} ; \frac{L_M}{a_s \mu} = \frac{\text{inertia force}}{\text{viscous force}} \quad (3.1)$$

$$\text{Froude number; } Fr = \frac{a_s L_M^2}{g \rho^2} = \frac{\text{inertia force}}{\text{gravity force}} \quad (3.2)$$

$$\text{Schmidt number; } Sc = \frac{\mu}{\rho D} = \frac{\text{momentum diffusivity}}{\text{mass diffusivity}} \quad (3.3)$$

$$\text{Sherwood number; } Sh = \frac{k d}{D}; \quad \frac{k}{Da_s} = \frac{\text{molecular mass transfer resistance}}{\text{convective mass transfer resistance}} \quad (3.4)$$

$$\text{Weber number; } We = \frac{L_M^2}{a_s \sigma \rho_L} = \frac{\text{inertia force}}{\text{tension force}} \quad (3.5)$$

$$\text{Wettability number; } Mo = \frac{\sigma_c}{\sigma_L} = \frac{\text{liquid tension force}}{\text{packing tension force}} \quad (3.6)$$

$$\text{Galilee number; } Ga = \frac{g \rho^2}{\mu^2 a_s^3}; \quad \frac{d^3 g}{v^2} = \frac{\text{gravity force}}{\text{inertia force}} \frac{\text{viscosity force}}{\text{tension force}} \quad (3.7)$$

$$\text{Surface tension number; } Ts = \frac{\mu_L^2 a_s}{\rho_L \sigma_L} = \frac{\text{viscosity force}}{\text{inertia force}} \frac{\text{viscosity force}}{\text{tension force}} \quad (3.8)$$

$$\text{Packing efficiency; } Er = \frac{1}{a_s Z}; \quad \frac{1}{a_s d} \quad (3.9)$$

Where d = packing characteristic diameter (L); k = mass transfer coefficients (L/T); a_s = specific surface area of packing (L^2/L^3); L_M = liquid mass flow rate per unit cross-sectional area (M/L^2t); G_M = gas mass flow rate per unit cross-sectional area (M/L^2t); ρ = density of the liquid or gas phase (M/L^3); D = liquid or gas diffusion coefficient (L^2/t); g = gravitational constant (L/t^2); σ_c = surface tension of packing material (M/t^2); σ_L = surface tension of liquid (M/t^2); μ = liquid or gas dynamic viscosity (M/Lt); and v = liquid or gas kinetic viscosity (t/L^2). The subscripts L and G refer to liquid and gas phases, respectively. These numbers can be liquid based or gas based.

Dimensional variables L_M , d , D , etc., that form the dimensionless groups, will vary with the particular situation. For example, the length d may be the packing diameter in one situation and the tower diameter in another, as in the case of E_r , the packing efficiency number in equation (3.9). Therefore, the reference flow rate L ; length d or Z ; and so forth must be specified.

Two cases are encountered when applying dimensional analysis. In the first case the governing differential equations are well known, whereas in the second case the governing differential equations are not known.

The Navier-Stokes equation is an example of the first case. This equation is given by

$$\frac{\partial v}{\partial t} = g - \frac{\nabla p}{\rho} + \nu \nabla^2 v \quad (3.10)$$

where v = velocity, m/s; p = pressure, N/m²; and ν = kinetic viscosity, s/m². ∇ and ∂ denote the gradient and the total derivative, respectively. Equation (3.10) can be dimensionally transformed into the following form (Welty et al., 1976)

$$\left[\frac{v^2}{d} \right] = \left[g - \frac{gp}{d\rho} + \frac{\nu v}{d^2} \right] \quad (3.11)$$

Equation (3.10) expresses both a dimensional and a numerical equality whereas equation (3.11) expresses a dimensional equality only. The use of dimensional analysis, as in equation (3.11), does not give an explicit relationship between the different variables. This means that equation (3.11) does not express a direct relationship between v , the velocity in the left hand side of equation (3.11), with any of the variables in the right hand side of the same equation. In addition to the formation of the various dimensionless groups, the dimensional analysis utilizing the governing differential equations provides physical interpretation to the dimensionless groups. For example, the Reynolds number expresses the ratio between the inertia forces and the viscous forces as previously indicated in equation (3.1).

Dimensional analysis can also be used even when the governing differential equations, which clearly describe the process under consideration, are not known by using the Buckingham theorem. The Buckingham theorem (Welty et al., 1976) provides a stepwise procedure that leads to the number and the form of the dimensionless numbers that are important for the particular problem. The Buckingham theorem states that if there are n dimensional variables in a dimensionally homogeneous equation, described by r fundamental dimensions, they may be grouped in i dimensionless groups by the following equation (Welty et al., 1976);

$$i = n - r \quad (3.12)$$

Unfortunately, the latter method does not give a physical interpretation to the resulting dimensionless numbers (Welty et al., 1976). The Reynolds number, for example, may not necessarily express the ratio between the inertia forces and the viscous forces.

There are many possible sets of independent dimensionless groups that can be used. According to Welty (1976), it appears desirable to have groups that depend on the presence of certain

variables: kinetic viscosity ν , gravity g , surface tension σ , and the mass transfer coefficient k , i.e., four dimensionless groups. The groups are usually chosen so that each of the variables μ , g , k , and σ would appear in one group only, i.e.,

$$N_1^k = f_1(N_2^\sigma, N_3^\mu, N_4^g) \quad (3.13a)$$

where N_1^k , N_2^σ , N_3^μ , and N_4^g = numbers that depend on k , σ , μ and g respectively. Treybal (1980) indicated that the transfer process in packed towers can be better described using a relationship that involves the three dimensionless numbers: the Reynolds number, the Schmidt number, and the Sherwood number, i.e.,

$$Sh = f_2(Re, Sc) \quad (3.13b)$$

where Sh = Sherwood dimensionless number, which is related to k . But the form of the functional relationship, i.e., f_1 or f_2 , that relates the dimensionless groups to each other is not provided, because it is not known, and no physical meaning could be attributed with certainty to the resulting dimensionless numbers.

Dimensional analysis can also be used in conjunction with the theoretical approach to obtain general equations. Examples of such an approach are the Davidson models (Davidson, 1959b).

3.3 THEORETICAL BASED APPROACHES

Mass transfer in moving liquids is directly related to the mechanism of the liquid movement itself. Flow of liquids over packing surfaces involves two regimes: a laminar regime and a turbulent regime with an intervening transition zone between the two regimes. It is natural, therefore, to attempt to describe the rate of mass transfer using the combination of laminar and turbulent mechanisms including the intervening transition zone.

The mechanism of mass transfer in the laminar region is controlled by molecular diffusion, which is well known (Treybal, 1980). However, the mechanism of the flow process which involves the movement of eddies in the turbulent and the transition regions is not thoroughly understood. The analysis of the boundary layer in a flow over flat plate, which is similar to the flow over packing surfaces, is a classical tool often used to illustrate the three flow mechanisms.

According to Prandtl (1928), the effects of fluid friction at high Reynolds numbers are limited to a thin layer near the boundary of the solid surface (Figure 3.1), hence the term boundary layer. In the laminar region the transfer is controlled by molecular diffusion, while in the turbulent region the transfer is controlled by both molecular and eddy diffusion.

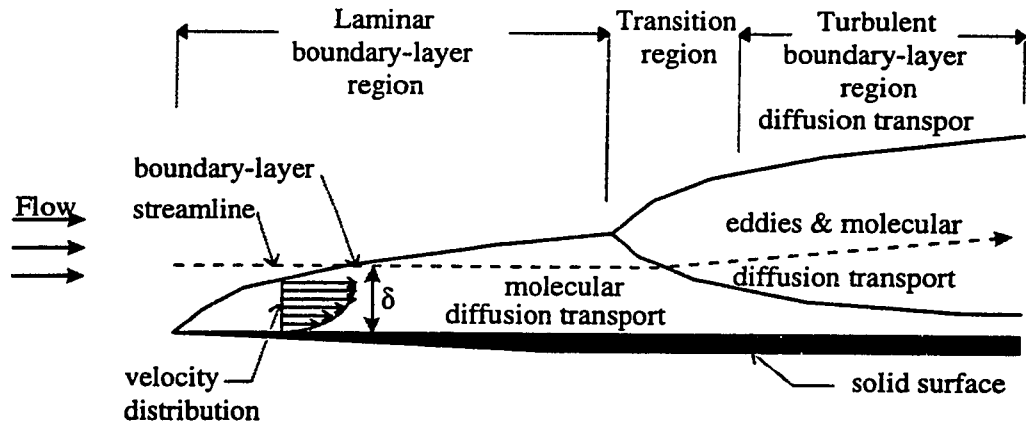


Figure 3.1 Boundary layer over a flat plate.

Treybal (1980) indicated that there is no theoretical answer to the problem of mass transfer between a solid surface and a fluid flowing above it, as shown in Figure 3.1. Nevertheless, solutions were obtained for simplified situations where a fully developed laminar flow condition was assumed such as the one presented in the following section.

3.3.1 Model for Laminar Mass Transfer

By assuming a laminar flow in the falling liquid layer and using streamline flow theory, the equation of motion can be written as follows (Treybal, 1980)

$$\mu \frac{d^2v}{d\delta^2} + g\rho = 0 \quad (3.14)$$

where δ = the liquid film depth and z = the vertical distance along the wall in the flow direction (Figure 3.2). The equation that governs the transport of mass is given by (Treybal, 1980)

$$v \frac{\partial C}{\partial y} = D_L \frac{\partial^2 C}{\partial z^2} \quad (3.15)$$

where D_L = liquid diffusion. With the assumption of steady state flow conditions, equations (3.14) and (3.15) can be simultaneously solved to yield the following equation (Treybal, 1980, Johnstone and Pigford, 1952),

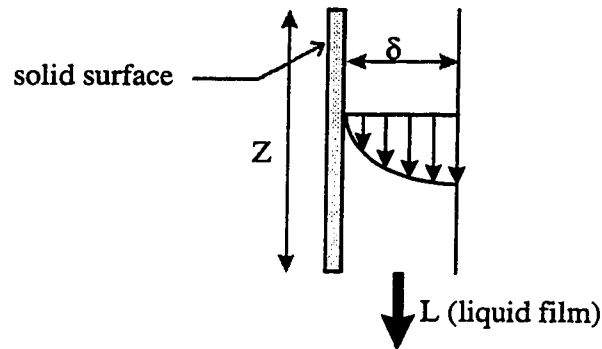


Figure 3.2 Laminar liquid film falling over a plate.

$$Sh_{avg} = \left(\frac{2}{3\pi} \frac{\delta}{Z} ReSc \right)^{0.5} \quad (3.16)$$

Using experimental data with high Reynolds number conditions, Sherwood and Pigford (1952) showed that the observed k_L may be larger than twice the theoretical values given by equation (3.16) due to ripples and waves formed on the liquid surface. Treybal (1980) and Welty et al. (1976) concluded that it is not possible to theoretically compute the mass transfer coefficient for turbulent flow conditions due to our inability to describe the flow mechanism mathematically. Also, the surface area becomes larger than the assumed smooth surface area because of the formation of ripples and waves on the liquid surface. To overcome these difficulties, some authors proposed simple models, which are described in the following sections.

3.3.2 Models for turbulent mass transfer coefficient

There are many models (theories) which "attempted" to interpret or explain the mechanism of interfacial mass transfer between liquid and gas phases especially in turbulent flow conditions. These models produced simple expressions for the mass transfer coefficient. In commenting on these models, Treybal (1980) stated the following:

"They are all (i.e., mass transfer models) speculations, and are continually being revised. It is helpful to keep in mind that

transfer coefficients for mass transfer are expediently used to deal with situations which are not well understood. ... The ultimate interpretation or explanation of the transfer coefficient will come only when the problems of fluid mechanics are solved, at which time, it will be possible to abandon the concept of transfer coefficient."

These classical mass transfer models are the two-film model, the penetration model, the surface renewal model and the film penetration model.

3.3.2.1 Film model. Lewis and Whitman (1924) assumed a time of exposure of the surface element sufficiently long for the concentration profile within a film to be characteristic of steady state. The entire concentration difference is attributed to molecular diffusion within an "effective" film of thickness δ (Figure 3.3). In such conditions, the local mass transfer coefficient k_L is given by the following equation.

$$k_L = \frac{D_L}{\delta} \quad (3.17)$$

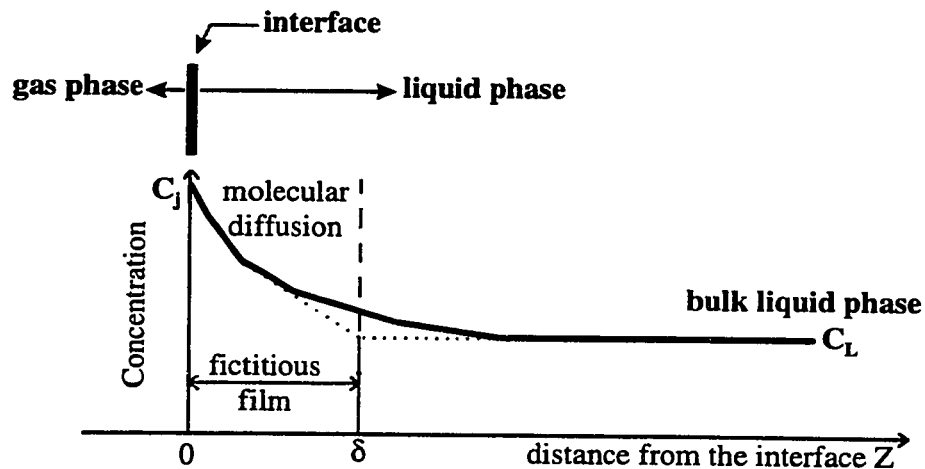


Figure 3.3 Film theory model.

In Figure 3.3, C_j = the liquid phase concentration that is in equilibrium with the gas phase concentration and C_L = the bulk liquid phase concentration. The concentration within the bulk liquid phase is assumed to be uniform.

3.3.2.2 Penetration model. The penetration model assumes the exposure time of fluid particles (within eddies) to the interface is too short for steady state to develop. Higbie (1935) pictured the absorption by the liquid phase as an unsteady state diffusion, or penetration, of eddies into a laminar layer of liquid flowing over the packing surfaces. He also assumed a constant time of exposure equal to θ for all eddies (Figure 3.4).

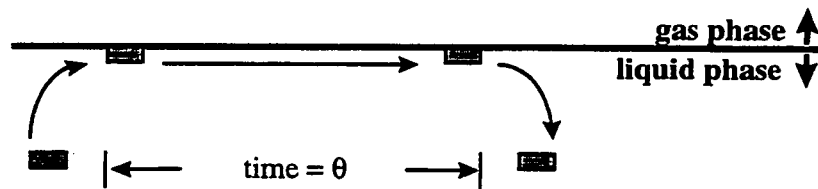


Figure 3.4 Penetration model.

For such conditions, the mass transfer coefficient averaged over θ is given by the following equation.

$$k_L = \sqrt{\frac{D_L}{\pi\delta}} \quad (3.18)$$

Using the penetration model, i.e., equation 3.18, and assuming a laminar stream flow in the falling liquid film inside a short pipe, Vivian and Peaceman (1956) developed the following equation.

$$k_L = 2\sqrt{\frac{D_L}{\pi Z} \left(\frac{9}{8} \frac{gL^2}{\rho_L \mu_L} \right)} \quad (3.19)$$

where L = liquid flow, Z = total height of the plate. Differences were observed between the values obtained by the above equation and experimental data. Vivian and Peaceman (1956) attributed these differences to the liquid film being finite in thickness and to the velocity distribution being parabolic as opposed to infinite liquid film thickness and uniform flow velocity that were assumed in the development of equation (3.19).

3.3.2.3 Surface renewal model. Dankwerts (1970) assumed the liquid-gas interface to be a mosaic of surface elements having different exposure time histories. He proposed the following equation

$$k_L = \sqrt{DS} \quad (3.20)$$

where S = the fraction of the total exposed surface area being renewed at each moment.

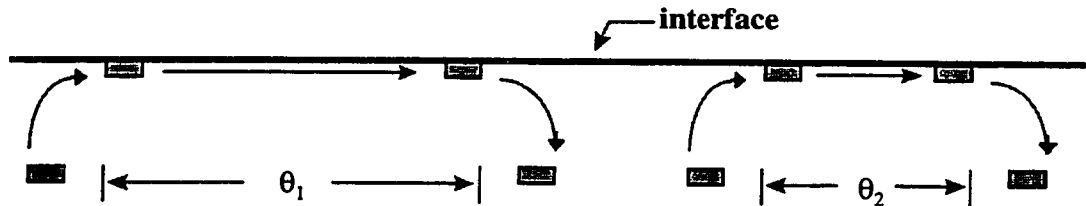


Figure 3.5 Film-surface renewal model.

The penetration and surface renewal theories assume the surface element to be essentially infinitely deep so that the diffusing solute never reaches the region of constant concentration, C_L .

3.3.2.4 Film-Surface renewal model. Toor and Marchello (1958) assumed the liquid concentration to be constant in the bulk liquid up to a certain distance, Z_b , from the interface, i.e., similar to the film theory. The upper part is similar to the penetration theory. For rapid penetration (large D_L) and small S or for thin surface element, the mass transfer coefficient takes on the character of the film model. Whereas, for slower penetration or rapid renewal the mass transfer coefficient follows the surface renewal model as shown in Figure 3.6.

Toor and Marchello (1958) proposed the following relationship.

$$k_L = \sqrt{DS} \coth \sqrt{\frac{SZ_b^2}{D}} \quad (3.21)$$

Obviously, the fictitious film thickness δ or Z_b , and the exposure time θ can never be measured since they do not exist. They are assumed concepts introduced to make the mathematical analysis of the proposed transfer models feasible.

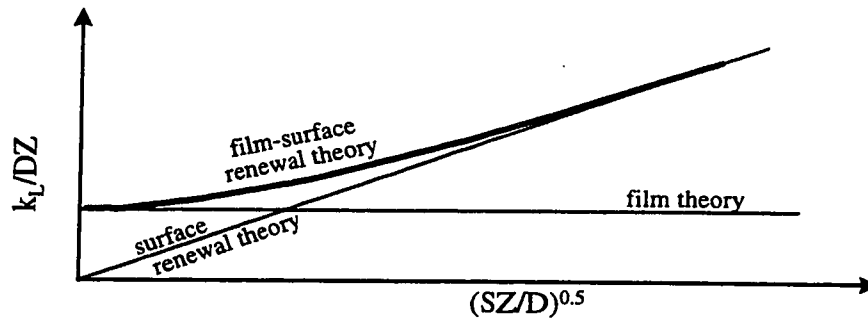


Figure 3.6 Film-surface renewal model.

The results of the different mass transfer models can not be generalized due to four principal reasons. First, the mass transfer coefficients resulting from these models include non-measurable quantities such as film thickness and exposure times. Second, the assumptions used in their development limit their applicability. Third, they do not account for the effect of other transport and hydrodynamic phenomena such as rippling and eddies. Finally, mass transfer equipment used in practice is very different from the simple geometry of the laboratory equipment used to derive the above mentioned models and theories. A more rigorous theoretical analysis was conducted by Davidson (1959b). He developed three models to represent random packing configurations.

3.3.3 Statistical Models of the Random Packing

Davidson (1959b) was the first to consider a comprehensive approach to predictive mass transfer correlations based on theory. In his three models the packing was assumed to be comprised of a large number of completely wetted plates. Liquid was assumed to run down the surfaces of the flat plates under laminar flow conditions and to completely mix at the packing junctions before passing to the next plate.

- model 1: The packing material is made up of vertical plates of constant height, d , that are completely and equally wetted. Based on these assumptions, Davidson (1959b) derived the following

$$\frac{H_L}{d} = 0.345 Sc^{\frac{1}{2}} Re^{\frac{2}{3}} Ga^{-\frac{1}{6}} \quad (3.26)$$

where H_L = the height of the transfer unit.

- model 2: The packing material is made up of plates of constant height, d . They are randomly oriented and completely and equally wetted. These assumptions lead to the following equation:

$$\frac{H_L}{d} = 0.244 Sc^{\frac{1}{2}} Re^{\frac{1}{3}} Ga^{-\frac{1}{3}} \quad (3.27)$$

- model 3: The packing material is made of plates with random height of less than a certain value d . These packings are randomly oriented, and completely wetted. These assumptions result in:

$$\frac{H_L}{d} = 0.1833 Sc^{\frac{1}{2}} Re^{\frac{1}{3}} Ga^{-\frac{1}{3}} \quad (3.28)$$

The last model is the most general amongst the three models. The weaknesses of Davidson's analysis are the assumptions of completely wetted packing and of laminar flow conditions. At low liquid rates, with large packing pieces, much of the packing is dry; while with small packing pieces, much of the void spaces are filled with liquid, so that interfacial area is less than the dry surface area of the packing. Thus, both these cases contradict Davidson's assumption. Au-Yeung and Ponter (1983) indicated that at low Reynolds number conditions, model 3 underpredicts the height of the transfer unit due to lack of complete mixing at the packing junctions; whereas, at high Reynolds number conditions the observed height of the transfer unit is lower due to rippling, which increases the surface area.

3.3.4 Mass Transfer from Theory to Practice

A likely explanation for the discrepancy between theory and experiments, even in well defined geometry and known effective surface area, may be found in the nature of the liquid flow itself. The true nature of the liquid flow over the surface of the packing as shown in Figure 3.1 is uncertain (Treybal, 1980). Vivian and Peaceman (1956) indicated that it is difficult to conceive that the liquid flowing over such a short flow path (the packing surface) will immediately establish a parabolic velocity distribution as suggested by the laminar stream flow theory (Figure 3.2). Flow in large-scale mass transfer devices such as packed columns is much more complex than the simple flow models presented so far. This is because it is difficult to determine the exact effective interfacial area and to mathematically describe the transfer process in turbulent flow conditions.

Most mass transfer research evaluated mass transfer coefficients in gas phase and in the liquid phase separately. According to the two film theory, the overall resistance to mass transfer is equal to the sum of the resistance in the gas film and the resistance in the liquid film. Therefore,

$$\frac{1}{K_L} = \frac{1}{k_L} + \frac{1}{Hk_G} \quad (3.22)$$

where K_L = the overall liquid-phase mass transfer coefficient; k_L = the individual liquid-phase coefficient; k_G = the individual gas-phase coefficient; and H = Henry's law constant. The resistance to mass transfer is proportional to the inverse of the mass transfer coefficient. The overall liquid-phase mass transfer coefficient is the coefficient used to describe the total resistance to mass transfer, i.e., that arising from both phases using the concentrations in a single phase. According to King (1964) equation (3.22) will hold true if the following conditions are satisfied:

- The interface is at equilibrium and H must be constant. If H is not constant, the value of the equilibrium line slope at the properly defined value of concentration must be employed.
- There must be no significant resistance present other than those represented by $1/k_L$ and $1/k_G$. The individual phase coefficients, k_L and k_G , are those measured in the absence or suppression of resistance in the other phase.
- The hydrodynamic conditions (interfacial area, etc.) must be the same as those prevailing during the measurements of individual phase resistance.
- The mass transfer resistance of the two phases must not interact, i.e., k_L and k_G are independent and the ratio k_L/k_G must be constant at all points of the interface.

King (1964) indicated that these conditions are rarely met in common mass transfer equipment, especially those which provide a wide distribution of liquid surface lifetimes, such as randomly-packed towers. In such equipment a wide variation in local values of k_L (and k_G) exists. Continuous change in effective surface area is expected even at a fixed flow rate. In a subsequent study, King (1965) concluded that the average overall mass transfer coefficient for an individual countercurrent surface exposure will be higher than the prediction of equation (3.22). However, the net observed over-all mass transfer coefficients for packed and plate towers appear to be less than the prediction of equation (3.22) (Dankwerts, 1951). Dankwerts (1951) and Emmert and Pigford (1954) associated this conflicting result with the possibility that gas-liquid

interface may not be in equilibrium as assumed by equation (3.22). In such case, the transfer of mass encounters higher interfacial resistance than predicted by equation (3.22).

In conclusion, theory falls short of producing a satisfactory mathematical description for the mass transfer coefficient in packed towers. Therefore several researchers have opted for the empirical approach based on parametric regression of experimental data.

3.4 REGRESSION BASED APPROACHES

The difficulty in determining the effect of the process variables, such as gas flow rate and packing surface area, on the transfer characteristics, compounded with the absence of the correct form of the relationship relating the dependent to the independent variables has resulted in the development of a huge number of different correlations. These correlations were obtained by regressing experimental data using an assumed relationship. Generation of experimental data is as important as developing a model itself because the latter depends on the former. Based on experimental and field data, the author devised a tool to predict and interpret the intrinsic relationship(s) that describe the process under investigation. The following section discusses the development of experimental data, and subsequent sections will discuss the development of models.

3.4.1 Experimental Data

The method used to obtain experimental data reflects our understanding of the transfer process and the ideas we have about the form of the relationship that describes the mass transfer coefficient. For example, if a variable is assumed to be insignificant, it will generally be ignored and left uncontrolled. When Sherwood and Holloway (1940) assumed the total resistance to mass transfer resides mainly in the liquid phase, they did not measure the resistance to mass transfer in the gas phase. A review of the literature showed that five main approaches are used to develop and use experimental data.

1. The first approach uses packing with simple geometry where the interfacial surface area is supposed to be known, such as for plates, cylinders and spheres (Welty et al., 1976; Davidson, 1959a; Fukushima et al., 1978; and Alper and Dankwerts, 1976 among others). In this case,

the mass transfer coefficient k_L and/or k_G is determined by dividing the observed $k_L a$ or $k_G a$ value by the “known” interfacial area. The experimental data are then regressed.

2. The second approach assumes k_G to be substantially the same for the same operating conditions in vaporization and in absorption (Shulman et al., 1955c; Puranik and Vogelpohl, 1974; Yoshida and Koyanagi, 1962, among others). First, k_{Gv} and k_{Ga} , the gas phase mass transfer coefficients for vaporization and absorption are determined for the same operating conditions, respectively. Data for the effective area for absorption, a , are then determined using the following equation:

$$\frac{\text{system specific during absorption}}{\text{system specific during vaporisation}} = \frac{k_G a}{k_G a_s} = \frac{a}{a_s}$$

where a_s = the dry surface area and a = the effective surface area during absorption.

3. The third approach conducts experiments in which the resistance to mass transfer is located in one phase only. To obtain k_G or k_L , the transfer is carried out using a pure solution in the liquid phase or the gas phase, respectively. Here the resistance to mass transfer resides in one phase, the solution, and no resistance is encountered in the pure liquid phase. Novella et al. (1992) determined k_L by absorbing pure CO_2 into water. This offers zero resistance in the gaseous phase. Shulman et al. (1955c) obtained k_{Ga} either from ammonia absorption experiments, or from measurements of the rate of evaporation from the flowing liquid into the air. In these experiments the liquid phase presented no resistance to the transfer of mass.
4. The fourth approach goes through the following steps (Shulman et al., 1955 a, b, and c and Davidson, 1959a):
 - a) First, k_G was obtained from the evaporation of naphthalene from Raschig rings and Berl saddles.
 - b) Second, the effective surface areas are obtained by comparing the k_G values from the previous step with the k_{Ga} values obtained from Fellingner (1941) data on ammonia absorption where the resistance to mass transfer in the liquid phase is assumed negligible.
 - c) $k_L a$ values are measured from liquid controlling experiments.
 - d) Finally, the values of k_L were calculated by dividing the measured $k_L a$ values by the effective area determined in the second step.

5. The fifth approach uses a well accepted correlation to determine one of the transfer components, i.e., a , k_L , or k_G . For example Ponter and Au-Yeung (1982) proceeded as follow:
- First, the interfacial areas were assumed to follow the Onda correlation for the wetted surface area (Onda et al., 1967).
 - Second, k_L data were obtained by dividing measured $k_L a$ values, from liquid phase controlling experiments, by the wetted areas as calculated in the first step.
 - Finally, k_G data were obtained by dividing measured $k_G a$, from gas phase controlling experiments, by the wetted areas a calculated in the first step.

The approaches presented above depend on the preconceived ideas the authors have vis-à-vis the transfer process. These ideas may affect the quality of the data and limit the applicability of the developed models. For example, if the Onda relationship for the interfacial surface area is not the true relationship, then the values of k_L and k_G obtained in step 2 and 3 of the last approach, as well as the resulting equations, will only be definitely reliable for the conditions for which they were developed. The resulting equation should not be used to draw conclusions and interpret the process. Whereas, if the Onda relationship for the surface area is the true relationship for the surface area, the k_L and k_G relationships from Onda et al. (1968) and from Au-Yeung and Ponter (1983) should be similar but they are not. This point is further illustrated by the resulting mass transfer and surface area correlations discussed in the following sections. The surface area correlations are considered first.

3.4.2 Interfacial Area

Several studies have been conducted using experimental setups with known interfacial areas, for example, wetted wall columns, cylinders, and flow over spheres. These setups have fairly well defined interfacial surface areas when they are completely wetted and when the liquid flow is smooth (laminar). Unfortunately, this is hardly achievable even in well controlled laboratory experiments and seldom represents the flow in existing packed towers. When the liquid flow is turbulent, or the packing is partially wetted, or the packing geometry is complex, the liquid flow hydraulics become complex. Generally the liquid flow includes the following components:

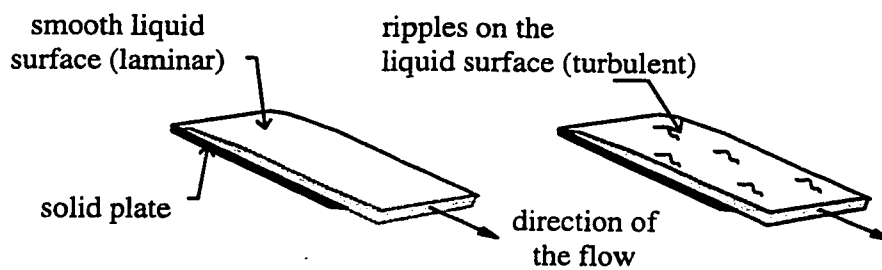


Figure 3.7 Flow over the surface of plates.

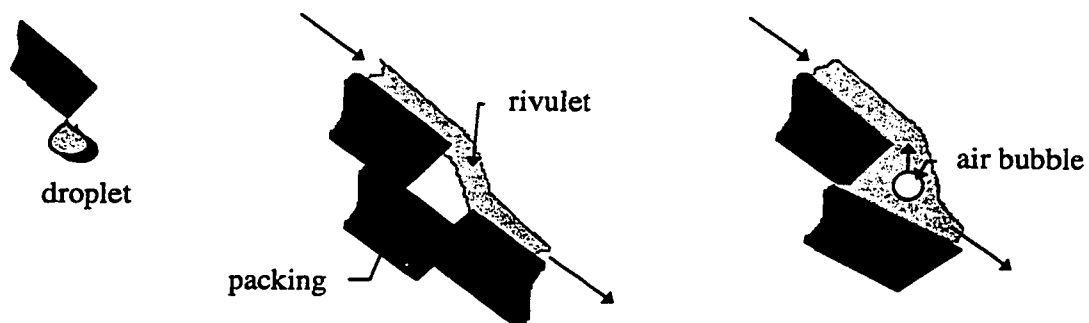


Figure 3.8 Air bubble, droplet, and rivulet flow patterns.



Figure 3.9 Mixing at the packing junction.

1. Flow over packing surface area (similar to the falling liquid film) shown in Figure 3.7.
2. Droplets and rivulets as shown in Figure 3.8.
3. Mixing at the packing junctions as shown in Figure 3.9.

The interfacial area in the above conditions is virtually impossible to measure. Moreover, flow patterns change from one packing type to another making a generalized correlation difficult to achieve. Visual inspection of flow patterns by Gossett et al. (1985) indicated that water flowing over saddles appeared to cascade in thin sheets from one piece of packing to the next. Flow over the rings seemed to be less cohesive. Water appeared to form small drops which fell from one piece of packing, and broke into smaller drops upon hitting the next piece of packing. This formation and reformation of drops would seem to renew the effective area for transfer much more efficiently than the sheeting flow pattern observed with saddles.

To overcome these difficulties, empirical equations have been developed. However, the form of the functional relationship that relates the interfacial surface area to the operating variables is not known. Consequently, several different configurations for the functional relationship have been proposed. Broadly, these configurations can be grouped into three forms.

- Form 1

This form consists of a product of dimensionless numbers raised to different exponents. This is the most often used form. An example of such form is the Novella et al. (1992) equation,

$$\frac{a}{a_s} = C_1 \text{Re}^{C_2} \text{Er}^{C_3} \text{Mo}^{0.18} \text{Ts}^{0.38} \quad (3.23)$$

where C_1 , C_2 and C_3 = packing dependent constants.

- Form 2

This is more general than form 1; it consists of the summation of different functional forms. An example of such equation is the Puranik and Vogelpohl (1974) equation. Puranik and Vogelpohl assumed the total surface area to be the sum of two components: a dynamic component due to the moving liquid, and a static component due to the stagnant liquid. In absorption applications without chemical reactions, Puranik and Vogelpohl assumed that only the dynamic area is involved in the transfer; while, the static surface area is considered a dead area and does not contribute to mass transfer. Accordingly they proposed the following equation,

$$\frac{a}{a_s} = C_1 \text{Re}^{C_2} \text{Er}^{C_3} \text{Mo}^{0.18} - C_4 + C_5 \ln \frac{\text{We}}{\text{Fr}} \quad (3.24)$$

This equation consists of a summation of three forms: a product of dimensionless numbers raised to different powers, $C_1 \text{Re}^{C_2} \text{Er}^{C_3} \text{Mo}^{0.18}$; a linear part represented by the constant, C_4 ; and a logarithmic function of dimensionless numbers, $C_5 \ln \frac{\text{We}}{\text{Fr}}$.

- Form 3

Onda et al. (1968) assumed the effective surface area and the wetted area to be the same. They also assumed that the wetted area approaches the packings dry area exponentially and they proposed the following equation,

$$a = a_s \left(1 - e^{-1.45 \text{Re}^{0.1} \text{We}^{0.2} \text{Fr}^{-0.05}} \right) \quad (3.25)$$

The correlations (models), equations (3.23), (3.24) and (3.25), have different forms as they were not developed based on first principles. These correlations, and similar ones, were based solely on statistical analysis of corresponding data (i.e., nonlinear regression) using a pre-assumed functional forms like those presented in equations (3.23), (3.24), and (3.25) or adjusted forms that describe the data better. The data with which these equations were developed were obtained in laboratory experiments. These data are different from full scale applications in many respects, for example the geometry, the values of the operational variables, and the contaminant characteristics, especially when it comes to the environmental applications of air stripping towers. As simple regression equations, these models should not be used outside the ranges of variable values of their developmental data set.

Experimental and theoretical developments gave some insight about the form of the relationships governing the mass transfer coefficients. Yet, the state of correlations for mass transfer coefficients is similar to the surface area correlations presented in the above. The following section discusses the correlations for mass transfer coefficient.

3.4.3 How Mass Transfer Correlations have Been Developed

Most investigators regressed equations formed of dimensionless numbers. They developed empirical correlations based on the theory by raising some dimensionless numbers to specific exponents. These exponents are similar (or in some case preset) to those obtained in the simple theoretical models presented earlier. The penetration theory, for example, with the assumption

of laminar flow between surface renewals predicts $k_L a$ to be proportional to the 1/3 power of the liquid flow rate and 1/2 power of the diffusion coefficient (Davidson, 1959b; Sherwood and Pigford, 1952). These findings lead one to assume that the correlation of packed tower absorption data on the basis of $k_L a$ should include Reynolds number to the 1/3 power and the Schmidt number to the 1/2 power. It is important to keep in mind that the validity of these results is directly dependent on the validity of the assumptions used in the development of these theories, namely the penetration model and the streamline flow model assumptions described in earlier sections.

Bravo and Fair (1982) stated that a functionality was *established and accepted to be representative* of the relationship between the variables that affect the transport process. This functionality has the following form for both liquid and gas phases,

$$Sh = c Re^\alpha Sc^\beta \quad (3.29)$$

where c , α , and β = parameters to be regressed. This form has been widely utilized to obtain regression equations. Different procedures have been used to obtain the final regression equations, but the main ones are the followings:

3.4.3.1 Novella et al. (1992). They built their correlation step by step by adding variables at each step. They used nonlinear multiple regression program to regress data of the absorption of pure CO₂ into water, therefore k_G is zero.

- step 1: liquid flow and packing depth: $k_L a = A_1 L^{0.8} Z^{-0.44}$ (3.30a)

- step 2: addition of packing diameter: $k_L a = A_2 (L^{0.8} Z^{-0.44}) d^{0.42}$ (3.30b)

- step 3: addition of surface tension effect

$$k_L a = A_3 (L^{0.8} Z^{-0.44} d^{0.42}) \left(\frac{\sigma_c}{\sigma} \right) \quad (3.30c)$$

- step 4: making the correlation dimensionless

$$\frac{k_L a}{D_L d^2} = C_1 Re^{C_2} Er^{C_3} Sc^\dagger Ga^{0.38} Ts^{0.8} Mo^{0.18} \quad (3.31a)$$

where C_1 , C_2 , and C_3 = regressed constants that are a function of the packing type. In the second stage, Novella et al. (1992) used spheres and cylinders of known surface area as packing. The data obtained were regressed as indicated above and the following equation was obtained,

$$\frac{k_L}{D_L a_s} = c_1 \text{Re}^{\frac{2}{3}} \text{Sc}^{\frac{1}{3}} \text{Ga}^{0.38} \text{Ts}^{0.42} \quad (3.31b)$$

After dividing equations (3.31a) and (3.31b) term by term the effective specific interfacial area is obtained

$$\frac{a}{a_s} = c_1 \text{Re}^{C_2} \text{Er}^{C_3} \text{Ts}^{0.8} \text{Mo}^{0.18} \quad (3.32)$$

where the C_i 's = packing type dependent constants.

3.4.3.2 Vivian and Peaceman (1956). Vivian and Peaceman (1956) followed the same procedure as Novella et al. (1992) and they generated the following dimensionally inconsistent equation:

$$k_L \sqrt{\frac{Z}{D}} = 7.13L^{0.4} \quad (3.33)$$

The authors then used dimensional analysis to obtain a dimensionally consistent equation. They arranged the variables that affect the process into four dimensionless groups: $\frac{k_L Z}{D}$, $\frac{\mu}{\rho D}$, $\frac{\rho^2 g Z^3}{\mu^2}$, $\frac{4L}{\mu}$. By substituting in these groups in equation (3.33), the following dimensionless equation was obtained,

$$\text{Sh} = 0.433 \text{Re}^{0.4} \text{Sc}^{\frac{1}{3}} \text{Ga}^{\frac{1}{3}} \quad (3.34)$$

3.4.3.3 Onda et al. (1967). Onda and his coworkers assumed a wetted area relationship similar to that of Fujita and Sakuna (1954) and included both the liquid surface tension and the surface energy of the packing materials:

$$\frac{a}{a_s} = 1 - \frac{1}{e^{1.45 \text{Re}^{0.1} \text{We}^{0.2} \text{Fr}^{-0.05}}} \quad (3.35)$$

k_L and k_G values were then obtained by dividing $k_L a$ and $k_G a$ values by the wetted surface area, a , values calculated using equation (3.35). $k_L a$ and $k_G a$ values are collected from reported data of gas absorption into water from different sources. The resulting data of k_L and k_G were then regressed, respectively, yielded the following correlations

$$k_L = 0.0051 \text{Re}^{\frac{2}{3}} \text{Sc}^{-\frac{1}{3}} \text{Er}^{0.4} \left(\frac{\rho_L}{\mu_L g} \right)^{-\frac{1}{3}} \quad (3.36)$$

$$k_G = c a_s D_G \text{Re}^{0.7} \text{Sc}^{\dagger} \text{Er}^{-2} \quad (3.37)$$

where c is a coefficient which depends on the packing diameter.

3.4.3.4 Bravo and Fair (1982). Bravo and Fair tried various combinations of dimensionless numbers to obtain the best grouping (fit) of the data. The Bravo and Fair correlations were obtained as follow. First, they determined the overall $k_L a$ data experimentally. Second, they calculated the individual k_L and k_G using the Onda correlations, equations (3.36) and (3.37).

Third, they calculated the effective surface area using $a = \frac{k_L a}{k_L}$. Finally, the area values were

then regressed to yield the following equation.

$$\frac{a}{a_s} = c(\text{ReGa})^{0.392} \frac{\sigma^{0.5}}{Z^{0.4}} \quad (3.38)$$

where c = coefficient. Equation (3.38) is not dimensionally consistent. To make it dimensionally consistent, the packing depth Z and the packing surface tension σ_c are replaced by $\frac{Z}{10}$ and $\frac{\sigma_c}{72}$, respectively, where 72 is the surface tension of water and the depth 10 is a randomly chosen value. If the Onda correlation for the wetted area (equation 3.35) is correct, equation (3.38) would be identical to equation (3.35), but it is not.

3.4.4 Discussion

The two-film theory suggested the diffusion exponent to be equal to one; whereas, the penetration and the surface renewal theories suggested a value of one-half. However, the film-surface-renewal model proposed a value intermediate between the values proposed by the two-film and the penetration models, respectively. This variation in the diffusion coefficient exponent confirms the conclusion of Bolles and Fair (1982) that the parameters of a parametric mass transfer correlation must change from one operating region to another to reflect the change in the transfer mechanism. This means that different liquid and gas flow rates, and so on as operating regions, should lead, within the same correlation, to different exponent values from one "operating region" to another. Unfortunately this is not incorporated in observed mass transfer correlations.

The correlation equations presented in previous sections are of the form of the Cobb-Douglas model (De Neufville, 1990), i.e.,

$$Y = C_0 \prod X_i^{C_i} \quad (3.38)$$

where Π = the multiplication of all X_i terms, C_i = model parameters (i.e., constants) to be estimated statistically to reflect reality, and X_i = independent variables that affect the regressed quantity Y . The Cobb-Douglas model dominated the literature and practice until the early 1970s, until its deficiencies become too obvious and practical alternatives became available through the development of high-speed computers. The Cobb-Douglas model has several attractive features (De Neufville, 1990):

- It can, by suitable choice of the parameters, C_i , represent a broad range of the important characteristics of the relationship sought.
- These parameters can be immediately interpreted in terms of the characteristics of the production functions, which is a great pedagogical and practical advantage.
- It is easy to estimate statistically. This is because the multiplicative equation can be transformed into a linear function by expressing variable in terms of their logarithms.

However the model inherently implies that certain features of the relationship remain the same regardless of the values of the variables. This general remark agrees with the conclusions of Bolles and Fair (1982).

The parameters of the model, a_i , are generally obtained using least squares regression, which has certain limitations and requires large sets of accurate data to yield satisfactory results. If the least squares regression is properly applied the following optimal properties are true for the developed model: (i) the estimates have maximum likelihood and highest posterior density; (ii) the estimates are unbiased; and (iii) the estimates have the minimum variances. But for these properties to be valid the following conditions must be satisfied first: (i) the values of the operating variables are exactly known; (ii) the model form is known; (iii) the errors and the observed responses at each set of operating conditions have the same variance; (iv) the errors (and the observed values of the responses) are not correlated and thus are statistically independent; (v) the errors are identically and normally distributed with zero mean and variance σ . It is obvious that the above assumptions are rarely satisfied. Despite the limitations and the drawbacks of the empirical approach, the latter is still largely used and has produced the most practical results.

A key assumption of least squares estimation is that the model form, i.e., the mathematical expression that describes the functional relationship must be known. However, this form is often unknown and always to some extent subjectively assumed (Adamowski, 1985, Silverman, 1986).

Table 3.1 Discrepancy between the exponents of important liquid variables in different correlations (from Manger and Ponter, 1980a).

Authors	Exponents of			
	Liquid flow	Diffusion	ρ Density	μ Viscosity
Higbie (1935)	<u>+0.33</u>	<u>+0.50</u>	-0.16	-0.16
Sherwood & Hollaway (1940)	+0.54	+0.50	-0.50	-0.04
Knoeder and Bonilla (1954)	+0.77	+0.53	-0.33	<u>+0.53</u>
Van Krevelen and Hoftijzer (1947)	+0.66	<u>+0.66</u>	-0.40	+0.33
Van Krevelen and Hoftijzer (1948)	+0.80	+0.60	-0.50	-0.40
Shulman et al. (1955)	+0.45	+0.50	-0.17	+0.05
Davidson (1959b)	+0.33	+0.50	-0.17	-0.16
Hikita (1960)	+0.45	+0.50	+0.16	-0.16
Onda et al. (1968)	+0.66	+0.50	+0.27	-0.82
Mohunta (1969)	+0.75	+0.50	-0.50	-0.80
Stephens and Morris (1951)	+0.70	+0.50	-0.50	-0.20
Taylor and Roberts (1956)	+0.40	+0.50	-0.50	+0.10
Taylor and Roberts (1956)	<u>+1.00</u>	+0.50	-0.50	+0.50
Normann and Sammak (1963)	+0.60	+0.50	-0.17	-0.44
Mika (1967)	+0.83	+0.50	<u>-0.99</u>	<u>-0.99</u>
Mika (1967)	+0.50	+0.50	-0.76	-0.43
Copp and Ponter (1972)	+1.00	+0.50	<u>+1.00</u>	-0.54

Actually, this is the main reason why so many different forms have been proposed. As a result, contradicting exponent values were obtained for the same variable in different regression equations. For example, the exponents of some variables in different correlations are identically preset to follow some "theory" while others are not. The exponent associated with molecular diffusion coefficient in the liquid is generally set at 0.5 as shown in Table 3.1. This is because the different mass transfer theories, from two-film to surface renewal (Toor and Marchello, 1958), suggest that the diffusion coefficient exponent should be between 0.5 and 1. However, the exponents of other parameters change from one correlation to another, sometimes in conflicting ways (Table 3.1). The liquid density exponent changes from -1 to 1. Thus, attempting to physically relate or interpret these correlations becomes almost impossible. This may be explained, in part, by the regression methods used that changed from being the least

squares method to simply a curve fitting procedure of a particular data set. Indeed, many parameters are freely changed to improve the fit of the correlation to its particular developmental data set. Each particular data set can be thought of as a sample (or a subset) from the population of all operating conditions.

Ponter and Au-Yeung (1982) stated that no reliable correlations are available to predict the mass transfer rate coefficient except for specific systems conducted under the same experimental conditions. Ponter and Au-Yeung relate the problem to the bad quality of the data, to insufficient quantity of the data, and to the model form being unknown. The assertion by Bravo et al. (1992) that the parameters have to change from one operating region to another is due to the high non-linearity of the as yet not well understood mass transfer mechanisms. Therefore, the form of the model must reflect these complexities. This also reveals the limitation of the current parametric regression-based approach to address this problem.

3.5 REVIEW OF CURRENT APPLICATION OF MASS TRANSFER CORRELATIONS

There is agreement in the recent literature that the Onda et al. (1968) model is the best model for air stripping applications (Roberts et al., 1985; Lamarche and Droste, 1989; Staudinger et al., 1990; and Dvorak et al., 1996). The original Onda work was based on 400 data points from engineered stripping, absorption and evaporation systems using liquid mass flowrates between 0.8 and 43 kg/m²/s and gas mass flowrates between 0.014 and 1.7 kg/m²/s. It consists mostly of data from laboratory experiments with primarily small packings. The majority of the data was for packings much smaller than 25 mm (1-inch) in diameter and made mainly of ceramic material. In addition, the Onda model was developed for solute of high concentrations encountered in chemical engineering applications. An important feature of this model is the independence of its parameters from the packing type and size. Onda and his coworkers claimed that their model gives results within $\pm 20\%$ range. As correlations, the Onda et al. model is limited to the packing and the ranges of the operating conditions within which it was either developed or verified.

The literature shows that the Onda model yields satisfactory results for lab data, i.e., conditions that are similar to those under which this model has been developed (Roberts et al., 1985;

Lamarche and Droste, 1989). Lamarche and Droste (1989) found that that 68% of the predicted values of their data lie within a factor of 1.18 from the observed values. Similarly, Roberts et al. (1985) found that 68% of the predicted values of their data lie within a factor of 1.21 from the observed values. This result is based on about 70% of the data. Roberts et al. (1985) eliminated more than 30% of the data because the stripping factors were smaller than 2. Roberts et al. (1985) warned against the use of the Onda model for stripping factors below one because it produces unpredictable results.

3.5.1 Current Application of the Onda Model

Current applications of air stripping towers utilize modern packings that have different shapes and have different hydraulic responses from those used to develop the Onda model (Billet and Bravo, 1989). Current air stripping applications use modern packings of 2.5 to 15.0 cm (1 to 6 in) in diameter and made of propylene. These modern packings have higher specific surface areas, lower pressure drops, and they can accommodate higher flow rates. Most applications of air stripping towers to strip VOCs from groundwater involves very small concentrations in the particle per billion range, i.e. orders of magnitude smaller than those used to develop the Onda model.

Recent studies show that 30 to 40 percent deviations from predictions are often reported in full-scale applications (Lenzo et al., 1990, Staudinger et al., 1990 and Djebbar and Narbaitz, 1995). Most studies that used full-scale data with modern, large size packings of more than 2 cm in size concluded that the Onda correlations overestimate the overall volumetric mass transfer coefficient (Djebbar and Narbaitz, 1995; Lenzo et al., 1990; Staudinger et al., 1990). Djebbar and Narbaitz (1995) found the average absolute error to be 40%. In the Djebbar and Narbaitz (1995) study, the Onda model overestimated observed $K_L a$ and the overestimation tends to increase with increasing packing diameter. Lenzo et al. (1990) found that for 81 out of 85 full-scale systems reviewed, the Onda predictions overestimated $K_L a$ with an average error of 35%. The error reported in the Lenzo et al. (1990) study should be even larger because of two reasons: (i) the experimental $K_L a$ values included end effects, and (ii) their calculation of the error was based on the deviation relative to the Onda predictions rather than to the experimental values. Staudinger et al. (1990) reported deviation in the Onda estimates in the order of 30% at the 90% confidence interval.

Only Gossett's study concluded that the Onda correlations underestimated the performance of two packings: the 50 mm (2 in) Pall Rings and Tripacks (Gossett et al., 1985). All other studies using large size packings reported overestimation of the transfer rate constant by the Onda correlations. The evaluation with lowest apparent error is that by Cummins (Djebbar and Narbaitz, 1995), but it is highly questionable as several other parameters were simultaneously adjusted. Without these adjustments, the Cummins study would result in an average error that is larger than 60%.

Considering the above, several authors attempted to improve the Onda model, but little success has been encountered. Among these are the works of Gossett et al. (1985) and Narbaitz and Djebbar (1995).

Roberts and coworkers (Roberts et al., 1985) asserted that gas phase resistance was underestimated by the Onda correlations. In an effort to build on this hypothesis, Gossett et al. (1985) sought to link transfer rate prediction to relative gas-phase resistance values using the following equation:

$$\%E = 100[(1 - a') - 1] + \%R_G \left[\left(\frac{1}{b'} \right) - \left(\frac{1}{a'} \right) \right] \quad (3.39)$$

in which %E = percentage difference between Onda-predicted $K_L a$ and measured $K_L a$, a' and b' = modification factors for the Onda individual liquid-phase and gas-phase mass transfer coefficients, respectively, and R_G = percent gas-phase control as predicted by the Onda correlations = $k_L a / (H k_g a)$ (Staudinger et al., 1986). The parameters a' and b' depend on packing type and can be arrived at using equation (3.39) given supporting data (Gossett et al., 1985). Because a' and b' are available for a limited number of packings, Gossett et al.'s (1985) correction has very limited application.

Moreover, the Gossett et al. (1985) correction did not improve the predictions in the Staudinger et al. (1990) data base. Staudinger (1986) pointed out that the Gossett modification is merely a curve fitting of their data. Actually Gossett et al. (1985) themselves indicated that any improvement to the Onda model should involve both a , k_L , and k_G correlations, and that more modifications than simple change of front-constants in the Onda expressions are needed.

Djebbar and Narbaitz (1995) found that the Onda model overestimates $K_L a$ for packings with large diameters, and that the overestimation increases non-linearly with the packing size. Therefore, they proposed the following equation to correct for the Onda predictions.

$$K_L a' = \frac{K_L a}{0.834 + 0.293 \ln(d)} \quad (3.40)$$

were d = the packing nominal diameter in cm; and $K_L a$ and $K_L a'$ = the Onda and the corrected Onda mass transfer coefficients, respectively. The result of applying this correction to experimental data from three different data bases, reduced the prediction errors from 35 to 17% (Djebbar and Narbaitz (1995)).

Although the Djebbar and Narbaitz (1995) modification was nonlinear, it did not improve the estimation of all studies used in Staudinger et al. (1986) data base. Table 3.2 shows examples of such results.

Data	Onda results	Corrected Onda results
Gossett et al. (1985)	20	30
Lang, K.C. (1991)	17	28

Gossett et al. (1985) and Djebbar and Narbaitz (1995) attempts failed to be general because they did not address the fundamental problems of the Onda model which are discussed in the following paragraphs.

3.5.2 Investigation of the Onda Model

Figure 3.10 shows the average error in the Onda model predictions resulting from different experimental studies. It clearly shows inconsistency in the Onda model performance, which greatly changes from one study to another. There are four plausible causes for the magnitude of the error and the variation of the magnitude of the error from one study to another. These are (i) column operational problems, (ii) data analysis problems, (iii) uncertainty in the variables values, and (iv) Onda correlations functionality problems. It is crucially important to distinguish between these errors. Failing to do so will lead to incorrect conclusions.

An important aspect which is frequently overlooked in the majority of published data is the error due to operational problems such as channeling, wall flow, and liquid maldistribution. Usually, authors tend to control their experiments well and to keep operational problems and their effects as small as possible. Unfortunately, operational problems do occur, but there are no estimates of their relative contribution in the total observed deviation. This situation is further complicated by two factors: (i) the difficulty to estimate these types of error, and (ii) the lack of detailed information in published data, which enable their estimation. Operational problems produce systematic errors, which make them difficult to estimate by only analyzing data from one specific source. This may explain, at least in part, the systematic higher or lower deviation in one study compared to another (Figure 3.10).

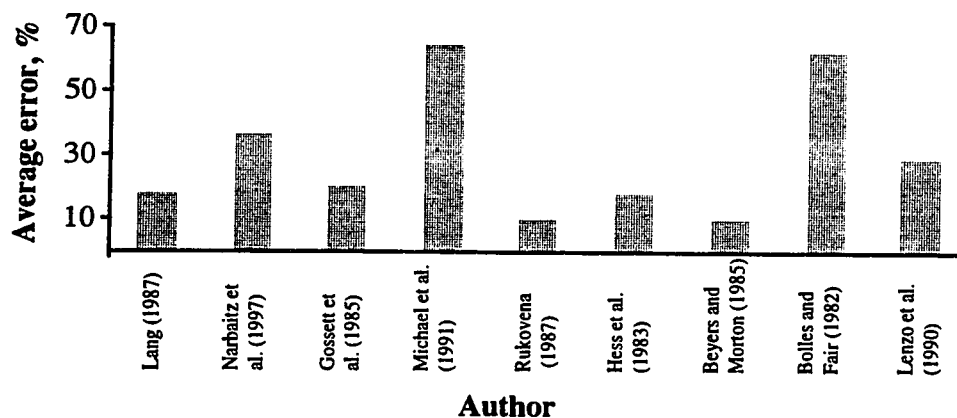


Figure 3.10 Change of the average error in the Onda prediction as a function of the data source.

The second cause of observed deviation would be mishandling and/or misanalysis of the data. Examples of such problems are end effects and the equation used to estimate mass transfer coefficient. The equation used to estimate the observed mass transfer coefficient in Gossett et al. (1985) was proven to be imprecise (Djebbar and Narbaitz, 1995). This equation produces observed $K_L a$ values that are 5 to 10% lower than “real” values when the influent air contains VOCs. The equation used by Gossett et al. (1985) to estimate experimental $K_L a$ does not handle influent air concentration that is different than zero. This explains in part the higher experimental $K_L a$ values reported by Gossett et al. (1985), and thus the smaller deviation reported in their study.

End effects may constitute up to 36% of the observed transfer (Spedding, 1988). Also, existing methods for estimating end effects are questionable (Djebbar and Narbaitz, 1995; Lamarche and Droste, 1989). Dvorak et al. (1996) neglected end effects on the basis that they are small. Therefore, they attributed any observed deviation in the Onda estimates to the Onda correlations themselves. Experimental studies that neglect end effects will end up with higher transfer rates than they are in reality.

The third source of error is the uncertainty in the values of the variables. At the 68% confidence level, Djebbar and Narbaitz (1995) found that typical errors in the variables used in the Onda model will produce 5 to 15% deviations in the predicted K_{La} values. Therefore, part of the observed deviation is attributed to the lack of fit of the Onda model, which points to the possibility of existence of a better model. This conclusion is true only if other sources of errors, such as end effects and operational problems, are negligible.

The above indicated sources of errors can be minimized through careful design and operation only, as described in Chapter 2.

The fourth possible cause of error would be the Onda correlations themselves, i.e., the adequacy of the Onda correlations to describe the transfer characteristics. The limitations of the Onda model that were identified in previous studies (Gossett et al., 1985; Staudinger et al., 1986; Bravo et al, 1992; Djebbar and Narbaitz, 1995; Dvorak et al., 1996) include mainly: (i) the effect of depth of the tower, packing diameter, and gas flow rate; (ii) the effect of the liquid distribution system; (iii) and the functional forms of the correlations. These limitations are further discussed in the following paragraphs.

The first point concerns packing depth of the tower, packing diameter, and gas flow rate. If a variable is not correctly characterized in the model, it will produce different and systematic errors that change depending on the real value of that specific variable. This type of error makes it difficult to compare and to transfer information from one study to another. In their study, Djebbar and Narbaitz (1995) found that K_{La} is not constant along the depth of the tower as assumed in theory. Gross and Termaath (1985) conducted experiments in which the only variable that changed was the packing depth. Gross and Termaath (1985) found that K_{La} decreases with the increase in the depth of the packing. The Onda model does not include the

packing depth as one of their variables. Also, Bravo et al. (1992) and Bravo and Fair (1982) indicated that the interfacial area available for mass transfer is function of the liquid and gas flow rates. Onda et al. (1968) assumed that the surface area varies only with the liquid flow rate. Dvorak et al. (1996) found that the gas phase mass transfer coefficient is overestimated at low gas loading rates, which resulted in an underestimation of the overall mass transfer coefficient. Also, they found that the Onda model was unable to reproduce the sharp increase in observed mass transfer coefficient at high gas loading rates. Dvorak et al. (1996) attributed this to the absence of the gas loading rate from the Onda surface area correlation. Finally the packing diameter which characterizes the size of the packing and contributes to differentiation between one packing type and another, with respect to the transfer characteristics, is questionable. Some packings have approximately the same size in all directions such as Tripac™, Norpac™, Hi-Flow Rings™, Flexirings™, and Lanpac™, while others do not, such as Snowflakes™, Cascade Minirings™, Tellerettes, and saddles which are quite flat. Therefore, the packing diameter definition and its relation to the transfer characteristics should be investigated.

The second point concerns the transfer characteristics in the upper part of the column and their relation with the liquid distribution system. These characteristics were observed to be different from those in the rest of the column depending on the “quality” of the liquid distribution system used (Perry et al., 1990; Djebbar and Narbaitz, 1995). Observed increase or decrease in $K_{L,a}$ in the upper part of the column is related to the adjustment of the wetted packing surface area associated with the shift from the liquid distribution pattern of the distributor to the natural flow distribution pattern of the particular packing type (Djebbar and Narbaitz, 1995). The depth of this upper part of the tower is, in large part, dictated by the liquid distributor characteristics. Therefore, the goodness of the liquid distribution system is not absolute. Actually the goodness of the liquid distribution at the top of the packing should be compared to the particular packing natural distribution frequency as far as its effect on the transfer is concerned. Some attempts have been made to characterize the effect of the liquid distribution system, but the results were too complex to be practical (Hoek et al., 1986).

The third point concerns the appropriateness of the functionality of the Onda correlations. Roberts et al. (1985), Gossett et al. (1985), and Dvorak et al. (1996) agreed that the source of error in the Onda model appears to be in the wetted surface area and/or in the gas-film resistance equations. In their study, Dvorak et al. (1996) concluded that the forms of the Onda correlations

are appropriate and that the parameters of the correlations only should be changed to reflect modern operating conditions. As indicated earlier, Dvorak et al. (1996) found that the Onda model does not handle correctly the effect of the gas flow rate. However, they concluded that the liquid loading effect is correctly characterized. To arrive at this conclusion, Dvorak et al. (1996) isolated the transfer components, a , k_L , and k_G , and investigated each component separately. Unfortunately, they used the Onda correlations themselves to separate the transfer components instead of an independent approach. For example, when they isolated the gas phase resistance, they used the Onda liquid and surface area correlations assuming that they are correct, an assumption that has yet to be proven.

In the evaluation of the functionality of the liquid loading, Dvorak et al. (1996) neglected the gas phase resistance. However, they indicated that the latter constitutes 4 to 54% of the total resistance. By eliminating gas phase resistance, Dvorak et al. (1996) obtained a simple linear relationship between the logarithm of liquid loading and the logarithm of overall mass transfer coefficient. If it is accepted that the gas phase resistance is relatively important, i.e., between 4 and 54%, then a linear relationship should not be obtained. If it is as found by Dvorak et al. (1996), then it should be concluded that the liquid loading functionality is not correct or at least, the assumption that the gas phase resistance is negligible is inadequate.

In estimating experimental mass transfer coefficients, Dvorak et al. (1996) neglected end effects. If the liquid distribution is excellent, as indicated by Dvorak et al. (1996), then end effects will be even higher. The subtraction of end effects from the total observed transfer will shift the observed $K_L a$ to lower values. This will result in the Onda $K_L a$ values being larger than observed $K_L a$ values not lower as suggested by Dvorak et al. (1996). If 15% of the removal is attributed to end effects in Dvorak et al. (1996) data, then the Onda model will overestimate $K_L a$ values by 20%, and 70% of the data will be overestimated. The analysis in Dvorak et al. (1996) was based on 76% of the data only, since 23% were discarded. The above raises questions about the findings of Dvorak et al. (1996) regarding the performance of the Onda model and the appropriateness of the liquid phase mass transfer correlation.

Bravo et al. (1992) indicated that a stronger influence of gas and liquid rates on interfacial area is expected for random packings. Also, they indicated that different (packing) surfaces and ranges of liquid flow rates can lead to different values of the exponent associated with the liquid flow

rate. This is not the case in current mass transfer correlations, where a single exponent is defined for each variable. This is one of the limitations of the parametric approach as discussed in previous sections.

Other studies avoided the approach of looking for general models by developing completely new correlations whose parameters depend on packing type and size. Obviously, these correlations are expected to produce better results for specific packings compared to the more general models such as the Onda model. Among these studies are the work of Sherwood and Holloway (1940), and more recently the works of Costa et al. (1992), Little and Selleck (1996) and Little and Mariñas (1997). This approach eliminated the need to characterize packing geometry-related variables on fundamental basis such as packing diameter and packing surface area. The parameters of proposed correlations depend on packing type and size. These parameters are available for a limited number of packings only, hence the limited application of proposed correlations.

Because of their generality, correlations like Onda's are more interesting and still draw much attention. There is agreement in the recent literature that the Onda model is appropriate, however, it needs to be ameliorated. Unfortunately, there is no concordance on the source of the deficiencies in the Onda model and how to curtail them. While claiming the appropriateness of the Onda liquid phase mass transfer equation, Little and Mariñas (1997) proposed a correlation for liquid phase mass transfer coefficient which is different from the Onda correlation. They did not provide clear reasons for their choice of a different model nor for the form of the proposed model.

One should not conclude from the above that the parametric approach is ineffectual. The parametric approach is the best approach if the form of the relationship is known, especially for explicitly understanding the cause effect relationship. Furthermore, it can be safely used within the conditions of the data with which it has been developed. Also they are easy to use with a calculator or spreadsheet. However, if this relationship is not known, such as the case of mass transfer in packed towers, other approaches may be preferable, especially when the number of independent variables is large and the degree of nonlinearity is high. The nonparametric approach is a promising alternative approach.

3.6 NONPARAMETRIC APPROACHES

In the parametric approach, the performance of a process (the dependent variables) is predicted using a mathematical function of a set of design variables (the independent variables) and a set of constants (parameters), such as,

$$y = \alpha x_1^\beta x_2^\gamma \dots \quad (3.41)$$

where y = the dependent variable being predicted; x_1 and x_2 = the independent variables; and α , β , and γ = the parameters. The parameters are usually determined by parameter estimation methods such as least squares regression.

The nonparametric methods are alternative methods that overcome some of the difficulties encountered with the parametric regression approach. The nonparametric approach frees discriminate analysis from rigid distributional assumptions, like those of the least squares method. The main advantage of these techniques is the avoidance of the explicit selection of a model form. In nonparametric approach a relationship of possibly complicated or unorthodox shape is generated by the data points themselves (Silverman, 1986). As stated by Silverman (1986), these techniques allow the data to “speak for themselves”. For these reasons, nonparametric techniques appear to be well suited for the analysis of air stripping K_{La} data.

Recently, two nonparametric methods have been applied by Djebbar and Narbaitz (1996) and Narbaitz and Djebbar (1996). These methods are the Nonparametric Kernel Regression and Neural Networks.

3.6.1 Nonparametric Kernel Regression

Simply stated, nonparametric kernel regression of a dependent variable y at a given value of the independent variable x can be estimated through a weighted average around x (Figure 3.11), that is:

$$E(y|x) = m(x) = \frac{1}{n} \sum_{i=1}^n w_i(x) y_i \quad (3.42)$$

where $m(x)$ = the expected value of the independent variable y at x ; n = the number of neighboring observations; y_i = the observation at x_i ; and w_i = weight.

The basic idea of the local average $m(x)$ is equivalent to the procedure of finding a local weighted least squares estimate (Härdle, 1989). As such, this estimate takes advantage of the fact that more information about $m(x)$ is contained in the surrounding of x rather than in points far away from x . Therefore more weight is given to the information contained in the neighborhood of x and less weight is given to the information contained in points far away from x . These weights are estimated, in nonparametric kernel regression, using probability density functions (Härdle, 1989) through nonparametric frequency techniques (Adamowski, 1985; Djebbar and Narbaitz, 1996). This nonparametric approach improved the K_L predictions in the Djebbar and Narbaitz (1996) study by more than 50% for the specific data base and methodology used.

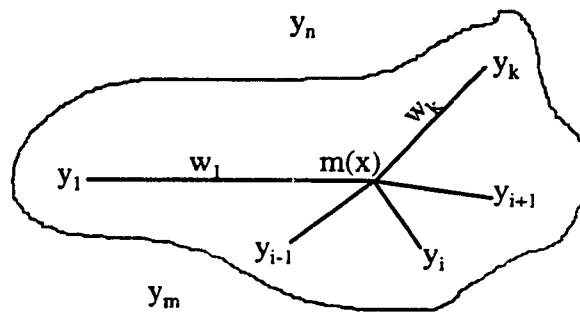


Figure 3.11 Concept of neighborhood in nonparametric regression.

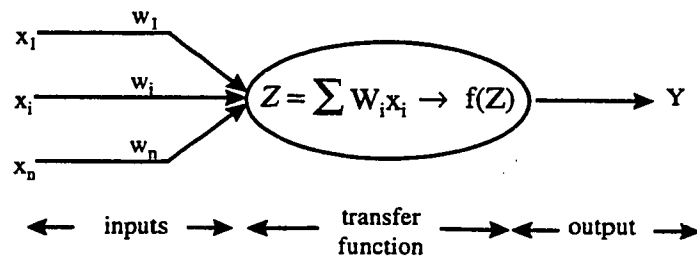
3.6.2 Neural Networks Method

Neural network is inspired by the functioning mode of an animal brain in which a great number of neurons are interconnected by their synapses. By analogy the neuron is defined as the basic unit of the network. This neuron can receive one or more inputs, calculate the weighted sum and produce a unique output through the transfer function (Figure 3.12).

A neural network can be defined as a highly parallel adaptive system capable of auto-improving by learning. The main concept of neural computing is the decomposition of the input-output relationship into a series of linearly separable steps using hidden layers, as shown in Figure 3.12.

Neural network can also be looked at as an association of neurons; therefore, several type of network architectures are possible.

a. neuron conceptualisation



b. architecture of neural network

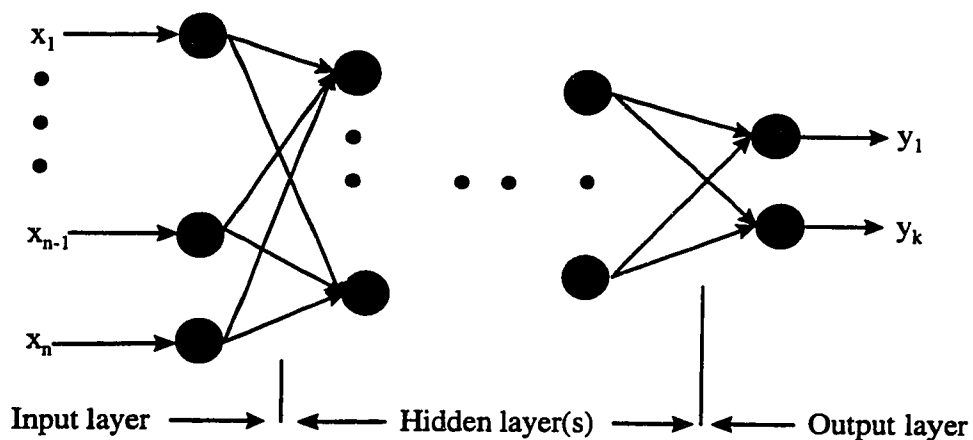


Figure 3.12 Concept of neural network.

There are two distinct steps in using neural networks. The first is the learning step in which the network is defined and trained to respond 'correctly' to the training data set. The second step is simply its application. The main difficulties with the neural network approach is the choice of the network architecture and to a lesser degree the training algorithm. Various neural network topologies have been proposed to date; however, recent success in neural network research is mainly attributed to the achievements of multilayer perceptrons with backpropagation training algorithms (Djebbar and Narbaitz, 1995). This neural network approach in the Djebbar and Narbaitz (1995) study improved the predictions by more than 50% for the same data base used to evaluate the nonparametric kernel regression. So both approaches yielded comparable results.

3.7 CONCLUSION

Despite its limitations, the parametric approach has led to a better understanding of the way some variables affect the transfer process. However, the high nonlinearity of the process, the high number of variables that affect the process, and the absence of the “true known” relationship that relates the variables to each other curbed the traditional parametric approach from providing totally satisfactory relationships, which, in some cases, were contradictory. Serious drawbacks are identified in the Onda model when used to design or analyze modern air stripping towers. These drawbacks need to be addressed using modern data through improving the Onda model or by proposing a new model.

The new nonparametric approaches proved to be more powerful and more robust than the traditional parametric approach in identifying and modeling complex relationships. These methods may overcome many of the shortcomings of the traditional approach. However, more investigation is required.

The lack of good predictive ability of existing mass transfer models and of the Onda model in particular, for full-scale applications is due to: (a) the extrapolative nature of the predictions; (b) the limited operating conditions in the databases used to develop the correlations; (c) the limitations of parametric regression techniques used to generate these models; and (d) the changing nature of mass transfer relationships from one set of operating conditions to another, that are not well understood and are poorly mimicked by current models (Djebbar and Narbaitz, 1995 and Bravo et al., 1992).

To avoid problems (a) and (b), in the above, newer predictive tools should be developed with a large high quality database that represents full-scale operating conditions. Extreme care should be taken to only use high quality data. This thesis will gather such a database to aid in the development of new predictive tools. It is obvious that to overcome problem (c) nonparametric approaches should be evaluated and refined further. This avenue of research is particularly promising given the great results of initial evaluations which used data from a single source (Djebbar and Narbaitz, 1995; Narbaitz and Djebbar, 1996). Accordingly this is one of the main thrusts of this thesis. Because parametric regressions are a better pedagogical tool, and are

much easier to use, i.e., they can be easily used with a calculator or a computer spreadsheet, the development of improved parametric regressions should not be abandoned. Given that there is a very large number of potential parametric models and the Onda model is considered the best among the large number of models developed so far, this thesis will use the new large quality database to calibrate a modified Onda model. The modifications will incorporate variables that the literature has identified as important, and are not part of the Onda model. A comparison of the predictive abilities of parametric and non-parametric approaches will determine which one is the preferred approach.

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CHAPTER 4

DATA SELECTION AND PARAMETERS ESTIMATION

This chapter discusses the data used in this study. First, a description of the data selection procedure is presented. The following section describes the main characteristics of the data such as the packings type and size, the VOCs removed, and the operating variables. The third section explains the method used to estimate experimental mass transfer coefficients. And the final section presents the methods used to estimate physical characteristics of water, air, and VOCs.

4.1 DATABASE DEVELOPMENT

Data on packed tower air stripping applications and their performance are abundant in the literature. However, it is difficult to obtain quality data which include: (i) detailed information on experimental conditions and operational variable values; (ii) information on the limitations and the problems encountered in conducting the experiments; and (iii) the degree of care taken in conducting the experiments and analyzing the results. Some of this information may be subjective to evaluation and reporting, however, the more is known, the better one is able to explain and analyze the response of the system to the operating variables.

Experimental data in the public domain were surveyed. When necessary, supporting information was obtained directly from the authors of the particular study. The following criteria were used to select the data:

- Full-scale operating conditions including packings with diameters that are mainly larger than 2.5 cm, tower to packing diameter ratios larger than eight (Treybal, 1980), and typical water and air loading rates (see section 2.4.3).

- Handling of end effects is described in detail.
- High level of care is taken in collecting the samples and analyzing the data.
- Explicit description of operating conditions, such as packing type and geometry; tower characteristics; liquid, gas, and temperature values; and type and characteristics of VOC(s) considered.
- Stripping factor should be greater than 2 (Roberts et al., 1985).
- For towers with only two sampling points, the effluent concentration must be greater than 1 $\mu\text{g/L}$.

The assembled database is summarized in Tables 4.1, 4.2 and 4.3. Table 4.1 lists the 12 studies used to build the database and the main characteristics of their respective experimental setups. In total, 21 packing types and sizes and 22 VOCs were considered. Table 4.2 contains the packing types along with their main characteristics, the source of the information about the individual packings is listed in Appendix A.1. Table 4.3 lists the main characteristics of the VOCs. The studies used in building this database encompass wide ranges of VOC air stripping operating conditions, and were conducted to mimic modern full-scale operating conditions (section 2.4.3).

Table 4.1 Summary of pilot-scale studies selected for the database.

#	Study	Number of data points	Tower		Loading rates		Air-to- water ratio
			height (m)	diameter (cm)	Air ($\text{kg/m}^2 \text{ s}$)	Water ($\text{kg/m}^2 \text{ s}$)	
1	Gossett et al. (1985)	271	2.44	44.5	0.06-1	10-23	10-170
2	Cummins (1988)	102	5.5	61	0.02-1.3	7.5-7.5	1.5-550
3	Cummins & Westrick (1983)	96	5.5	61	0.03-1.5	1.6-43.5	5-42
4	Gross & Termaath (1985)	54	2.4-1.2	19	0.4-0.4	14.5	37.8
5	Raczko et al. (1985)	16	3.05	30.5	0.3-1.2	11-31	7-103
6	Hess et al. (1983)	59	3.05	30.5	0.2-0.9	6-43	40-160
7	Cline et al (1985)	15	3.05	30.5	0.1-0.7	8.6-24	18-85
8	Umpres et al. (1982)	12	2.34	30.5	0.3-1.3	2.6-11	8
9	Narbaitz et al. (1998)	698	4.6	76.2	0.15-1.3	5.5-27.5	8.5-42
10	Lang (1991)	67	2.7-5.2	61, 91.5	0.6-4.5	2-24	2.5-20
11	Rukovena (1987)	54	3.05-5.2	43, 89	0.2-5.6	4.3-28.5	1-80
12	Michael et al. (1991)	6	1.22	61	0.3-0.8	6.5	8-27

Table 4.2 Names and main characteristics of packings in the database.

Packing	Diameter (cm)	Surface area (m ² /m ³)
Random packing		
Rashig Rings	1.3	400
Ceramic Saddles	1.3, 2.5	466, 259
Pall Rings;	1.6, 2.5, and 5	341, 220, 108
Tellerettes	2.5 and 5	180, 125
Norpac	3.8 and 5	145, 100
Hi-Flow Rings	5	97
Flexiring	5	115
Tripac	5	157
Cascade Minirings	5 and 7.6	210, 141
Flexisaddles	7.6	88.6
LANPAC TM	8.9	137
Snowflakes	9.4	91.8
Structured packing		
Munters	1.6	420
Flexipac	5	131

Table 4.3 List of VOCs used in this study and their characteristics according to Haarhoff and Cleasby (1990).

Compound name	Chemical formula	Henry's Law Const. at 20°C (atm. m ³ liquid/m ³ air)	A*
Dichloromethane	CH ₂ Cl ₂	0.0725	3817
Bromoform	CHBr ₃	0.028	4399
Chloroform	CHCl ₃	0.11677	4612
Bromodichloromethane	CHCl ₂ Br	0.095	4375
Dibromochloromethane	CHClBr ₂	0.036	4375
Carbon Tetrachloride	CCl ₄	0.985	4411
Chloroethane	C ₂ H ₅ Cl	0.3968	3120
1,1-Dichloroethane	C ₂ H ₄ Cl ₂	0.182	4128
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	0.059	3620
1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	0.561	4133
1,1,2,2-Tetrachloroethane	C ₂ H ₂ Cl ₄	0.016	4375
Vinyl chloride	C ₂ H ₃ Cl	0.923	3729
cis-1,2-Dichloroethylene	C ₂ H ₂ Cl ₂	0.125	4192
Trichloroethylene	C ₂ HCl ₃	0.302	4780
Tetrachloroethylene	C ₂ Cl ₄	0.557	4918
1,2-Dichloropropane	C ₃ H ₆ Cl ₂	0.096	4375
Benzene	C ₆ H ₆	0.23	3680
Chlorobenzene	C ₆ H ₅ Cl	0.16	4375
m-Dichlorobenzene	C ₆ H ₄ Cl ₂	0.15	4375
Toluene	C ₆ H ₅ CH ₃	0.19	8100
m-Xylene	CH ₃ C ₆ H ₄ CH ₃	0.45	4375
Ethylbenzene	C ₈ H ₁₀	0.27	4375

*Henry's Law temperature constant in Equation 4.3

The data pertain primarily to modern large size packings with nominal packing diameters between 2.3 and 9.4 cm. The liquid loading rate varies between 0.4 and 2 m³/m²min (2 and 43 gpm/ft²), the gas flow rate varies between 0.06 and 5.7 m³/m²min (1 to 120 gpm/ft²), and Henry's Law constant values at 20°C range between 0.015 and 1.4 atm. m³ water /m³ air. Stripping factors resulting from these operating conditions range between 2 and 500. The towers used in these studies have total packing depths that vary between 1.2 and 5.2 m. The liquid phase temperature range between 7 and 30°C. In addition this database includes performance data on two structured packings.

The total number of data points amounts to 1450, which is about three times the Onda et al. (1968) developmental database. To the author's knowledge, this is the most comprehensive database gathered to date. It should provide a solid means for the development of a versatile model, and for an extensive evaluation of the proposed model.

4.2 ESTIMATION OF OVERALL MASS TRANSFER COEFFICIENT $K_L a$

Great care was taken in determining the observed mass transfer coefficient. The concentrations used were those at the top and bottom of the packings or, for a small portion of the data, in and out concentrations corrected for end effects. The observed mass transfer coefficient is determined using the generalized equation which accepts influent air with a VOC concentration greater than zero (Djebbar and Narbaitz, 1995):

$$K_L a = \left[\frac{L}{z} \right] * \left[\frac{R}{R-1} \ln \left\{ \frac{c_i (1-1/R) + c_e / R}{c_{i+1} (1+1/R) + c_e / R} \right\} \right] = [\text{HTU}] * [\text{NTU}] \quad (4.1)$$

where (Figure 4.1) $R = \frac{HG}{P_i L}$ = the stripping factor (dimensionless); HTU = the height of a transfer unit (m); NTU = the number of transfer units (dimensionless); c_e = the liquid effluent VOC concentration which corresponds to depth Z, the bottom of the packing media in Figure 4.1, kg/m³; H = the Henry's law coefficient on a volume to volume basis, atm. m³ water /m³ air; P_i = the total operating pressure, atm; L = the liquid volumetric flow rate per unit cross sectional area, m³/m²s; G = the gas volumetric flow rate per unit cross sectional area, m³/m²s; K_L = overall liquid phase mass transfer coefficient, m/s; a = effective interfacial surface area, m²/m³; and c_i and c_{i+1} =

the VOC concentrations in the liquid in kg/m^3 at both ends of the packing depths z_i , z_{i+1} , respectively.

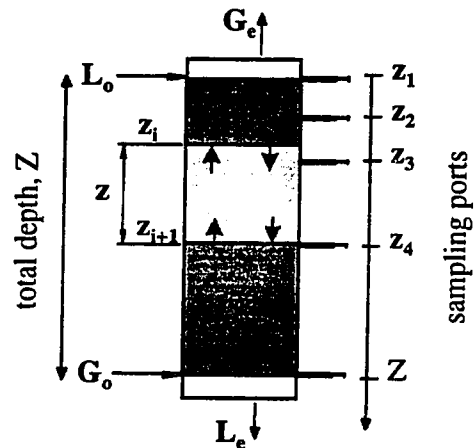


Figure 4.1. Definition of tower parameters used in the analysis.

Most mass transfer data use influent and an effluent sampling points. If the influent and effluent samples are not taken from the packed zone, then the resulting estimated transfer would include end effects. Such data must be corrected for end effects before it can be used in the analysis of mass transfer characteristics.

4.3 ESTIMATION OF END EFFECTS

Mass transfers that occur inside the column, above and below the packing, are called end effects. It has been customary to express end effects in terms of an equivalent height of packing. End effects are accounted for using one of two methods. The first method assumes that end effects are equal to the transfer that occurs in a short empty column. In the second method, the observed total number of transfer units, NTUT, is estimated for different packing depths Z . The intercept with the ordinate in the plot of NTUT vs. Z gives the number of transfer units due to end effects, NTUE. Therefore, the net number of transfer units due to the packing only is given by the following equation,

$$\text{NTU} = \text{NTUT} - \text{NTUE} \quad (4.2)$$

The value of NTU indicates the difficulty in removing the solute from the liquid phase. Both NTU estimation methods are based on the assumption that mass transfer inside and outside the packing are additive and linear in nature. Both methods have been applied to the same system,

but yielded different results. The differences are believed to be caused by the flow being too different from the plug flow assumption for NTUs to be additive (Lamarche and Droste, 1989). The second method is sound only if the rate of mass transfer varies with liquid and gas rates in the "end effects" region exactly the same way as it varies in the packed section. Yoshida and Koyanagi (1962) showed experimentally that both gas and liquid flow rates affect NTUE and NTU differently. Roberts et al. (1985) failed to formulate a truly predictive model because the phenomena contributing to end effects are not understood adequately from a theoretical viewpoint.

According to Staudinger (1986), end effects are significant in laboratory experiments, i.e., using small columns, but they are rather small in pilot and full-scale systems. The majority of existing mass transfer correlations were based on laboratory experimental setups, which used mainly small columns. Spedding (1988) indicated that end effects may represent 10 to 36% of the total transfer. Error in accounting for end effects will produce similar errors in the calculated transfer characteristics.

The data used in this study were scrutinized for end effects. Only data which did not include end effects or were "corrected" for end effects were included. Among the selected studies, only Cummins's (1988) data were corrected for end effects. Cummins (1988) used five sampling ports, however, the first sampling port was from the influent line, not from the top of the packing. The concentration at the top of the packing was extrapolated using the depth vs. concentration distribution within the column.

4.4 ESTIMATION OF PACKING AND FLUIDS PARAMETERS

Adequate interpretation of results requires the values of certain physical properties, for example liquid density, diffusion coefficient, Henry's Law constant, and critical surface tensions. These physical properties were carefully estimated, because they affect the resulting mass transfer coefficient considerably. These characteristics are shown in Table 4.2 and Table A2 in Appendix A2. The packing parameters, i.e., packing diameter and dry surface area, are readily available from the selected studies and are based upon manufacturers' specifications. Table A.1 in Appendix A1 presents a list of packings with their main characteristics. The physical properties of air and water are also described in the following sections.

4.4.1 Henry's Law Constants

Henry's law constant was discussed in section 2.2. The values of Henry's Law constant were obtained from experimental studies, such as Haarhoff and Cleasby (1990), Gossett (1987), and Lamarche and Droste (1989). The temperature dependence of Henry's Law constant is estimated using the following equation (Haarhoff and Cleasby, 1990),

$$H_T = H_{20} \left(\frac{293}{273 + T} \right)^{10^A \left(\frac{1}{293} - \frac{1}{273 + T} \right)} \quad (4.3)$$

where A = constant; T = temperature in °C; and H_T and H_{20} = Henry's Law constants at temperature T and 20 °C, respectively (atm. m³ liquid/m³ air). Values of H_{20} and A for different VOCs are presented in Table A2 in appendix A. Haarhoff and Cleasby (1990) recommend the use of $A = 4500$ when the experimental value is not available.

4.4.2 Molecular Diffusion Coefficients

After Henry's Law constant, the molecular diffusion coefficient is probably the most important physical parameter in the transfer process. Diffusion is the mass transport of species relative to the environment on a molecular scale. Alper and Dankwerts (1976) indicated that diffusion in liquid is more difficult to assess than diffusion in gases because of additional complexities introduced by the liquid structure, molecular motions, and intermolecular forces.

If the liquid diffusion coefficient at 20°C, $D_{L,20}$, is known, then the diffusion coefficient at a temperature T , $D_{L,T}$, can be estimated using the following simple equation (Treybal, 1980);

$$D_{L,T} = D_{L,20} \frac{(T + 273)}{\mu_a} 10^{-16} \quad (4.4)$$

where $D_{L,T}$ = diffusion in water at specified temperature, m²/s, and μ_a = water viscosity, Ns/m². Likewise, the diffusion in the air at temperature T , $D_{G,T}$, is estimated by the following equation (Treybal, 1980),

$$D_{G,T} = D_{G,20} \left(\frac{T + 273}{293} \right)^2 \quad (4.5)$$

The slower rate of diffusion is expected to result in lower mass transfer rates in packed towers. Values of $D_{L,20}$ and $D_{G,20}$ for different compounds are given in Table A2, Appendix A2.

4.4.3 Viscosity

The viscosity of a fluid is a measure of its resistance to shear or angular deformation. It results from the cohesion and momentum interchange between molecules within the fluid. As the temperature increases, the viscosities of all liquids decrease, while the viscosities of all gases increase. The following equations are used to estimate liquid and air viscosities. For air, the equation from Lamarche and Droste (1989) was used,

$$\mu_G = (1.71 + 0.005 T) 10^{-5} \quad (4.6)$$

For water, the equation from Kreider (1985) was used,

$$\frac{0.1}{\mu_L} = 2.1482 \left[(T - 8.435) + \sqrt{8078.4 + (T - 8.435)^2} \right] - 120 \quad (4.8)$$

where T = temperature in °C, and μ_L , μ_G = viscosities in kg/ms for water and air, respectively.

4.4.4 Packing Critical Surface Tension

Surface tension is another property of considerable importance in the aeration process. Surface tension plays an important role in drop and air bubble formation, and in determining the wetted surface area. Table 4.4 presents the values of critical surface tension for water and different packing materials used in this study (Dvorak et al., 1996; Staudinger, 1986).

Table 4.4 Critical surface tension for different material.

Material	Critical surface tension, N/m
Water	0.075
Ceramic	0.062
Polypropylene	0.0285
Polyethylene	0.033

4.4.5 Water and Air Densities

Air density is estimated using the following equation from Robertson and Crowe (1980),

$$\rho_G = 1.30 - 4.5 \times 10^{-3} T \quad (4.9)$$

whereas, water density is calculated using the following equation from Heggen (1983),

$$\rho_L = 1000 \left(1 - 0.000019549 (T - 4)^{1.68} \right) \quad (4.10)$$

where T = temperature in °C, ρ_G and ρ_L = gas and liquid densities, respectively, kg/m³.

4.5 DATA ANALYSIS AND USE

This database covers modern application and operation of air stripping towers for VOC removal. This database is used in the following chapters to analyze mass transfer in packed towers for air stripping and to develop a new approach for estimating mass transfer coefficient. The methods used to estimate physical characteristics of water, air, VOC and packings are those frequently applied in air stripping applications. They are not exhaustive, as there are several other methods.

Chapter 6 and 7 use all of the database. However, Chapter 5 uses part of Narbaitz et al. (1998) data only. Several computer programs were written to help prepare, analyze, and present the data and the results.

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CHAPTER 5

EVALUATION OF THE ONDA MASS TRANSFER CORRELATIONS

Paper published in the Environmental Progress Journal, Vol. 14, No. 3, pp. 137-145, 1995
under the title of: "Mass Transfer Correlations for Air Stripping Towers."

"... The problem with statistics was that anyone could get a model that was fitted to less than 1 % error in the past, and as soon as you went two months into the future it was 50 % out because you were just mining a spurious correlation out of your data... "

Michiel Hazewinkel

MASS TRANSFER CORRELATIONS FOR AIR STRIPPING TOWERS**Yassine Djebbar and Roberto M. Narbaitz**

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ABSTRACT

The overall liquid phase mass transfer coefficient, $K_{L,a}$, is the most important parameter in the design of air strippers. Designers frequently estimate $K_{L,a}$ using a mass transfer correlation to avoid the cost of pilot tests. This paper evaluates the well-accepted Onda correlation using a newly developed data base. Predictions based on the Onda correlation systematically overestimated $K_{L,a}$ for packings typically used in full-scale applications. They had an average error of $\pm 40\%$ and an average standard deviation of $\pm 47\%$. The overestimation was a function of the packing diameter. A simple equation was developed to correct the Onda overestimation for packings larger than 1 inch (2.54 cm) in diameter, and it yielded predictions within $\pm 20\%$ range. The experimental $K_{L,a}$ values obtained in this study varied with packing depth contradicting a basic assumption of the mass transfer theory, i.e., that $K_{L,a}$ is spatially constant. Also, the effect of measurement errors of the variables involved in the calculation of both the experimental and the predicted $K_{L,a}$ values were investigated. A large part of the observed difference between experimental and Onda predictions was attributed to a lack of fit of the Onda model. Thus, the quality of the predictive correlations can be improved.

INTRODUCTION

Air stripping of volatile organic compounds (VOCs) from contaminated ground water has become a well-accepted treatment method. Compared to other ground water treatment technologies, air stripping is very attractive because of its low cost, ease of operation and high efficiency especially for VOCs with a low affinity for adsorption. The most important parameter in the design of an air stripping tower is the mass transfer coefficient $K_L a$. Engineers often calculate $K_L a$ using a mass transfer correlation to avoid costly pilot scale tests. Tens of correlations have been developed but the Onda model (Onda et al. [17]) is considered the best set of mass transfer correlations for dumped packings in air stripping applications (Lamarque and Droste [11], Roberts et al., [19], and Staudinger et al., [21]). Model predictions have been satisfactory for laboratory studies that used primarily small size packings of traditional shapes. Current applications, however, utilize modern packings of 2 to 6 inches (5.08 to 15.24 cm) in size that have different shapes and have different hydraulic responses. Evaluations using large modern packings in full scale air strippers have been rather limited and some are of questionable quality. A recent pilot-scale air stripping study led to the development of a unique database that includes many VOCs, numerous operating conditions, various modern large size dumped packings and has extensive quality control (Narbaitz et al., [16]). The objectives of this study are as follows. First, to evaluate the Onda correlation using this new data base. Second, to assess the impact of packing depth, a factor not considered by current mass transfer correlations. And third, to assess the impact of experimental errors. This will help determine the relative contribution of both measurement errors and the Onda model's lack of fit to the total observed deviation.

MASS TRANSFER IN PACKED TOWERS

The theory of air stripping in packed columns has been well documented in the engineering literature (Treybal [23], Kavanaugh and Trussell [10]). Using the Kavanaugh and Trussell [10] approach, the packing depth element z , i.e. from depth z_1 to z_2 (Figure 1), is given by:

$$z = \int_{z_1}^{z_2} dz = \frac{L_f}{K_L a \rho_L} \int_{c_1}^{c_2} \frac{dc}{c - c^*} \quad (1)$$

where ρ_L = the liquid density (M/L^3); c^* = the VOC concentration in liquid phase that is in equilibrium with the VOC concentration in the gas phase (M/L^3); c_1 and c_2 = the VOC

concentrations in the liquid at the depths z_1 and z_2 , respectively (M/L^3); and L_f = the liquid mass flow rate per unit cross sectional area (M/L^2T). M , L and T refers to mass, length and time units, respectively. Using some simple mathematical manipulations, Equation 1 yields:

$$z = \left[\frac{L_f}{K_L a \rho_L} \right] * \left[\frac{R}{R-1} \text{Ln} \left\{ \frac{c_1 (1-1/R) + c_o / R}{c_2 (1+1/R) + c_o / R} \right\} \right] = [\text{HTU}] * [\text{NTU}] \quad (2)$$

where $R = \frac{HG}{P_t L}$ = the stripping factor (dimensionless); HTU = the height of a transfer unit (L);

NTU = the number of transfer units (dimensionless); c_o = the liquid effluent VOC concentration at depth Z , the bottom of the packing media (Figure 1) (M/L^3); H = the Henry's law coefficient on a volume to volume basis (atm); P_t = the total operating pressure (atm); and G = the gas mass flow rate per unit cross sectional area (M/L^2T).

For the total packing height, Z , Equation (2) becomes:

$$Z = \left[\frac{L_f}{K_L a \rho_L} \right] * \left[\frac{R}{R-1} \text{Ln} \left\{ \frac{c_1 / c_o (R-1) + 1}{R} \right\} \right] = [\text{HTU}] * [\text{NTU}] \quad (3)$$

where c_1 is the liquid influent concentrations at $z = 0$ (M/L^3). This is the most frequently used equation. The mass transfer coefficient $K_L a$ can be obtained from either equations 2 or 3, as

$$K_L a = \frac{L_f}{z \rho_L} \text{NTU} \quad (4)$$

In a column with multiple sampling ports, when the section of the column being analyzed does not include the bottom of the column as shown in Figure 1, the gas phase concentration entering this section is not zero, and Equation 2 must be used to calculate $K_L a$. Equation 3 is only valid for an inflow gas concentration equal to zero. Rearranging Equation (4) gives;

$$\text{NTU} = K_L a \left\{ \frac{z \rho_L}{L_f} \right\} \quad (5)$$

A plot of NTU versus $\left\{ \frac{z \rho_L}{L_f} \right\}$ should give a straight line if the assumption of constant $K_L a$ with depth is valid. The slope of this line is the experimental $K_L a$. It should be noted that generally only two data points, an influent sample and an effluent sample, are used in the $K_L a$ determination.

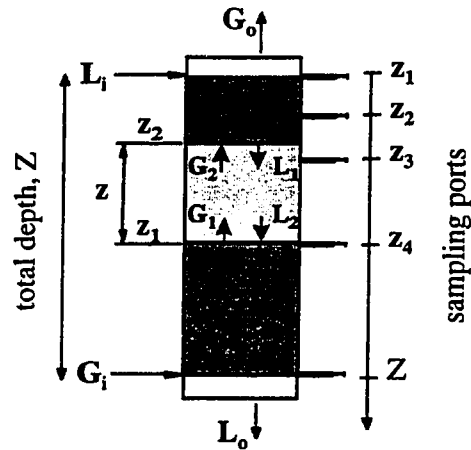


Figure 1. Definition of tower parameters used in the analysis.

Most available mass transfer correlations include an adjustable set of parameters that are functions of packing size and type. Unfortunately, the parameter values for modern packings are lacking, therefore, the corresponding mass transfer correlations cannot be used.

Despite the large number of studies dealing with mass transfer in packed towers, discrepancies, misunderstandings and misapplications of the results are still encountered. For example, the exponents of some parameters in different correlations are identically preset to follow some theory while others are not. The exponent associated with chemical diffusion coefficient in liquid is generally set at 0.5 as shown in Table 1. This is because the different mass transfer theories, from two-film to surface renewal (Toor and Marchello [22]), suggest that the diffusion coefficient exponent should be between 0.5 and 1. However, the exponents of other parameters change from one correlation to another, sometimes in conflicting ways (Table 1). The liquid density exponent changes from -1 to 1, thus attempting to physically relate or interpret these correlations is almost impossible. This may be explained, in part, by the regression methods used in the development of the correlations. Indeed, many parameters are freely changed to improve the fit of the correlation to its particular developmental data set. Each particular data set can be thought of as a sample from the population of all operating conditions. Au-Yeung and Ponter [1] stated that no reliable correlations are available to predict the mass transfer rate coefficient except for specific systems conducted under the same experimental conditions. Bravo et al. [3] has shown that the parameters change from one operating region to another, which means that different packing surfaces and gas flow rates, as operating regions, can lead to different exponent values in the same correlation. This results from the high non-linearity of the

complex mass transfer mechanisms that are not totally understood. It also reveals the limitation of the current regression-based approach to address this problem. In addition, existing correlations, such as the Onda model, were developed in laboratory conditions with concentrations in the percent range using mainly traditional packings of less than 1 inch (2.54 cm) in size. Current VOC air stripping applications, however, involve concentrations in the parts per billion level and use modern packings of large size diameters. These modern packings have higher specific surface areas, lower pressure drops, and they can accommodate higher flow rates. These new operating conditions are obviously different than those used in the correlations' development. Yet, mathematical correlations are still the instrument of choice in the design of stripping towers, because of the high cost of pilot-scale studies. Among all of the existing models, there is agreement in the recent literature that the Onda model [17] is the best mass transfer correlation.

Table 1. Discrepancy between the exponents of important liquid variables in different correlations (from Manger and Ponter, 1980)

Authors	Exponents of			
	L Liquid flow	D Diffusion	ρ Density	μ Viscosity
Higbie (1935)	<u>+0.33</u>	<u>+0.50</u>	-0.16	-0.16
Sherwood & Hollaway (1940)	+0.54	+0.50	-0.50	-0.04
Knoeder and Bonilla (1954)	+0.77	+0.53	-0.33	<u>+0.53</u>
Van Krevelen and Hoftijzer (1947)	+0.66	<u>+0.66</u>	-0.40	+0.33
Van Krevelen and Hoftijzer (1948)	+0.80	+0.60	-0.50	-0.40
Shulman et al. (1955)	+0.45	+0.50	-0.17	+0.05
Davidson (1959)	+0.33	+0.50	-0.17	-0.16
Hikita (1960)	+0.45	+0.50	+0.16	-0.16
Onda et al. (1968)	+0.66	+0.50	+0.27	-0.82
Mohunta (1969)	+0.75	+0.50	-0.50	-0.80
Stephens and Morris (1951)	+0.70	+0.50	-0.50	-0.20
Taylor and Roberts (1956)	+0.40	+0.50	-0.50	+0.10
Taylor and Roberts (1956)	<u>+1.00</u>	+0.50	-0.50	+0.50
Normann and Sammak (1963)	+0.60	+0.50	-0.17	-0.44
Mika (1967)	+0.83	+0.50	<u>-0.99</u>	<u>-0.99</u>
Mika (1967)	+0.50	+0.50	-0.76	-0.43
Copp and Ponter (1972)	+1.00	+0.50	<u>+1.00</u>	-0.54

EVALUATION OF THE ONDA CORRELATIONS

The Onda model

The Onda correlation consists of three separate equations. They provide for independent calculation of the individual liquid and gas phase mass transfer coefficients, k_L and k_G , as well as the wetted specific interfacial surface area for mass transfer, a_w . These equations are:

$$k_L = .0051 (L_f / a_w \mu_L)^{2/3} (\mu_L / \rho_L D_L)^{-1/2} (a_t d_p)^{0.4} (\rho_L / \mu_L g)^{-1/3} \quad (6)$$

$$k_G = c a_t D_G (G_f / a_w \mu_G)^{0.7} (\mu_G / \rho_G D_G)^{1/3} (a_t d_p)^{-2} \quad (7)$$

$$a_w = a_t \left\{ 1 - \exp \left[-1.45 (\sigma_c / \sigma_L)^{0.75} (\text{Re}_L)^{0.1} (\text{Fr}_L)^{-0.05} (\text{We}_L)^{0.2} \right] \right\} \quad (8)$$

in which k_L = chemical-specific liquid phase mass transfer coefficients (L/T); k_G = chemical-specific gas phase mass transfer coefficients (L/T); a_w = wetted specific surface area of the packing (L^2/L^3); a_t = total specific surface area of packing (L^2/L^3); L_f = liquid mass flux (M/L^2T); G_f = gas mass flux (M/L^2T); ρ_L = density of the liquid (M/L^3); ρ_G = density of the gas (M/L^3); D_L = liquid diffusion coefficient (L^2/T); D_G = gas diffusion coefficient (L^2/T); d_p = nominal packing diameter (L); g = gravitational constant (L/T^2); c = constant = 2 if $d_p < 15$ mm otherwise $c = 5.23$; σ_c = surface tension of packing material (M/L^2); σ_L = surface tension of liquid (M/L^2); $\text{Re}_L = L_f / a_t \mu_L$ = liquid phase Reynolds number (dimensionless); $\text{Fr}_L = L_f^2 a_t / \rho_L^2 g$ = liquid phase Froude number (dimensionless); $\text{We}_L = L_f^2 / a_t \rho_L \sigma_L$ = liquid phase Weber number (dimensionless); μ_L = liquid viscosity (M/LT); and, μ_G = gas viscosity (M/LT).

The two phase resistance theory postulates that the total resistance to interfacial mass transfer is equal to the sum of the individual liquid phase and gas phase resistances, therefore:

$$\frac{1}{K_L a} = \frac{1}{k_L a} + \frac{1}{H k_G a} \quad (9)$$

where H is the Henry's constant expressed as the ratio of the mass concentration in the gas phase to that of the liquid phase. The original Onda work was based on 400 data points from engineered stripping systems. It consists mostly of data from laboratory experiments and it uses traditional packings of less than 1-inch (2.54 cm) in size. Onda and his coworkers claimed that their model gives results within $\pm 20\%$.

Application of the Onda model is limited to the ranges of the operating conditions within which it has been either developed or verified. It cannot be used reliably outside these ranges. According to Au-Yeung and Ponter [1], the Onda model does not express the correct fundamental dependency of the local liquid phase mass transfer coefficient, k_L , on system

properties and operating conditions. In addition, Roberts et al. [19] recommended not to use this model for stripping factors (R) below 1.0 because it produces unpredictable results. Fortunately, air stripping columns are usually operated at R values larger than 2.

Until now, the Onda model has been mainly assessed using smaller packings under laboratory scale operating conditions (Roberts et al., [19] and Lamarche and Droste [11] among others). The only comparable large scale data sets that the authors are aware of, at least those which include 2 inch (5.08 cm) packings, are the Lenzo et al. [12], Cummins [5], Cline et al. [4] and Gossett et al. [6] data bases. Table 2 presents a summary of these studies, Gossett et al.'s and Cline et al.'s studies are included in Staudinger's evaluation [20]. In previous studies [12, 5, 20] test samples were collected from the influent line rather than at the top of the packed bed. Thus, they included end effects and they resulted in higher experimental K_{La} values. Cummins adjusted the top of packing concentrations and the Henry's law constant to obtain a minimum deviation from the Onda predictions. Also, a delay of up to four weeks in conducting the VOC analysis renders Cummins' results questionable. Many researchers, therefore, have expressed the need for new evaluations using modern large diameter packings under full-scale operating conditions. The data base described in the following section is developed for this purpose.

Table 2 Results of previous investigations on Onda correlation.

Author	# data points	ASD*	Remarks on analysis	Remarks on data
Onda et al. [17]	400	20%	Chemical Eng. systems, small d	Laboratory data, $d^{**} \leq 1"$
Cummins [5]	126	8%	Henry's constant manipulated to better fit the data, large d	Pilot scale, $d \leq 3"$
Bolles and Fair [2]	545	62%	small and large d	Pilot and laboratory, $d \leq 2"$
Lenzo et al. [12]	569	29%	large d	Pilot and full-scale data, $d \leq 2"$
Staudinger et al. [21]	449	17%	small and large d	Pilot scale, mainly $d = 1"$

* Results corresponds to a 68% confidence level of the difference between the model predictions and the experimental data (one standard deviation).

**Diameter of packing used in data base.

Description of the data base

A new data base has been developed by Narbaitz et al. [16] in a large pilot-scale study using several modern large diameter packings and numerous full scale operating conditions. A schematic representation of the tower is shown in Figure 1. It consists of a 30-inch- (0.76 m) diameter tower, with a total height of 29 ft (8.84 m) and filled with 15 ft (4.57 m) of packing. This tower can treat up to 200 gpm. It has five sampling ports within the packing located at 0, 2, 4, 8 and 14 ft (0.0, 0.61, 1.22, 2.44 and 4.27 m) from the top of the packed zone, respectively. To

break any wall flow, the column is equipped at 4 ft (1.22 m) intervals with aluminum redistributor rings that extend 3 inches (7.62 cm) inwards from the column wall. The characteristics of the packings tested are summarized in Table 3.

Table 3 Characteristics of the packing materials used in the Narbaitz et al. data base.

Packing name	Company	diameter cm(in)	surface area (m ² /m ³)
Cascade Mini-Rings #2	Glitsch Inc.	7.62 (3)	150.86
Flexirings #2	Koch	5.08 (2)	114.78
Flexisaddles #3	Koch	7.62 (3)	88.55
Tripacks #1	Jeager Inc.	5.08 (2)	157.42
Nor-Pac #3	NSW	3.8 (1.5)	144.5
Nor-Pac #4	NSW	5.08 (2)	100.3
Snowflakes	Glitsch Inc.	9.4 (3.7)	91.83

Table 4 Characteristics of the chemical compounds in the data base.

Group	Compound Name	Formula	Diffusion (m ² /s)		H (20 °C)
			Gas E-10	Water E-6	m ³ liq./m ³ gas
GI	Chloroform	CHCl ₃	9.23	9.18	0.117
	1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	8.13	8.28	0.561
	Carbon Tetrachloride	CCl ₄	8.18	8.22	0.986
	Trichloroethylene	C ₂ HCl ₃	8.45	8.46	0.302
	Tetrachloroethylene	C ₂ Cl ₄	7.61	7.59	0.557
GII	Chloroform	CHCl ₃	9.23	9.18	0.117
	Bromodichloromethane	CHCl ₂ Br	9.09	8.72	0.095
	Chlorodibromomethane	CHBr ₂ Cl	8.96	8.37	0.036
	Bromoform	CHBr ₃	8.83	8.08	0.028
GIII	Toluene	C ₆ H ₇ N	7.98	8.31	0.190
	Chlorobenzene	C ₆ H ₅ Cl	7.48	7.7	0.160
	M-Xylene	C ₃ H ₃	7.21	7.52	0.450
	M-Dichlorobenzene	C ₆ H ₄ Cl ₂	7.29	7.24	0.150

The VOCs were studied in three multicomponent mixtures (Table 4) consisting of approximately 100 µg/l of each VOC. At these low solute concentrations, the Henry's law constant is not affected by the presence of other compounds as reported by Munz and Roberts [15] and Mackay and Shiu [13]. Table 4 also lists the Henry's law constants and the diffusion coefficients of the VOCs considered, as reported by Gossett [7] and Haarhoff and Cleasby [9]. The minimum stripping factor was three, well above the critical value of one. More details about this data base can be found in Narbaitz et al. [16]. The experimental K_{La} values were based on concentrations strictly within the packing media, so they are free of end effects. Thus, the Narbaitz et al. [16]

data base has a particular advantage over previous ones, in that the data are used directly in the analysis without correcting for end effects.

Results of the Onda correlations' evaluation .

The evaluation of the Onda correlations was conducted using basic statistical tools. The absolute average error, AAE, is given by:

$$AAE = \frac{1}{n} \sum_{i=1}^n \frac{|(K_L a)_{exp} - (K_L a)_{pre}|}{(K_L a)_{exp}} \quad (10)$$

and the average algebraic error, AGE, is given by:

$$AGE = \frac{1}{n} \sum_{i=1}^n \frac{(K_L a)_{exp} - (K_L a)_{pre}}{(K_L a)_{exp}} \quad (11)$$

where n = the number of data points; and, $(K_L a)_{exp}$ and $(K_L a)_{pre}$ = the experimental and the predicted mass transfer coefficients, respectively. AAE is a measure of average absolute deviation. AGE measures the overall over- or under-estimation. As suggested by Roberts et al. [19] and Bolles and Fair [2] the standard error of $K_L a$ should be based on its logarithm transform, SEE;

$$SEE = \left\{ \frac{1}{n} \sum_{i=1}^n (\text{Log } (K_L a)_{exp} - \text{Log } (K_L a)_{pre})^2 \right\}^{0.5} \quad (12)$$

Finally, the interval limited by one standard deviation defines the expected 68% confidence level and it is given by:

$$F = 10^{SEE} \quad (13)$$

This air stripping tower has multiple sampling ports (Figure 1), therefore, Equation 2 must be used to calculate the observed mass transfer coefficient. Previous works (Gross and TerMaath [8]) used Equation 3 instead which is only valid for zero inflow gas concentration. With the Narbaitz et al. [16] data a difference of 4 to 5% between the results of equations 2 and 3 is obtained. Figure 2 presents the Narbaitz's experimental $K_L a$ values (based on concentrations at five packing depths) versus the Onda predicted $K_L a$ values. Based on this graph the Onda predictions consistently overestimated experimental $K_L a$ values. Equation 10 gives an average error of 40%. Overall, 90% of the data are overestimated with a 43% AGE. Finally, a factor $F = 1.47$ will account for 68% of the predicted values. As shown in Figure 3, the average error varies from 10% for Flexirings to 56% for Tripacks #1. The percent of the data overestimated ranged

from 45% for Flexirings to 100% for both 2 inch (5.08 cm) Nor-Pac and 3 inch (7.62 cm) Flexissadles. An overestimation of K_{La} is unacceptable because it results in an undersized treatment system.

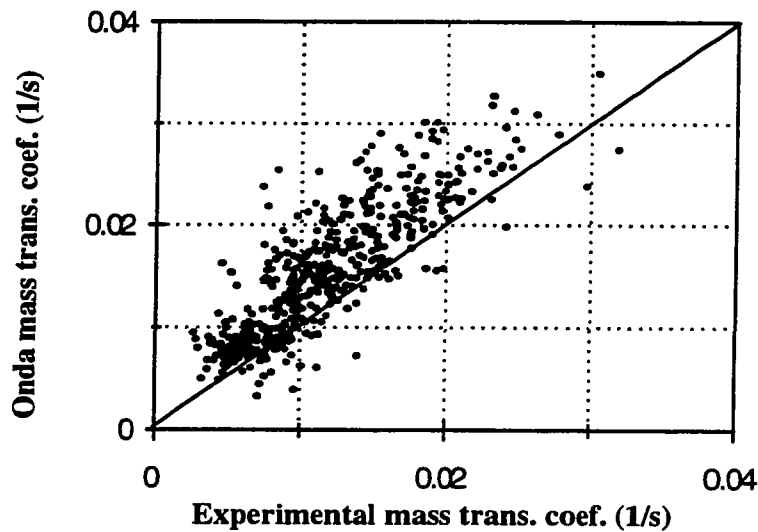


FIGURE 2. Experimental vs. predicted mass transfer coefficient for the Narbaitz et al. data base (538 data point).

Only Gossett's study concluded that the Onda correlation underestimated the performance of the 2 inch (5.08 cm) Pall Rings and Tripacks [20]. All other studies using large size packings, including this one, report overestimation of the transfer rate constant by the Onda correlation.

Lenzo et al. [12] found that for 81 of 85 full-scale systems reviewed, the Onda predictions overestimate the K_{La} with an average error of +35%. The error in the Lenzo study must be even larger because of the experimental K_{La} included end effects. Also, their calculation of the error was based on the deviation relative to the Onda predictions rather than to the experimental values as in Equation 10. The evaluation with lowest apparent error is that by Cummins [5], but it is highly questionable as several other parameters were simultaneously adjusted. Without these adjustments, the Cummins study will result in an average error larger than 60%. To compensate for the inaccuracies of the Onda correlations and to insure that the designs are conservative, engineers have been using safety factors of at least 1.5. The latter is determined from previous experience.

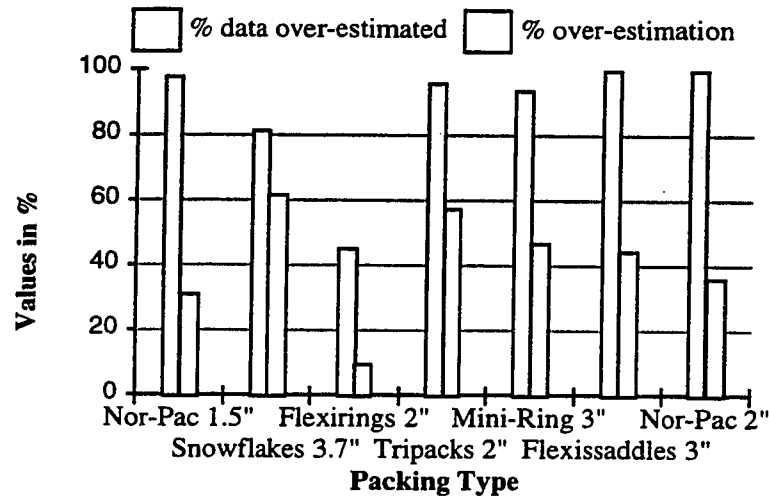


FIGURE 3. Onda simulation results for individual packing.

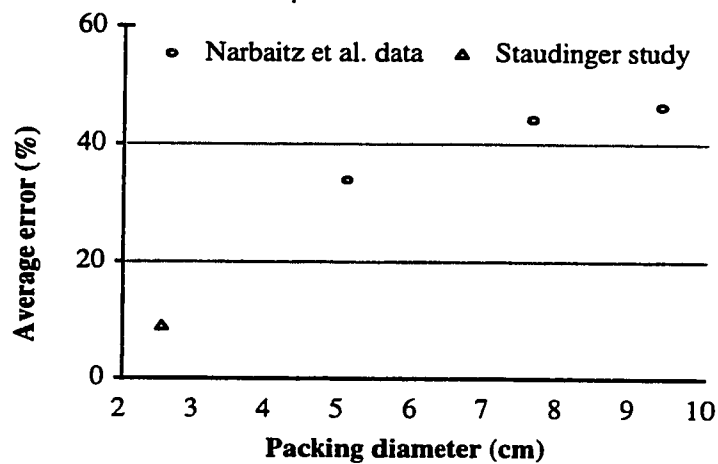


FIGURE 4. Average error of the Onda correlation versus packing diameter.

Figure 4 presents the average algebraic error (AGE, Equation 11) as a function of nominal packing diameter. Each AGE data point represents the result of several packings of the same diameter. The result for one inch (2.54 cm) packing is taken from Staudinger et al. [21] while the rest of the points are from Narbaitz et al. [16] data analysis. This figure confirms the claim that the Onda model tends to overestimate the mass transfer coefficient when the packing diameter increases. This explains, at least in part, the relatively higher error obtained in this study compared to previous ones with smaller packings. In fact this claim is implicitly recognized in

the Onda correlation itself. The coefficient c in Equation 7 for the calculation of the local gas phase mass transfer coefficient changes abruptly from 2 to 5.23 when the nominal packing diameter changes from less than 15 mm to larger than 15 mm. Other than fitting reasons, there is no clear physical explanation for this change. The change in c within Equation 7 is intended to reflect a variation in the character of the transfer process, therefore the latter is anticipated to be gradual rather than discontinuous. Based on the Onda model predictions, the data in Figure 4 were regressed resulting in the following equation:

$$K_L a' = \frac{K_L a}{0.834 + 0.293 \ln(d)} \quad (14)$$

were d = the packing nominal diameter in cm; and $K_L a$ and $K_L a'$ = the Onda and the corrected Onda mass transfer coefficient, respectively. This correction is applicable to packings larger than 1" (2.54 cm) in diameter. The result of applying this correction to Narbaitz's data for a 1.5" (3.8 cm) packing, Cline's data for a 2" (5.08 cm) packing and to Cummins' data for a 2" packing are presented in Table 5. A clear improvement in the predictions is evident.

Table 5. Assessment of the correction (Equation 14) of the Onda predictions.

Author	Packing	Before correction	After correction
Narbaitz et al. (1998)	1.5"	31%	7%
Cummins (1988)	2"	60%	22%
Cline et al. (1985)	2"	15%	-12%

IMPACT OF PACKING DEPTH

Some factors are known to affect the transfer process in packed columns, but, they are either ill-considered or completely ignored by mass transfer correlations. Among these factors are channeling, end effects, and liquid distribution systems. There are no reliable models to describe their impacts.

The mass transfer calculations in packed columns assume a constant mass transfer coefficient throughout the column height. This assumption, however, has been proven to be invalid at least at the entrance of the column up to a certain depth. Perry et al. [18] showed that a natural frequency of distribution will develop in packed beds of sufficient height. This height is referred to as the bed depth required to reach the packing's natural distribution frequency. Beyond this

depth the mass transfer coefficient is supposed to become constant. Most previous studies were conducted in laboratory-scale conditions where the concentration gradient, the change in concentration gradient and the packing depth were small and this may have masked the impacts upon variables that are function of the operational scale.

The Narbaitz et al. [16] experimental packed column is divided into 10 segments as shown in Figure 5. The order of these segments, from 1 to 10, is based on decreasing mean gradient of the logarithm transform of the concentrations. Figure 6, 7 and 8 show three typical patterns of experimental $K_L a$ (Equation 2) variations with respect to depth segments. The Onda predictions and the overall experimental mass transfer coefficients, which are independent of the packing depth, are also shown for comparative purposes. Figure 6 shows the case where the initial liquid distribution coincides with the natural frequency distribution of the packing. In this case, the $K_L a$ decreases gradually immediately below the distribution system as it does further downstream. Figure 7 shows the impact of a liquid distribution system that has a distribution capacity superior to the natural liquid distributing capacity of the packing. This leads to a sharp decrease in experimental $K_L a$ in the upper part of the column. In the type III behavior, the liquid distribution system offers a poorer distribution than the natural packing distribution.

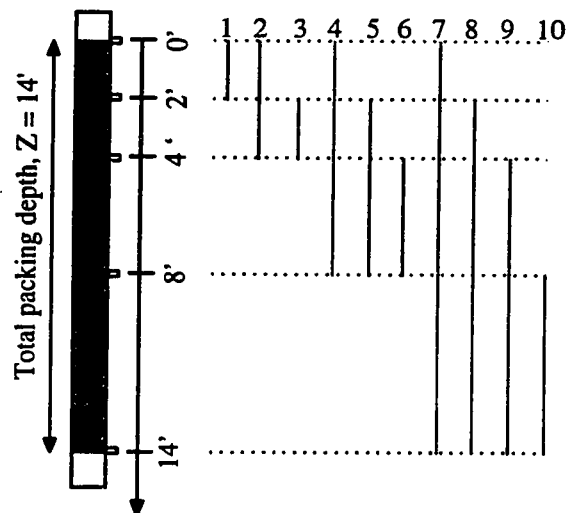


Figure 5. Depth segment with decreasing mean concentration gradient (order from 1 to 10).

However, after the packing's natural distribution frequency is reached, the three types of graphs show a gradual decrease in mass transfer coefficient with increasing segment number, i.e., decreasing mean concentration gradient. However, it is not yet clear if the observed variations (Figure 6, 7 and 8) are related to the depth or to the concentration gradient change or to both. This contradicts the assumption of constant mass transfer coefficient $K_L a$ when varying the packing depth. After the packing natural distribution frequency is reached, the flow pattern should be constant, therefore, the interfacial area should also be constant. Thus, the changes in $K_L a$ with depth must be related to the mass transfer coefficient K_L , rather than to the effective surface area a .

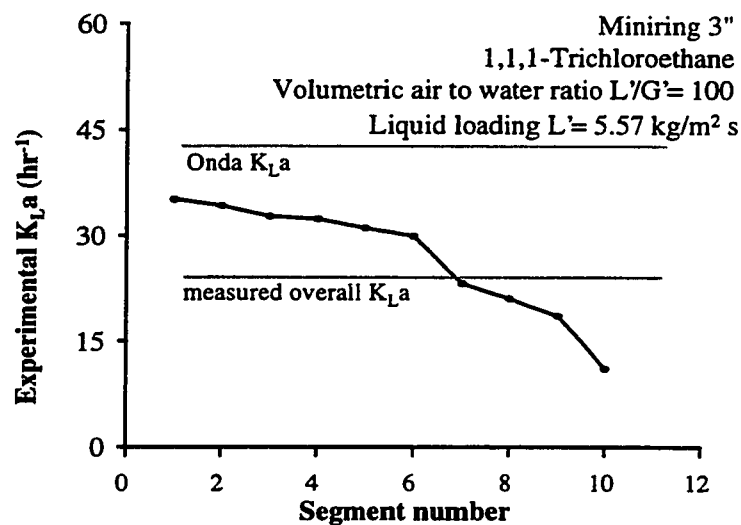


FIGURE 6. $K_L a$ versus segment depth for the case where the initial liquid distribution coincides with the packing's natural distribution frequency (Type I).

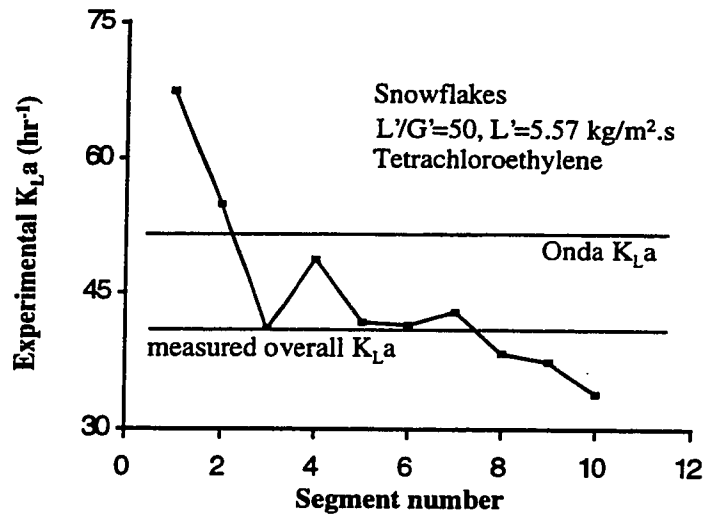


FIGURE 7. $K_{L,a}$ versus segment depth for the case where the initial liquid distribution has a distribution capacity higher than the packing's natural distribution frequency (Type II)

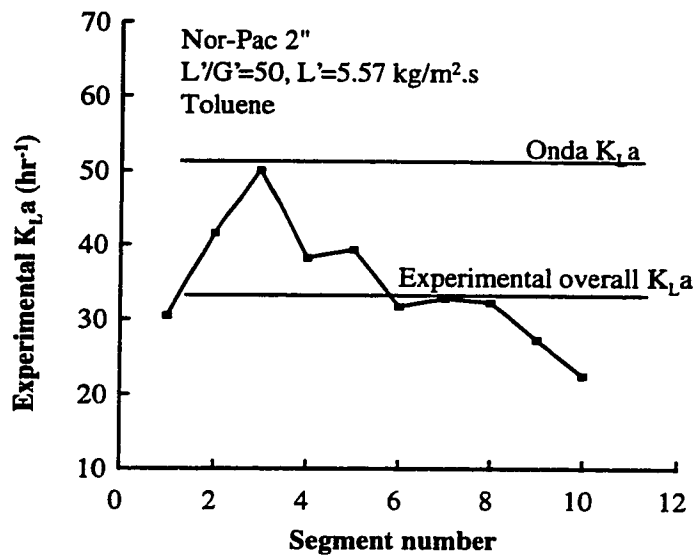


FIGURE 8. $K_{L,a}$ versus segment depth for the case where the initial liquid distribution has a distribution capacity lower than the packing's natural distribution frequency (Type III).

GENERAL VARIABLES ERROR ANALYSIS

Models do not always describe experimental data well because: (a) the data contain experimental errors; (b) the model's assumptions are rarely attained; and (c) extraneous disturbance or noise. Therefore, model predictions can not be exact. There always are extraneous variables, i.e., variables not considered by the model, and in this case they include end effects, channeling, liquid distribution, etc. If the model form is assumed adequate and errors due to extraneous variables are negligible, the observed deviation in the predictions result from two main sources: (i) the measurement error in the variables within the model; and (ii) the values of the model's parameters are imprecise. Not only does the error exist in the variables' estimate, which contradicts a basic assumption in model development, but also it is usually difficult to determine the precision of these variables. However, an assessment of the order of magnitude of each source of error can be made.

The expected error of the Onda model is not well established. Staudinger et al. [21] and Roberts et al. [19] studied the effect of errors in the stripping factor and in the influent and effluent concentration measurements. They found that the error in the experimental $K_L a$ becomes quite significant for stripping factors below 1.5. According to Staudinger et al. [21] the cause of the deviation between the experimental $K_L a$ values and the Onda predictions at stripping factors larger than 1.5 is most likely related to the Onda correlation predictive capacity itself or to other factors, such as column channeling and liquid distribution system, rather than to errors in the values of the variables such as inaccurate measurement of the VOC concentrations and the stripping factor. The ratio of packing diameter to the column diameter (Treybal [23]) and the redistribution system used in the Narbaitz et al. [16] tower are believed to ensure an even liquid distribution throughout the column height and to minimize the channeling. Given the high stripping factors, any deviation between the Onda predictions and the experimental data can be attributed to the Onda model's lack of fit or to the variable measurement errors or to both.

In the following paragraphs the expected deviation due to typical errors in the variables (Table 6) in both the experimental and the predicted $K_L a$ expressions are evaluated. First, a larger data base is constructed. It is composed of Narbaitz et al. [16] and Lamarche and Droste [11] data bases. The latter is added to cover laboratory scale conditions with small variable values. According to Bolles and Fair [2] the error in the experimental $K_L a$ is a function of the magnitude of the variables.

Error estimation

The maximum observed variance in a function $y = f(x_1, \dots, x_n)$ is proportional to the variances associated with the several variables used in its calculation, x_i . If the variables x_i can be assumed independent, then, the off diagonal terms of the covariance matrix are negligible. And the expected variance of y , σ_y , is given by:

$$\sigma_y^2 = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2 \sigma_{x_i}^2 \quad (15)$$

where x_i is the i^{th} independent variable; n is the total number of independent variables; and σ_{x_i} is the variance associated with the independent variable x_i .

Results and Analysis

Equation 15 was applied to the Onda correlation equations 6, 7 and 8 separately using the typical error values given in Table 6. The estimated order of magnitude of the deviations are $\sigma_{k_o}^2 \propto 10^{-9}$, $\sigma_{k_L}^2 \propto 10^{-6}$, $\sigma_w^2 \propto 10^{-4}$ (in m, s and kg units) in the local gas phase, local liquid phase and the surface area, respectively. This implies that the major part of the observed deviations in the Onda model is due to the surface area calculation in Equation 6.

Table 6 Commonly reported errors in air stripping variables.

Variable name	Error %
Henry's constant	20
Liquid diffusivity	10-5.8
Gas diffusivity	7-4.3
Temperature	0.1
Concentration	5.0
Liquid flow	1.0
Gas flow	1.0
Length	1.0
Experimental K_{La}	8-15

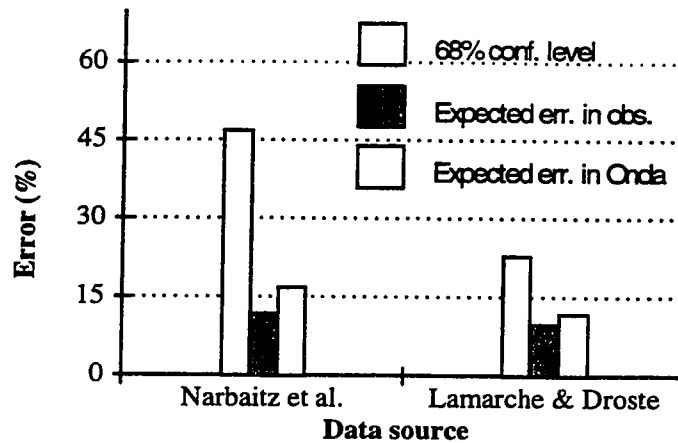


FIGURE 9. Comparison between the expected error in the Onda predictions, the expected error in the experimental K_{La} and the difference between the Onda and the experimental K_{La}

The expected deviations in the Onda correlation predictions and the experimental mass transfer coefficients are calculated by applying Equation 15 to Equations 4 and 9. The results of these calculations are shown in Figure 9 along with the expected 68% confidence level of the difference between the Onda predictions and the experimental K_{La} s (Equation 13). The expected deviation in the experimental K_{La} due to errors in the variables is in good agreement with the reported values in the literature (Table 6). Repeat testing at individual air strippers conducted by Lenzo et al. [12] resulted in 8 to 15% standard deviation in the experimental K_{La} values. These deviations are most likely due to sampling and analytical technique errors or to typical measurement errors of other variables involved in the K_{La} calculations.

As shown in Figure 9, the two data bases produced similar results. Lamarche and Droste data show that observed deviations could be explained by the combination of the errors in variable measurements in both experimental and Onda correlations predictions. This is in line with previous laboratory studies that used small packing diameter. However, in Narbaitz data, the potential deviations which are caused by errors in variables are 12 and 18% in the experimental data and in the Onda correlations predictions, respectively. The latter are much lower than the observed deviation which is 47%. At this confidence level, neither the potential deviations in the experimental data nor in the predicted K_{La} s or the combination of both could explain the total observed deviation in the Onda correlations. Therefore, improvement of mass transfer correlations is still possible. Of course, the large data set needed and the severely limiting

presuppositions of the model form will always be the major difficulties in undertaking such a task.

CONCLUSIONS

- The well accepted Onda correlation was evaluated using a new data base that involves full scale operating conditions and uses large size packing materials. The Onda correlation systematically overestimates the mass transfer coefficient $K_{L,a}$ for larger diameter packings that are typically used in full-scale applications. The average error is found to be 40% and a safety factor of 1.47 would be required to account for 68% of the data.
- A complementary equation which further accounts for the impact of packing diameter yielded predictions within $\pm 20\%$.
- The experimental mass transfer coefficient $K_{L,a}$ is found to decrease with decreasing mean driving force or possibly depth. This phenomenon is not accounted for by present correlations.
- Observed increases and decreases in $K_{L,a}$ in the upper part of the column are related to the adjustment of the wetted packing surface area associated with the shift from the liquid distribution pattern of the distributor to the natural flow distribution pattern of the packing.
- At the 68% confidence level typical errors in the variables accounts for only a part of the total observed deviation in the Onda correlation. Large part of this deviation is attributed to lack of fit of the Onda model. Hence, improving mass transfer correlations is still possible.

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CHAPTER 6

IMPROVED ONDA CORRELATIONS FOR VOC AIR STRIPPING IN PACKED TOWERS

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IMPROVED PARAMETRIC MODEL FOR VOC AIR STRIPPING IN PACKED TOWERSYassine Djebbar¹ and Roberto M. Narbaitz²¹*S&DD, Greater Vancouver Regional District, 4330 Kingsway, Burnaby, BC, Canada, V5H 4G8*²*Dept. of Civil Engineering, Univ. of Ottawa, P.O. Box 450, Stn. A, Ottawa, ON, Canada, K1N 6N5***ABSTRACT**

A comprehensive database for volatile organic compound (VOC) air stripping in packed towers was gathered from 12 field and pilot-scale studies. The main aims of this database are to analyze mass transfer characteristics, and to develop new correlations. The new correlations address several of the shortcomings of the Onda et al. (1968) model that were identified in previous studies. The predictions by the improved correlations were superior to those of the Onda correlations. For the validation database, the average absolute error of the improved correlation's predictions was less than 23% while it was 29% for the Onda model. The improved correlations also estimated well the mass transfer characteristics of structured packings. However, there are a few observed characteristics of mass transfer that are still not described well by the improved correlations such as the effect of high gas flow rates on mass transfer characteristics.

KEYWORDS: Volatile Organic Compounds, Packed Tower, Air Stripping, Onda Correlations, Random Packing, Structured Packing, Mass Transfer Coefficient Correlations.

INTRODUCTION

Air stripping towers are frequently used to remove volatile organic compounds (VOCs) from contaminated ground water. The design of these towers requires an estimate of $K_{L,a}$, the overall liquid-phase-based mass transfer coefficient. Pilot-scale studies are a relatively expensive method of determining $K_{L,a}$. A more common and affordable alternative is to use mass transfer correlations in conjunction with a safety factor to compensate for possible inaccuracies in the correlations. Tens of correlations have been developed in the past fifty years (Au-Yeung and Ponter, 1983). However, only a few have been tested for the removal of VOCs at the $\mu\text{g/L}$ level that is frequently encountered in contaminated ground water applications.

There is agreement in the recent literature that the Onda et al. (1968) model is the best model for air stripping applications (Staudinger et al., 1990; Roberts et al., 1985 and Lamarche and Droste,

1989). The literature shows also that this model yields satisfactory results for lab data, i.e., conditions that are similar to those under which this model has been developed. However, 30 to 40 percent deviations from predictions are often reported in full-scale applications (Lenzo et al., 1990, Staudinger et al., 1990 and Djebbar and Narbaitz, 1995). Several attempts have been made to improve the Onda model, but they have had limited success. Among these are the works of Gossett et al. (1985) and Djebbar and Narbaitz (1995). Other researchers have proposed completely new correlations that are packing dependent (Costa et al., 1992; and Little and Mariñas; 1997). These new correlations can only be used for a limited number of packings, hence they are not general. Because of its generality, correlations like the Onda's are more useful and still draw much interest.

The lack of good predictive ability of existing models is attributed to four main factors: (a) the quality of developmental and verification data, principally those related to operational problems, experimental errors and data manipulation which impact the values of the experimental $K_{L,a}$ s; (b) the data with which these correlations have been developed only cover a limited set of operating conditions, thus, many predictions are extrapolative in nature; (c) the limitations of parametric regression techniques used to develop these models; and (d) the changing nature of mass transfer relationships from one set of operating conditions to another that are not well understood and are poorly mimicked by current parametric models (Djebbar and Narbaitz, 1995; Bravo et al., 1992).

The objective of this paper is to address some of the above concerns by developing an improved parametric-regression-based model using a large and new air stripping database.

ONDA MODEL

The Onda model consists of three separate equations for the calculation of the individual liquid and gas phase mass transfer coefficients, k_L and k_G , as well as the wetted specific interfacial surface area for mass transfer, a_w . These equations are (Onda et al., 1968):

$$k_L = 0.0051(L_f / a_w \mu_L)^{2/3} (\mu_L / \rho_L D_L)^{-1/2} (a_t d_p)^{0.4} (\rho_L / \mu_L g)^{-1/3} \quad (1)$$

$$k_G = ca_t D_G (G_f / a_w \mu_G)^{0.7} (\mu_G / \rho_G D_G)^{1/3} (a_t d_p)^{-2} \quad (2)$$

$$a_w = a_t \left\{ 1 - \exp \left[-1.45 (Mc)^{0.75} (Re_L)^{0.1} (Fr_L)^{-0.05} (We_L)^{0.2} \right] \right\} \quad (3)$$

in which k_L = chemical-specific liquid phase mass transfer coefficient (L/T); k_G = chemical-specific gas phase mass transfer coefficient (L/T); a_w = wetted specific surface area of the packing (L^2/L^3); a_t = total specific surface area of packing (L^2/L^3); L_f = liquid mass flux (M/L^2T); G_f = gas mass flux (M/L^2T); ρ_L = density of the liquid (M/L^3); ρ_G = density of the gas (M/L^3); D_L = diffusion coefficient of the contaminant within the liquid phase (L^2/T); D_G = diffusion coefficient of the contaminant within the gas phase (L^2/T); d_p = nominal packing diameter (L); g = gravitational constant (L/T^2); c = constant = 2 if $d_p < 15$ mm, otherwise $c = 5.23$; $Mc = \sigma_c/\sigma_L$; σ_c = surface tension of packing material (M/T^2); σ_L = surface tension of liquid (M/T^2); $Re_L = L_f/a_t\mu_L$ = liquid phase Reynolds number (dimensionless); $Fr_L = L_f^2 a_t/\rho_L^2 g$ = liquid phase Froude number (dimensionless); $We_L = L_f^2/a_t\rho_L\sigma_L$ = liquid phase Weber number (dimensionless); μ_L = liquid viscosity (M/LT); and, μ_G = gas viscosity (M/LT). M, L, and T refer to mass, length, and time units, respectively. Notice that equation 1 is dimensionally inconsistent.

The two-phase resistance theory postulates that the total resistance to interfacial mass transfer is equal to the sum of the individual liquid phase and gas phase resistances, therefore:

$$\frac{1}{K_L a} = \frac{1}{k_L a} + \frac{1}{H k_G a} \quad (4)$$

where H = the Henry's Law constant expressed as the ratio of the mass concentration in the gas phase to that of the liquid phase, and a = the interfacial area, which is assumed to be equal to the wetted area, a_w , of the Onda model. The original work by Onda and his coworkers was based on 400 data points from engineered stripping and absorption systems. It consisted of data from laboratory experiments and it used traditional packings of small sizes. Only 2 out of 25 packing materials available to the Onda et al. (1968) had diameters greater than 25 mm. The development of the Onda model went through two stages. First, Onda et al. (1967) proposed equation (3) to estimate a_w . Then, based on this equation, Onda et al. (1968) developed correlation equations (1) and (2) to estimate the liquid and gas film coefficients k_L and k_G , respectively. Onda and his co-workers (1968) claimed that their model gives results within a $\pm 20\%$ range. In Roberts et al. (1985) and Lamarche and Droste (1989) studies, the Onda correlations yielded an average standard deviation in the $\pm 20\%$ range for packings with diameters smaller than 15 mm and made mainly of ceramic material. Both studies contain data for operating conditions that are typical of laboratory-scale stripping columns similar to those used to develop the Onda correlations.

RECENT EVALUATIONS OF THE ONDA MODEL

Most current air stripping applications use modern types of packings made of propylene or other plastics. These modern packings have different shapes, higher specific surface areas, lower pressure drops, and can accommodate higher flow rates. Recent studies found that the Onda correlations systematically overestimate K_La for packings with large diameters that are typically used in current full-scale applications (Staudinger et al., 1990; Lenzo et al., 1990; and Djebbar and Narbaitz, 1995). Staudinger et al. (1990) reported that the deviation in the Onda estimates at the 90% confidence interval was in the order of 30%, while Lenzo et al. (1990) reported a value of 35%. The error reported in the Lenzo et al. (1990) study should be even larger for two reasons: (i) their calculation of the error was based on the deviation relative to the Onda predictions rather than relative to the experimental values, and (ii) the experimental K_La values included the removal achieved above and below the packing, i.e., end effects. Djebbar and Narbaitz (1995) found that the average error in the Onda predictions was 40%, and that the Onda model overestimated K_La . Also, they found that the degree of the overestimation increases with increasing packing diameter. Only Gossett et al. (1985) and Dvorak et al. (1996) have claimed that the Onda correlations underestimate the experimental mass transfer coefficients for a few packings. However this may be due to the way the end effects were handled in both studies.

Two main attempts have been made to improve the predictions of the Onda model for air stripping applications (Gossett et al., 1985 and Djebbar and Narbaitz, 1995). Roberts and his co-workers concluded that the gas phase resistance was underestimated by the Onda gas phase resistance correlation. In an effort to build on this hypothesis, Gossett et al. (1985) sought to link transfer rate predictions to the relative contribution of the gas-phase resistance using the Onda correlations. The computed adjustment values of k_G improved the fit of the Onda model for the Gossett et al. (1985) data. However, these modifications did not improve the predictions in the Staudinger et al. (1990) database. This points to the data-fitting-based character of the Gossett improvement, which Staudinger (1986) characterized as non-fundamental. In fact, Gossett et al. (1985) indicated that the modifications should also involve the a_w and k_L correlations. Also, they indicated that modifications more radical than simple change of the front-constants in the Onda expressions were needed, because when the values of the variables changed the error of the Onda predictions changed in a nonlinear fashion. These findings were echoed by those of Djebbar and Narbaitz (1995), who found that the Onda model overestimates K_La for larger packing diameters,

and that this overestimation increased non-linearly with the packing diameter. Subsequently, Djebbar and Narbaitz (1995) proposed a diameter dependent equation to correct for the Onda predictions. Although this modification was nonlinear, it did not improve the predictions for all the data gathered by Staudinger (1986). The Djebbar and Narbaitz (1995) and the Gossett et al. (1985) attempts to improve the Onda correlations failed to be general because they did not address the fundamental problems of the Onda model. The following paragraphs discuss some of these main problems.

Figure 1 shows the average error in the Onda predictions resulting from different experimental studies. There is a large variation in the error of the Onda estimates from one study to another. There are four plausible causes for these errors; namely, (i) column operational problems, (ii) the extrapolative nature of some predictions and experimental errors, (iii) data analysis problems, and (iv) the Onda model's functionality deficiencies. It is crucial to differentiate between these errors, because failing to do so will lead to incorrect conclusions.

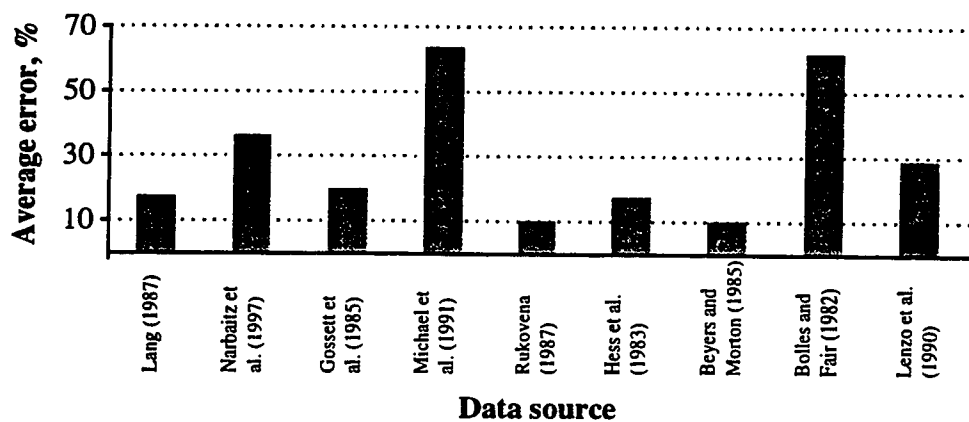


Figure 1. Average error of the Onda predictions for data from various sources.

The first source of errors are column operational problems. These are important aspects which are frequently overlooked in the majority of published data; they include channeling, wall flow, and liquid maldistribution. Also, as many random packing materials are not symmetrical, filling the stripping tower via different procedures or even on two different occasions may result in different mass transfer coefficients (Hoek et al., 1986). There is no estimate of the relative contribution of operational problems to the total observed deviation. This aspect is further

complicated by two factors. First, it is difficult to estimate this type of error. Second, detailed information on the experiments that enable estimation of this type of error is usually lacking. Operational problems produce systematic errors, which make them difficult to estimate by just analyzing data from one specific source. This may explain, at least in part, the systematically higher or lower deviation of results from one study compared to another (Figure 1). Fortunately, in preparing data to develop a new model or to verify an existing one, authors tend to control well their experiments, and thus, keep these errors to a minimum.

The second plausible source of the discrepancies are experimental errors and the extrapolative nature of some predictions. Experimental errors include representative sample collection, appropriate sample storage, and chemical analysis. Most models have been developed for laboratory scale data using small ceramic packings, while modern applications of air stripping towers use new and large packings which are made of plastic materials. Therefore most current predictions are extrapolative in nature.

The third cause of observed deviation would be mishandling and/or misanalysis of the data. For example, the equation used to estimate the observed mass transfer coefficient in the Gossett et al. (1985) was incorrect because it does not handle air concentrations that are different than zero. It produces observed K_{La} values that are 5 to 10% higher than "real" values as calculated by the equation developed by Djebbar and Narbaitz (1995). This partly explains the higher experimental K_{La} values reported by Gossett et al. (1985). Another frequently mishandled problem is end effects. End effects may constitute more than 30% of the observed transfer (Spedding, 1988). Also, existing methods for estimating end effects are fundamentally questionable (Djebbar and Narbaitz, 1995; Lamarche and Droste, 1989).

The three preceding sources of errors will always exist to a certain extent. Their relative effect on measured mass transfer coefficient can amount up to $\pm 50\%$ of the "true" value. These sources of error and their effect on experimental K_{La} can be minimized and confined to a negligible amount only through sound design and careful operation. This was assumed to have been done in the data used in this study.

The fourth possible cause of error comes from the Onda correlations themselves, i.e., the inadequacy of the Onda correlations to describe the transfer characteristics. For example, if a

variable is not correctly characterized in the model, the deviation between observed and model-predicted K_{La} s will be a function of the variable's value. This variable will be constant in data from one study, but it will be different in another data from a different study resulting in different errors. Such errors will make it difficult to compare and to transfer information from one study to the another, because the error will be attributed to the wrong reason. Some of the deficiencies of the Onda model that were identified in previous studies include: (i) the effect of packing depth; (ii) the effect of the liquid distribution system, (iii) the effect of packing diameter, and (iv) the functionality of the correlations (Djebbar and Narbaitz, 1995; Staudinger, 1986; Gossett et al., 1985; Dvorak et al., 1996). These limitations are discussed in the following paragraphs.

In independent studies, Gross and Termaath (1985) and Djebbar and Narbaitz (1995) found that K_{La} is not constant along the depth of the tower as assumed by current models. Gross and Termaath (1985) conducted experiments in which the only variable that changed was the packing depth and found that K_{La} decreases with an increase in the depth of the packing. Similarly, Djebbar and Narbaitz (1995) found that K_{La} decreases with increasing packing depth. Existing correlations do not include the packing depth as one of their variables.

The second limitation of the Onda correlations is their incognizance of the effect on mass transfer characteristics of the quality of the liquid distribution achieved by the liquid distribution system at the top of the column. This quality is often different from that of the packings. Using the same liquid distributor and flow conditions, Djebbar and Narbaitz (1995) found that K_{La} increased or decreased in the upper part of the column depending on the type of packing tested. This behavior is related to the adjustment, in the upper part of the tower, of the wetted packing surface area associated with the shift from the liquid distribution pattern of the distributor to the natural flow distribution pattern of the packing (Harriott, 1989; Perry et al., 1990; Djebbar and Narbaitz, 1995). The depth of the upper part of the tower is mainly dictated by the liquid distributor characteristics. Some attempts to characterize the effect of the liquid distribution have been made, but the results were too complex for any practical purpose (Hoek et al., 1986).

The third potential deficiency of the Onda model relates to its use of the nominal packing diameter, d_p , and specific surface area to characterize the geometry, interfacial area, and therefore mass transfer characteristics of a given packing. Theoretically d_p should be an extremely important variable if used to determine dimensionless numbers. Unfortunately, there

is no clear definition of d_p . Many packings have approximately the same size in all directions such as Tripac™, Norpac™, Hi-Flow Rings™, Flexirings™, and Lanpac™, so there is little ambiguity. However, other packings, such as Snowflakes™, Cascade Minirings™, Tellerettes™, and saddles are quite flat. In the latter case, it is not clear how to define the nominal diameter and often the largest dimension is used.

The fourth point concerns the appropriateness of the functionality of the Onda correlations to model mass transfer characteristics. Bravo et al. (1992) indicated that the Onda model neglected the effect of gas flow rate on the effective surface area. Little and Selleck (1991) found that the Onda model overestimates their experimental gas-phase resistance data by 40 to 50%. Dvorak et al. (1996) experimental data showed that at high gas loading rates, the observed mass transfer coefficient increases sharply, which is not reflected by the Onda correlations (Dvorak et al., 1996). However, they found that the gas phase mass transfer coefficient is overestimated at low gas loading rates, which resulted in underestimation of the overall mass transfer coefficient. The problems associated with the gas phase resistance may be due to the absence of the gas loading rate from the Onda surface area correlation.

Dvorak et al. (1996) indicated that the liquid loading effect is correctly characterized, and concluded that the forms of the Onda correlations are appropriate, but the parameters of the correlations should be changed to reflect modern operating conditions. Roberts et al. (1985), Gossett et al. (1985), and Dvorak et al. (1996) agreed that the source of error appears to be in the wetted surface area and/or in the gas-film resistance equations. To arrive at this conclusion, Dvorak et al. (1996) isolated the transfer components, a_w , k_L , and k_G , and investigated each component separately. Unfortunately, they did so using the Onda correlations themselves rather than an independent approach. When they isolated the gas phase resistance, they used the Onda liquid and surface area correlations assuming that they were correct. While this may be the only practical avenue of analysis, the assumption that the correlation for a_w is accurate is questionable. While claiming the appropriateness of the Onda liquid phase mass transfer equation, Little and Mariñas (1997) who extensively used the Dvorak et al. (1996) study, proposed correlations for the height of liquid and gas-side transfer units that are different from those based on the Onda correlations. They did not provide clear reasons for their choice of a different model form, nor for the form of the proposed model.

In conclusion, there is agreement in the recent literature that there is a need to improve the Onda correlations. However, there is no clear consent on the source of the deficiencies of the Onda model and how to curtail them, but from the preceding, it appears that: (i) although far from being perfect, the best available functional relationships to describe the transfer characteristics are the ones proposed by Onda and his co-workers (Onda et al., 1968); (ii) the depth of the tower should be included in the correlations; (iii) the various potential definitions of packing diameter should be investigated; (iv) the parameters of the three correlations should be modified to reflect current applications of air stripping towers; (v) gas loading should be included in the surface area correlation; and (vi) modifications of the Onda model should be undertaken using data from several sources to reduce the impact of systematic errors. To address these concerns a database that is both comprehensive and representative of real world applications is necessary.

DATABASE

Experimental data in the public domain were surveyed and evaluated against strict criteria. These criteria include the following: (i) full-scale operating conditions, such as packing of large diameters and large tower sizes; (ii) correct handling of end effects; (iii) high level of care in sample collection and analysis, as well as the analysis method itself; and (iv) explicit description of the operating conditions, such as packing type and geometry, tower characteristics, liquid and gas flow rates, operating temperature values, and type and characteristics of the VOC(s) considered. When necessary, supporting information was obtained directly from the researchers who generated the data. This led to the development of the database, which is summarized in Tables 1, 2 and 3. The selected studies were conducted with modern full-scale operating conditions in mind. They include new types of packing media, optimum VOC air stripping factors in the range of 2 to 7, typical liquid loading rates of 2 to 43 kg/m²s, Henry's Law coefficients between 0.02 and 1.4 atm. m³ liquid/m³ air, gas flow rates between 0.06 and 5.7 kg/m²s, with an air to water ratio between 2 and 500 and total packing depth between 1.2 and 5.2 m, liquid phase temperature between 7 and 30 °C, and packing nominal diameters mainly between 2.54 and 9.4 cm. As far as the authors are aware, this database is the most comprehensive gathered to date. The total number of data points is 1450. The effective number of data points used in the analysis is 1252, which is about three times the number used by Onda et al. (1968) to develop their correlations. It was collected from 12 different sources. Table 1 lists the studies used to build the database and the main characteristics of their respective experimental setups. Table 2 contains the packing used in this database with their main

characteristics. Finally, Table 3 contains the VOCs used in this database with their main characteristics. As indicated in Table 2, the database contains air stripping results using two structured packings.

To interpret results adequately, certain physical properties are required, for instance, the liquid density, diffusion coefficient, Henry's Law constant, and critical surface tensions. Great care had to be taken in determining these physical properties because they considerably affect the resulting mass transfer coefficient.

The temperature dependence of Henry's Law constant is estimated using the following equation (Haarhoff and Cleasby, 1990),

$$H_T = H_{20} \left(\frac{293}{T} \right)^A 10^{\left(\frac{1}{293} - \frac{1}{T} \right)} \quad (5)$$

where A = constant; T = temperature in °C; and H_T and H_{20} = Henry's Law constants (atm. m³ liquid/m³ air) at temperature T and 20 °C, respectively. Table 3 shows values of H_{20} and A for different VOCs are presented in.

Henry's Law constant values and the equations to predict them at the experimental temperatures were obtained from experimental studies such as Haarhoff and Cleasby (1990), Gossett (1987), and Lamarche and Droste (1989). The liquid and gas phases diffusion values were determined using the diffusion values at 20°C from Hayduk and Laudie (1974) and Lyman et al. (1990), respectively. These values were then corrected for the liquid temperature (Treybal, 1980). Values of 0.75 and 0.033 N/m were used for the critical surface tensions of water and plastic packing, respectively (Staudinger, 1986).

Observed mass transfer coefficients were estimated using carefully determined concentrations. Concentrations used are those at the top and bottom of the packings or those corrected for end effects. Observed mass transfer coefficients are determined using the generalized equation which accepts influent air with a concentration greater than zero (Djebbar and Narbaitz, 1995):

$$z = \left[\frac{L}{K_L a} \right] * \left[\frac{R}{R-1} \ln \left\{ \frac{c_1 (1-1/R) + c_o / R}{c_2 (1+1/R) + c_o / R} \right\} \right] = [\text{HTU}] * [\text{NTU}] \quad (6)$$

Table 1 Summary of pilot-scale studies selected for the test database.

Study	Number of data points	Tower		Loading rates		Air-to-water ratio
		height (m)	diameter (cm)	Air (kg/m ² s)	Water (kg/m ² s)	
Gossett et al. (1985)	271	2.44	44.5	0.06-1	10-23	10-170
Cummins (1988)	102	5.5	61	0.02-1.3	7.5-7.5	1.5-550
Cummins & Westrick (1983)	96	5.5	61	0.03-1.5	1.6-43.5	5-42
Gross & Termaath (1985)	54	2.4-1.2	19	0.4-0.4	14.5	37.8
Raczko et al. (1985)	16	3.05	30.5	0.3-1.2	11-31	7-103
Hess et al. (1983)	59	3.05	30.5	0.2-0.9	6-43	40-160
Cline et al (1985)	15	3.05	30.5	0.1-0.7	8.6-24	18-85
Umphres et al. (1982)	12	2.34	30.5	0.3-1.3	2.6-11	8
Narbaiz et al. (1998)	698	4.6	76.2	0.15-1.3	5.5-27.5	8.5-42
Lang (1991)	67	2.7-5.2	61, 91.5	0.6-4.5	2-24	2.5-20
Rukovena (1987)	54	3.05-5.2	43, 89	0.2-5.6	4.3-28.5	1-80
Michael et al. (1991)	6	1.22	61	0.3-0.8	6.5	8-27

Table 2 Names and main characteristics of packings in the database.

Packing	Diameter (cm)	Surface area (m ² /m ³)
Random packing		
Rashig Rings	1.3	400
Ceramic Saddles	1.3, 2.5	466, 259
Pall Rings;	1.6, 2.5, and 5	341, 220, 108
Tellerettes	2.5 and 5	180, 125
Norpac	3.8 and 5	145, 100
Hi-Flow Rings	5	97
Flexiring	5	115
Tripac	5	157
Cascade Minirings	5 and 7.6	210, 141
Flexisaddles	7.6	88.6
LANPAC™	8.9	137
Snowflakes	9.4	91.8
Structured packing		
Munters	1.6	420
Flexipac	5	131

Table 3 List of VOCs used in this study and their characteristics (Haarhoff and Cleasby, 1990).

Compound name	Chemical formula	Henry's Law Const. at 20°C (atm. m ³ liquid/m ³ air)	A*
Dichloromethane	CH ₂ Cl ₂	0.0725	3817
Bromoform	CHBr ₃	0.028	4399
Chloroform	CHCl ₃	0.11677	4612
Bromodichloromethane	CHCl ₂ Br	0.095	4375
Dibromochloromethane	CHClBr ₂	0.036	4375
Carbon Tetrachloride	CCl ₄	0.985	4411
Chloroethane	C ₂ H ₅ Cl	0.3968	3120
1,1-Dichloroethane	C ₂ H ₄ Cl ₂	0.182	4128
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	0.059	3620
1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	0.561	4133
1,1,2,2-Tetrachloroethane	C ₂ H ₂ Cl ₄	0.016	4375
Vinyl chloride	C ₂ H ₃ Cl	0.923	3729
cis-1,2-Dichloroethylene	C ₂ H ₂ Cl ₂	0.125	4192
Trichloroethylene	C ₂ HCl ₃	0.302	4780
Tetrachloroethylene	C ₂ Cl ₄	0.557	4918
1,2-Dichloropropane	C ₃ H ₆ Cl ₂	0.096	4375
Benzene	C ₆ H ₆	0.23	3680
Chlorobenzene	C ₆ H ₅ Cl	0.16	4375
m-Dichlorobenzene	C ₆ H ₄ Cl ₂	0.15	4375
Toluene	C ₆ H ₅ CH ₃	0.19	8100
m-Xylene	CH ₃ C ₆ H ₄ CH ₃	0.45	4375
Ethylbenzene	C ₈ H ₁₀	0.27	4375

*Henry's Law temperature constant in Equation 2

where $R = \frac{H G}{P_t L}$ = the stripping factor (dimensionless); HTU = the height of a transfer unit (m);

NTU = the number of transfer units (dimensionless); c_o = VOC's concentration in the effluent liquid at depth Z, the bottom of the packing media in Figure 2 (kg/m³); H = the Henry's Law constant (atm. m³ liquid/m³ air); P_t = the total operating pressure (atm); and L = the liquid volumetric flow rate per unit cross sectional area (m³/m² s); and G = the gas volumetric flow rate per unit cross sectional area (m³/m² s).

DEVELOPMENT OF IMPROVED MASS TRANSFER CORRELATIONS

Narbaitz and Djebbar (1998) enumerated five approaches to develop new correlations. The fifth approach consisted of utilizing a well-accepted model to estimate two of the three transfer components, e.g., a_w and k_L , a_w and k_G , or k_L and k_G . These components are called "part one" components. The remaining transfer component, or "part two", is determined using the experimental mass transfer coefficients and the estimated "part one" components. Then, the "part two" of the transfer is subsequently regressed to produce new correlations, or to improve an

existing one. This process is repeated until satisfactory results are obtained for each of the three transfer components, a_w , k_L , and k_G . The final result is a new correlation for each of the three components.

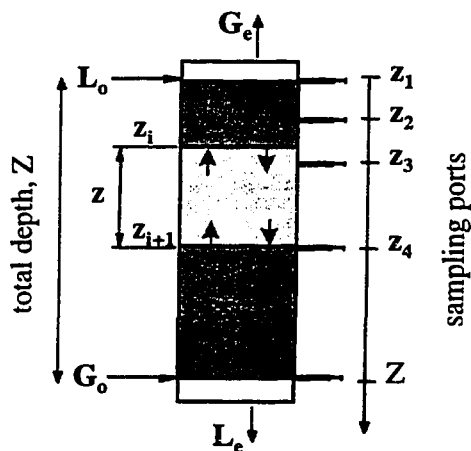


Figure 2. Definition of tower parameters used in the analysis.

This approach was adopted in this study. The nonlinear regression analysis was performed using the statistical software STATGRAPHICS™, which is based on the algorithm of Marquardt (Manugistics, 1993). The Onda model is used to estimate “part one” components for three reasons: (i) it was recognized as the best existing model, (ii) there is no convincing reason that points to a different model form, and (iii) development of new model forms for a_w , k_L , and/or k_G would require data for the individual transfer components that do not exist, are expensive to obtain, and may be difficult to justify given the wealth of different model forms that already exist. Therefore, no attempt was made to search for a different model form and the following modifications were introduced to overcome some of the Onda model shortcomings. First, the liquid phase mass transfer correlation was rendered dimensionless through the use of the liquid-based Sherwood number, $Sh_L = k_L/D_L a_i$. Second, the dimensionless number $Ge = Z/d_p$, i.e., packing height divided by the packing diameter was added to the liquid phase mass transfer coefficient and to the surface area correlations. Finally, the gas phase Reynolds number was added to the surface area correlation.

For the purpose of estimating the model's parameters and to validate the new model, the database is randomly divided into two groups: one part was used to develop a new model, while the second part was used to validate the new model. Structured packing data, which accounts for 157 data points, were used in the validation stage only.

The evaluation of results was conducted using basic statistical tools. The average absolute error, AAE, is given by:

$$AAE = \frac{1}{n} \sum_{i=1}^n \frac{|(K_L a)_{\text{exp}} - (K_L a)_{\text{pre}}|}{(K_L a)_{\text{exp}}} \quad (7)$$

and the average algebraic error, AGE, is given by:

$$AGE = \frac{1}{n} \sum_{i=1}^n \frac{(K_L a)_{\text{exp}} - (K_L a)_{\text{pre}}}{(K_L a)_{\text{exp}}} \quad (8)$$

where n = the number of data points; and, $(K_L a)_{\text{exp}}$ and $(K_L a)_{\text{pre}}$ = the experimental and the predicted mass transfer coefficients, respectively. AAE is a measure of average absolute deviation, while AGE measures the overall over- or under-estimation. Roberts et al. (1985) suggested that the standard error of estimates of $K_L a$ should be based on its logarithm transform, i.e.;

$$SEE = \left\{ \frac{1}{n} \sum_{i=1}^n (\text{Log } (K_L a)_{\text{exp}} - \text{Log } (K_L a)_{\text{pre}})^2 \right\}^{0.5} \quad (9)$$

Using equation 9, the interval limited by one standard deviation defines the expected 68% confidence level and it is given by (Roberts et al., 1985):

$$F = 10^{SEE} \quad (10)$$

Initially, all of the data was regressed to investigate any particular trend or obvious anomalies. Two main conclusions were drawn from this exercise. First, the deviation between Cummins's experimental and Onda predicted $K_L a$ data was particularly high compared to the rest of the data. The average deviation was about 70% in Cummins and Westrick (1983) and Cummins (1988) data, while it was in the 35% range with the rest of the data. Staudinger (1986) indicated that there were serious flaws with the Cummins data. Therefore the Cummins data were excluded from the data in the following analysis.

The second conclusion was drawn from the plot shown in Figure 3, which precludes Cummins and structured packing data. The wetted surface area and the gas mass transfer coefficient were estimated using the corresponding Onda correlations. Then, using experimental $K_L a$, k_L values were estimated, regressed, and the results were presented in Figure 3 as a plot of observed versus regressed liquid Sherwood number, $Sh_L = k_L / (a_s D_L)$. Figure 3 shows two distinct regions with two different trends. The first region corresponds to data with packing diameters that are smaller than 25 mm while the second region corresponds to data with packing diameters that are larger than, or equal to 25 mm. A plot of the results with other variables did not show as strong a trend as the one shown in Figure 3. Consequently, the database was divided into two groups: the first group, with 176 data points, had packings with diameters smaller than 25 mm, and the second group, with 919 data points, had packings with diameters larger than, or equal to 25 mm.

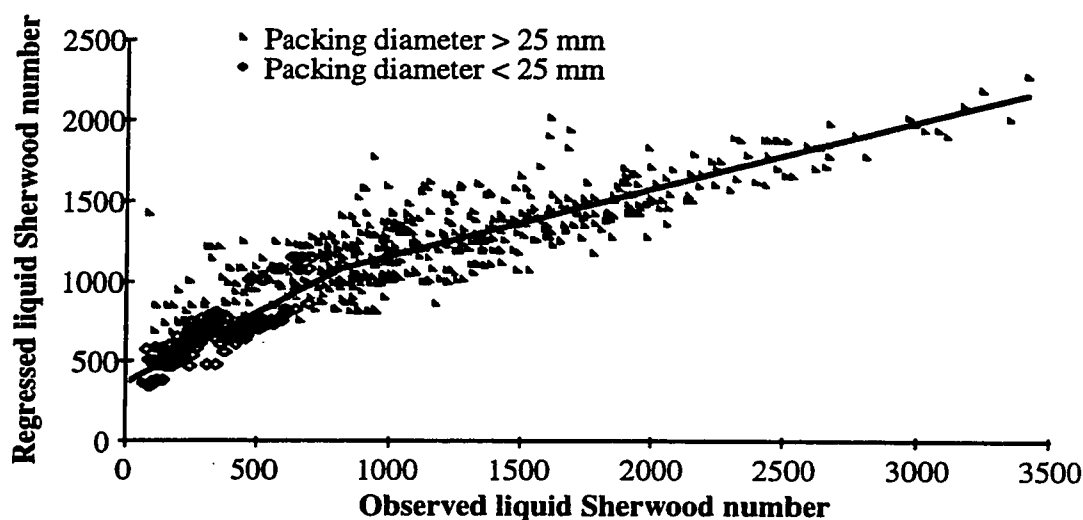


Figure 3. Regressed versus observed liquid phase Sherwood number.

Modern applications of packed towers rarely use packing with small diameter, therefore, the data with small packing diameter may not be of great practical importance. Furthermore, previous studies concluded that the Onda correlations are reasonably accurate for packings with small diameters (Roberts et al., 1985; Lamarche and Droste, 1989). Roberts et al. (1985) found that 68% of the predicted values of their data lie within a factor of 1.21 from the observed values. This result is based on about 70% of the data, as more than 30% of the data were eliminated from the analysis because the stripping factors were smaller than 2. The Roberts et al. (1985) assessment of the Onda correlations agrees closely with that of Onda and his coworkers (Onda et

al., 1968). The Onda correlations were used to estimate mass transfer coefficients for the 176 data points that pertain to packings with a nominal diameter of less than 25 mm. The average absolute error was 26%, the average algebraic error was 18% and the factor that delineates 68% of the data was 1.33. Thus, the Onda model was assumed to be reasonably accurate for packing with diameter smaller than 25 mm (1 inch), and is adopted for air stripping applications that use small packing diameters.

The following series of simulations investigated several potential definitions of packing diameter. Four definitions of the packing diameter were used; namely, (i) nominal packing diameter, (ii) average diameter, $(d_{\max}+d_{\min})/2$, (iii) geometric mean diameter, $(d_{\max}d_{\min})^{0.5}$, and (iv) diameter of the sphere that has the same surface area of the packing. d_{\max} , and d_{\min} are the largest and smallest dimensions of the packing, respectively. The data were regressed using each of the four packing diameter definitions. Obviously, the parameters of the correlations changed depending on the packing diameter definition used. However, no one definition produced particularly better correlations. The error was in the 4% range from one definition to another (Table 4). Therefore, the traditional nominal packing diameter was used in the rest of the analysis to define the packing diameter.

Table 4. Average absolute error for different packing diameter definitions.

Diameter definition	Average Absolute Error, %
nominal packing diameter	29
average diameter, $(d_{\max}+d_{\min})/2$	34
geometric mean diameter, $(d_{\max}d_{\min})^{0.5}$	33
diameter of the sphere that has the same surface area of the packing	31

The data used in the following development does not include packings that are smaller than 25 mm in diameter or Cummins data. This data contain 1078 data points and was divided randomly into development and validation data sets of 500 and 578 data points, respectively. Structured packing data of large diameter was part of the validation data set. The development data were regressed using the Onda model form including the modifications indicated earlier, and the following correlations were obtained,

$$a_w = a_t \left\{ 1 - \exp \left[-0.095 (\text{Re}_L)^{0.41} (\text{Re}_g)^{0.01} (\text{Fr}_L)^{-0.48} (\text{We}_L)^{0.38} (\text{Er})^{0.56} (\text{Mc})^{0.75} \right] \right\} \quad (11)$$

$$\frac{k_L}{a_t D_L} = (0.15 \times 10^{-8}) (L_f / a_w \mu_L)^{0.65} (\text{Sc}_L)^{1.15} (\rho_L / \mu_L g)^{1.8} (\text{Er})^{1.4} (\text{Ge})^{-0.6} \quad (12)$$

$$\frac{k_G}{a_t D_G} = 0.97 (G_f / a_t \mu_G)^{0.6} (\text{Sc}_G)^{1.5} (\text{Er})^{0.43} \quad (13)$$

where $\text{Sc}_L = \mu_L / D_L \rho_L =$ liquid phase Schmidt number (dimensionless); and $\text{Sc}_G = \mu_G / D_G \rho_G =$ gas phase Schmidt number (dimensionless). Equations 11, 12, and 13 represent the improved model.

Figure 4 shows the results of goodness of fit tests for the 500 data points that constitute the developmental data set. The improved correlations produced an average error of 23.5%, with 68% of the data within a band limited by a factor of 1.29 from the best fit line. The developmental data set as a whole is slightly overestimated with an average algebraic error of 13%.

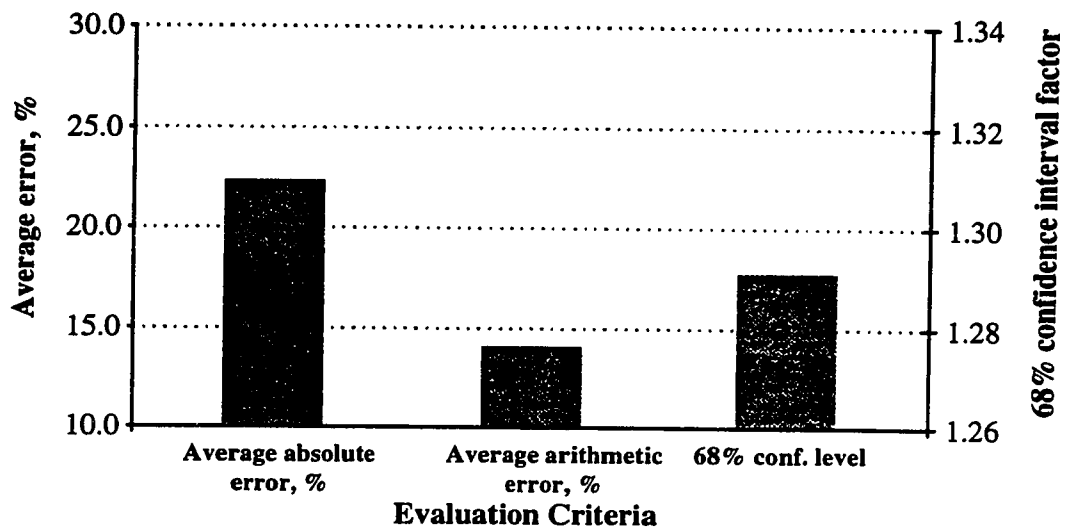


Figure 4. Results of the improved correlations using the developmental data set.

The following paragraphs analyze the results of the Onda model and the improved correlations using the 578 validation data points. Figure 5 presents a comparison between the Onda and the improved models. None of the validation data points was excluded. The results of the improved

model are similar to those of the developmental data set, indicating stability in the results. The average absolute error is 22% for the improved correlations while it is 29% for the Onda model. As expected, the Onda correlations overestimated the mass transfer coefficient, and the average overestimation was 24%. The improved correlations barely overestimated the results (AGE = 0.7%).

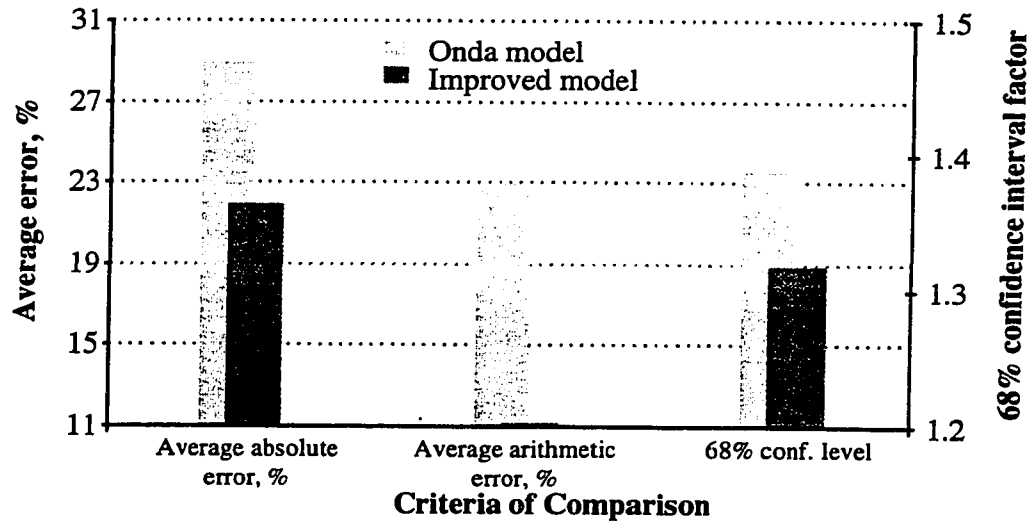


Figure 5. Average errors and F factor for the validation data set.

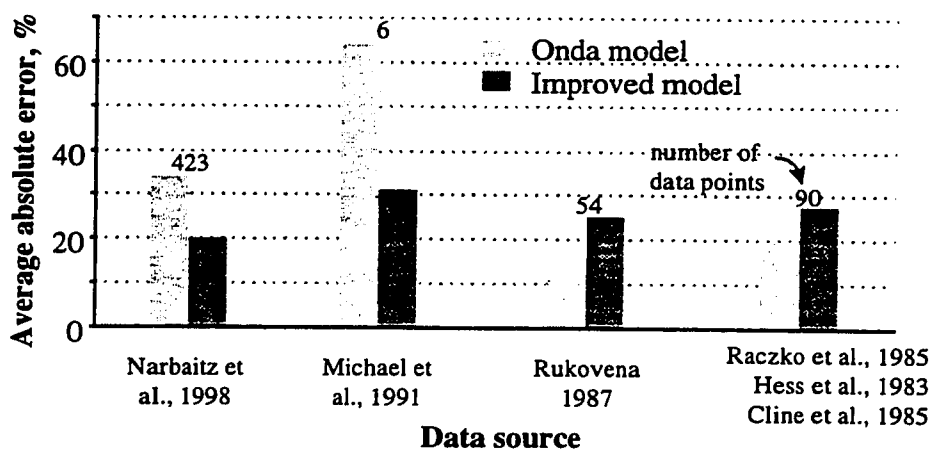


Figure 6. Average absolute error for individual data sources of the validation data set.

Figure 6 compares the Onda and the improved models based on the source of the data. Two factors should be considered in analyzing these results. The first factor is the expected minimum

error. Djebbar and Narbaitz (1995) found that a deviation of 10 to 15% in the Onda estimates can be expected based on anticipated measurement errors in the variables within the correlations. The second factor is the number of data points considered in the analysis. The Onda correlations show high variation in the results from one author to the other, while the improved model shows certain consistency. Being the largest in number, the Narbaitz et al. (1998) data demonstrates a marked improvement of the new correlations over the Onda correlations.

Figure 7 shows the variation of the error as a function of the liquid loading. The Onda correlations show a fairly systematic decrease in the deviation as the liquid loading increases. It has been speculated that this pattern may be attributed to two reasons. The first one is the Onda liquid-phase mass transfer correlation which may not describe well the liquid phase resistance to mass transfer at small liquid loading rates. The second potential reason is related to the surface area formation mechanism. As the liquid loading increases, the resulting surface area more closely follows a trend that is represented by the Onda surface area correlation, resulting in a decrease in the total observed error. The first explanation was proposed by Staudinger et al. (1990), while the second explanation was proposed by Dvorak et al (1996). Even though a similar trend can be observed in the improved correlations results, this trend is not as marked.

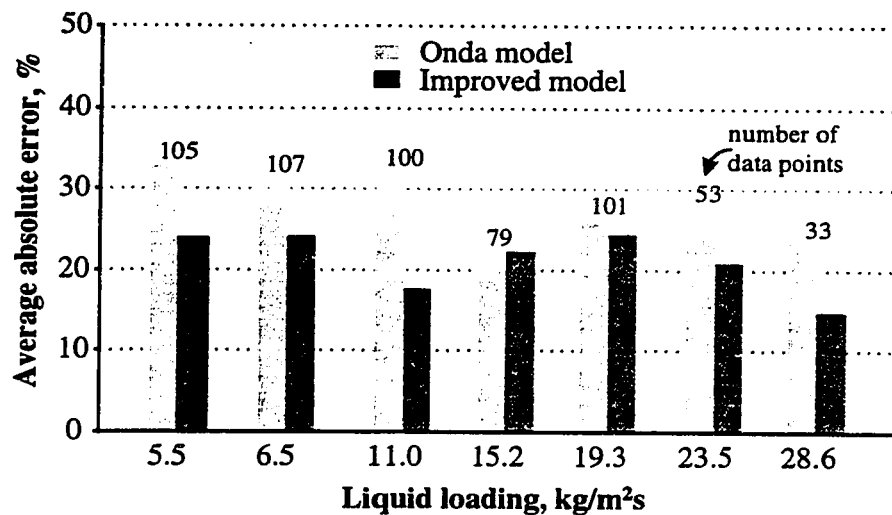


Figure 7. Average absolute error of the Onda and improved model as a function of the liquid loading for the validation data set.

Figure 8 shows the variation of the error with the packing diameter. The Onda model predictions show a general increase in the deviation as the packing diameter increases. This trend is not followed by the 12 points of 88.9 mm diameter data that pertains to a single packing material, Lanpac™. However, this is a small number of data points compared to 50 data points for the next smallest number of data for an individual packing. This trend was explained in previous studies by the inability of the Onda correlations to describe well the process of mass transfer occurring in larger packing diameters (Djebbar and Narbaitz, 1995; Staudinger, 1986; Lenzo et al., 1990). On the other hand, the improved correlations show a U shaped trend in the deviation as a function of the packing diameter. The higher errors are associated with larger and smaller diameters while smaller errors are associated with mid sized packings. In all cases, the error is smaller than 30%. No reasonable explanation was found for the U shaped trend observed in Figure 8.

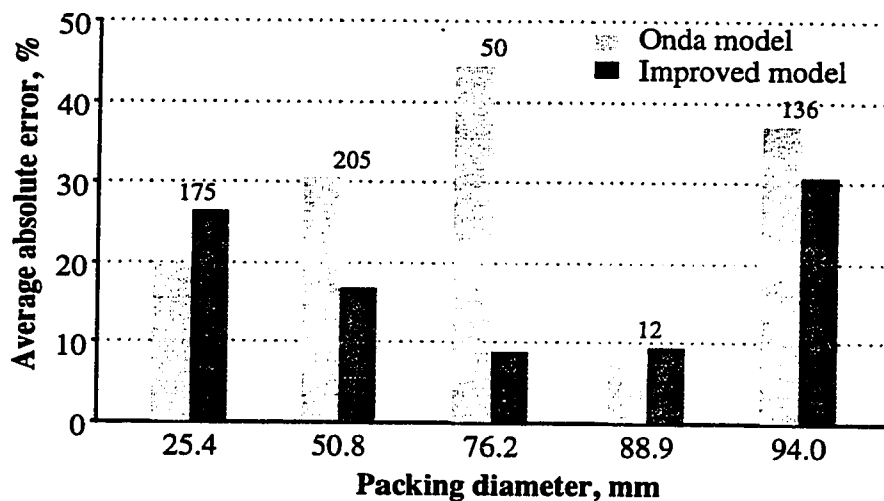


Figure 8. Average absolute error of the Onda and improved model as a function of the packing diameter for the validation data set.

A series of runs using both the Onda and improved models showed that both correlations are not very sensitive to the change in the packing diameter. A variation of 20% in the packing diameter produced 1.4% variation in the improved correlations predictions and 4.5% in the Onda correlations predictions. The problem of variation in the Onda error as shown in Figure 8 may not be related to the packing diameter. Rather, the trend shown in Figure 8 is likely related to the interfacial surface area formation and its relation to the variation of the transfer characteristics

which is accompanied by, but poorly related to the increase in the packing diameter. The above analysis may explain the low sensitivity of the Onda correlations to the different definitions of packing diameter tested previously. This weak relationship between d_p and mass transfer may also explain why the improvement introduced by Djebbar and Narbaitz (1995) did not work as expected for some other databases. Therefore, the packing diameter as considered in both the Onda and the improved models is not as good an indicator of the transfer characteristics, as previously thought.

Figure 9 shows the variation of the error with the packing depth. The Onda correlations are independent of the packing depth and, hence, produce a constant value, while the improved model's predictions vary with the packing depth. The improved correlations tend to overestimate K_{La} at low packing depth. This may be due to residues of end effects in the data which are more important in short columns. Also, It may be due to the effect of liquid distribution system. Djebbar and Narbaitz (1995) found that the liquid distribution system highly affects the transfer characteristics in the upper parts of the tower, and therefore it has a higher impact in short columns.

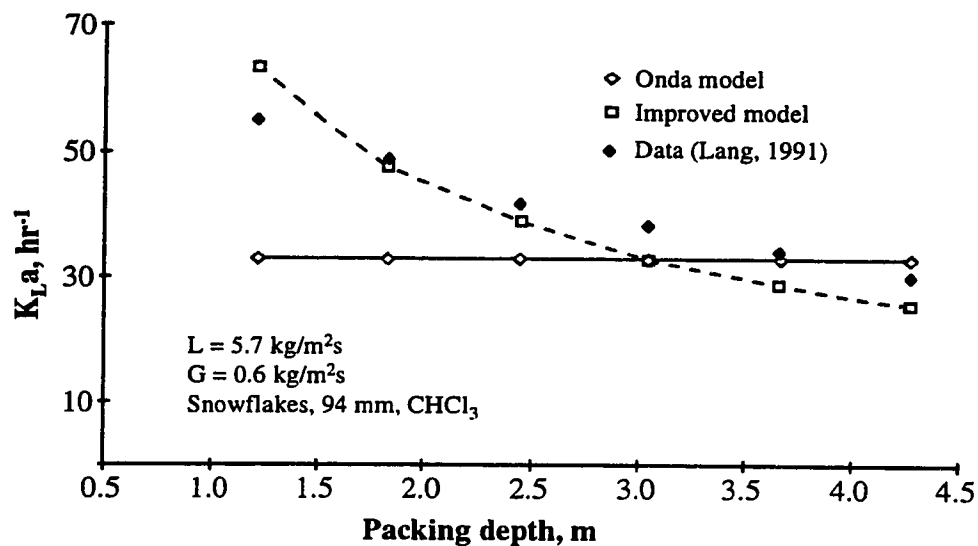


Figure 9. Effect of packing depth on simulated K_{La} .

Figure 10 shows the effect of the liquid loading on the mass transfer coefficient as well as its impact on the Onda and improved models predictions. Both models predict less than linear

increases in $K_L a$ with increasing liquid loading and the predictions can be modeled as a power function of the liquid loading as shown in Figure 10. The rate of $K_L a$ change with the liquid loading is a function of the gas loading and the packing surface area. However, the variation of the rate of change of $K_L a$ with these two variables is relatively small. These results triggered further simulations of $K_L a$ using the Onda and improved correlations for hypothetical operating conditions where only the liquid flow was varied. Then, resulting $K_L a$ values were regressed using the equation form shown in Figure 10. For the predictions by the improved correlations, the values of the regressed exponents changed from 0.65 to 0.69 when the gas loading rate changed from 0.4 to 1.2 $\text{kg}/\text{m}^2\text{s}$, respectively. Higher exponent values are associated with higher gas flow rates. The values of the same exponents for the Onda predictions changed from 0.67 to 0.73. For the conditions shown in Figure 10, the observed values exhibit two distinct regions. These two regions cannot be represented accurately with one regression equation of the form shown in Figure 10. However, the improved model results are closer to observed data than the Onda model predictions.

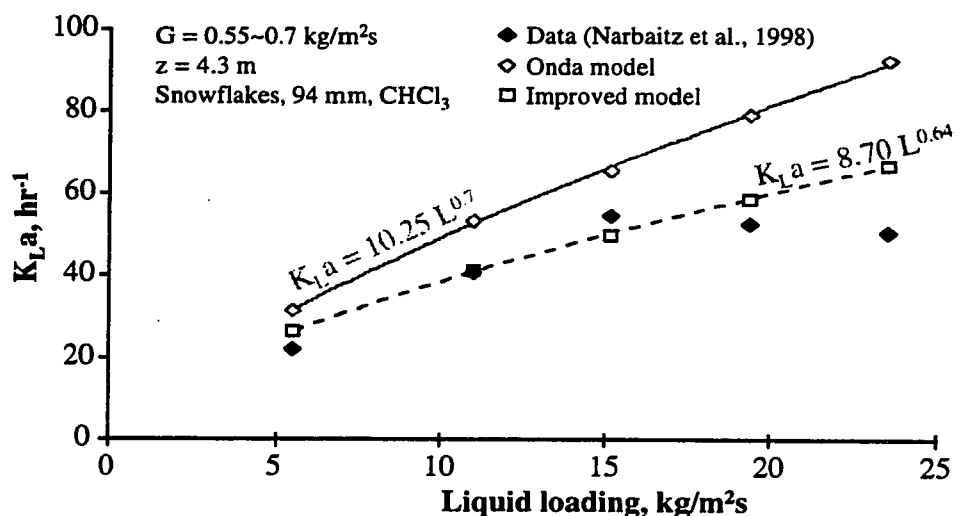


Figure 10. Effect of liquid flow on $K_L a$.

Figure 11 shows the effect of the gas loading on the mass transfer coefficient. In general, the improved correlations predict more accurately the transfer characteristics compared to the Onda correlations. However both models were unable to predict the sharper increases in $K_L a$ at very high gas flowrates. Previous studies showed that the Onda correlations were unable to model the

observed increase in the mass transfer coefficient at high gas flow rates (Staudinger, 1986; Gossett et al, 1985; and Dvorak et al., 1996).

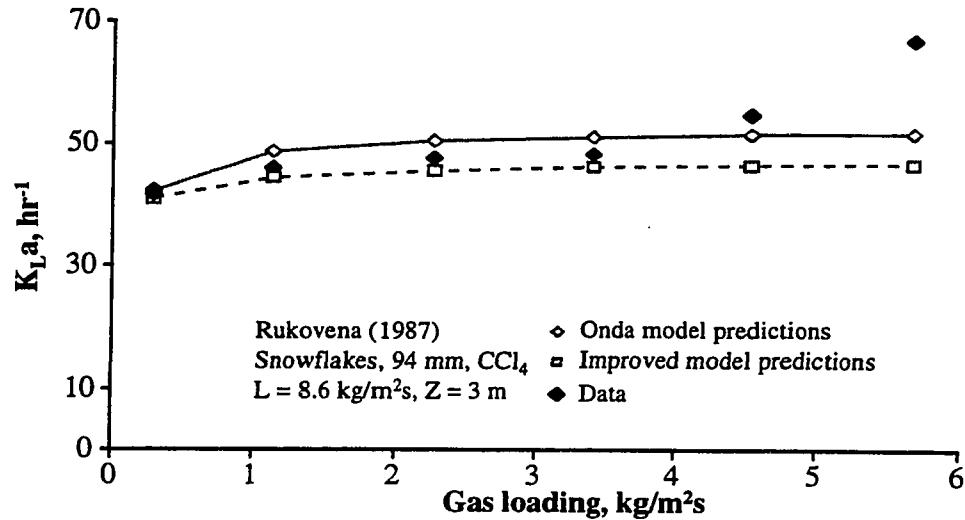


Figure 11. Effect of gas loading rate on simulated $K_L a$.

This lack of sensitivity to gas flow rate at high loading rates has important practical implications. Designs based on these models at very high gas flowrates would be unnecessarily tall. Fortunately, most packed towers are operated at lower gas loading rates in the range of 1 to 3 kg/m²s. This is because increased gas flowrates result in significant increases in pressure drop and blower costs, and these additional costs are much greater than the savings achieved in tower costs via improved mass transfer. Thus, this deficiency in the correlations, which must be considered, is generally avoided through the economic analysis during the design.

Finally, the database gathered for this study contains performance data using two structured packings: Flexipac and Munters. The authors are not aware of any study that looked at performance data of structured packings using traditional correlations. The average absolute error and F factor of the estimated mass transfer coefficients for the two structured packings are shown in Figure 12. The Onda correlations produced results that are within the expected Onda results using random packings. The improved correlations produced an average error of 18.5%, with 68% of the data within a band limited by a factor of 1.29 from the best fit line. These results show that the improved correlations can be used to estimate the performance of structured

packings. However, due to the limited validation data for structured packings in this database, further investigations are required before drawing definitive conclusions.

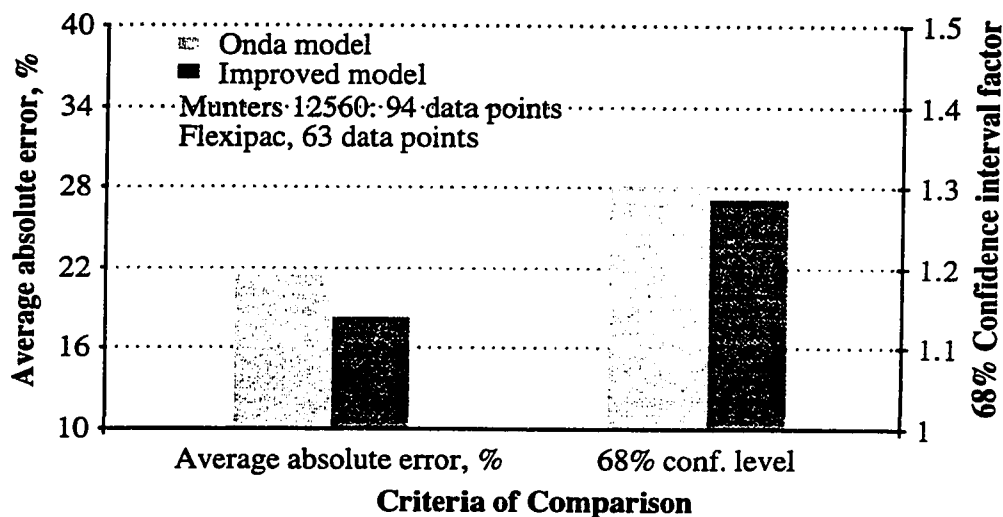


Figure 12. Average absolute error and F factor for structured packings data.

CONCLUSIONS

A database formed from full-scale experiments was assembled from different sources. This database is comprehensive and representative of current applications of VOCs stripping in packed towers. It was used in this study to develop and validate new correlations

The new correlations addressed several shortcomings of the Onda correlations identified in previous studies such as relative insensitivity to packing depth and a tendency to overestimate K_{La} . The average absolute error for the validation, as well as for the development data, was found to be less than 24% with 68% of the data within a factor of 1.3 from the best fit. The same parameters for the Onda model were 29% and 1.39 for the validation data set, respectively. Thus, for the large data set studied, the modified correlations are better than the Onda correlations.

However, some drawbacks of the Onda correlations remain. These may be due to the inherent limitation of parametric regression with large uncertainty regarding the functional form of the correlations. These include the effect of gas loading at high gas flow rates and the effect of

packing diameter. The packing diameter as considered in both the Onda and the improved models is not as good an indicator of the transfer characteristics, as previously thought.

The improved model shows that it can predict mass transfer in structured packings. Because the data on structured packing is limited in this database, further testing is required before drawing final conclusions.

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CHAPTER 7

ARTIFICIAL NEURAL NETWORKS PREDICTION OF $K_L a$ IN AIR STRIPPING TOWERS

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“... Traditional (parametric) statistics deals with methods and problems in estimation on the basic assumption that the underlying statistical probability distribution is one of a family depending on just a few parameters. This is an assumption which is often violated and is, in fact, in my circumstances not a very reasonable assumption. That is where nonparametric and robust methods come in. Here, roughly, nonparametric statistics makes almost no assumption at all beyond, say, as in this book, smoothness of the underlying distribution...”

Michiel Hazewinkel

NEURAL PREDICTIONS OF AIR STRIPPING $K_{L,a}$

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ABSTRACT

Design of air stripping packed towers used to remove volatile organic compounds (VOCs) requires an estimate of the overall mass transfer coefficient ($K_{L,a}$), which is frequently estimated via physically-based parametric correlations. Parametric correlations have some shortcomings and produce predictions with relatively large deviations for full-scale, modern application of air stripping towers. In this study neural network technology, a powerful new nonparametric approach, is used to analyze mass transfer characteristics in air stripping towers and to simulate $K_{L,a}$. A large database that is representative of current applications of air stripping towers was assembled for this analysis. The $K_{L,a}$ predictions by neural networks were superior to both the Onda model and an improved Onda model, the best existing parametric models for air stripping applications. The average absolute error for the validation, as well as for the development data, was found to be less than 19%. The NN model was able to simulate the sudden increase in $K_{L,a}$ at high gas loading rates. Also, it simulated more realistically the effect of the packing depth and liquid flow.

KEYWORDS: Air Stripping, Mass Transfer Coefficients, Neural Networks, Parametric Regression, Nonparametric Regression, Volatile Organic Compounds.

INTRODUCTION

The design of air stripping towers requires an estimate of $K_{L,a}$, the overall liquid-phase-based mass transfer coefficient. Pilot-scale studies are a relatively expensive method of determining $K_{L,a}$. A more common and affordable alternative is to use mass transfer correlations. There is agreement in the recent literature that the Onda et al. (1968) model is the best model for air stripping applications (Staudinger et al., 1990; Roberts et al., 1985 and Lamarche and Droste, 1989). The literature shows also that this model yields satisfactory results for lab data, i.e., conditions that are similar to those under which this model has been developed. However, 30 to 40 percent deviations from predictions are often reported in full-scale applications (Lenzo et al., 1990, Staudinger et al., 1990 and Djebbar and Narbaitz, 1995).

The lack of good predictive ability of existing parametric models is attributed to four main factors: (a) the quality of developmental and verification data, principally those related to operational problems, experimental errors and data manipulation which impact the values of the experimental K_{La} s; (b) the data with which these correlations have been developed only cover a limited set of operating conditions, thus, many predictions are extrapolative in nature; (c) the limitations of parametric regression techniques used to develop these models; and (d) the changing nature of mass transfer relationships from one set of operating conditions to another that are not well understood and are poorly mimicked by current parametric models (Djebbar and Narbaitz, 1995; Bravo et al., 1992).

Djebbar and Narbaitz (1998) proposed an improved correlation using the Onda model form using a large and new database. However, the proposed model still have some shortcomings (Djebbar and Narbaitz, 1998). The Djebbar and Narbaitz (1998) study addressed points (a) and (b). The objective of this paper is also to address points (c) and (d) by using neural networks (NN) technology to analyze and estimate mass transfer coefficient K_{La} .

EXISTING PARAMETRIC ESTIMATION METHODS

Many problems fall short of satisfactory theoretical solutions because of the problem's complexity, the uncertainty in the values of the response and the variables, and our limited knowledge of the processes involved. Most often, the need to deal with these problems in practice requires functional relationships that relate the dependent variables to the independent variables for prediction purposes. The absence of a theoretical relationship, or the real function, is "overcome" by assuming a relationship based on some theory, observations, and sound engineering judgment, making this relationship subjective to a certain extent. The parameters of the relationship are determined using one of several parameter estimation methods, such as the least squares regression, which has certain limitations and requires large sets of accurate data to yield satisfactory results (Bates and Watts, 1988). For the optimal properties of the least square estimates to be valid in the parametric approach, it is essential that the following assumptions hold: (i) the values of the operating variables are exactly known; (ii) the errors and the observed responses at each set of operating conditions have the same variance; (iii) the errors (and the observed values of the responses) are not correlated, thus, are statistically independent; (iv) the

errors are identically and normally distributed with zero mean and variance σ^2 ; and (v) the model form is known (Bates and Watts, 1988). It is obvious that the above assumptions are almost never satisfied. If the first four assumptions are usually partly satisfied, the fifth assumption, however, remains controversial. A key assumption of parametric modeling is that the model form, i.e. a mathematical expression that describes the relationship between the dependent and the independent variables, is known. However, this form is often unknown and always to some extent subjectively assumed (Adamowski and Feluch, 1991). Once regressed, these models can be readily applied using a simple calculator. It is also important to note that the smoothing process in parametric regression considers the entire data set, which makes it vulnerable to outliers (Adamowski, 1989).

An additional disadvantage of current parametric models is that they inherently imply that certain features of the relationship remain the same regardless of the values of the variables (De Neufville, 1990). This is in disagreement with the conclusions of Bravo et al. (1992) and Bolles and Fair (1982) who indicated that the nature of mass transfer correlations, including the parameters of the correlations, should change with the values of the variables.

The mass transfer coefficient in packed towers for air stripping lacks a theoretical solution. Treybal (1980) indicated that the ultimate interpretation or explanation of the transfer coefficient will come only when related fluid mechanics problems are solved. Over the past fifty years, research has produced tens of parametrically regressed correlations to predict $K_L a$. The functional relationship for mass transfer coefficient in packed towers is usually assumed to have the following form (Welty et al., 1976),

$$K_L a = b_0 (X_1)^{b_1} (X_2)^{b_2} \dots = g(X_1, X_2, \dots, b_0, b_1, b_2, \dots) \quad (1)$$

where X_1 and X_2 = dimensionless numbers, such as the Reynolds and the Schmidt numbers, which are functions of the operating variables; and b_0 , b_1 , and b_2 = regression parameters. The parametric approach is the method of choice when the real form of the functional relationship that relates the variables is known, or when the number of independent variables is manageable, say less than five. Unfortunately, this is often not the case.

EXISTING PARAMETRIC ESTIMATION METHODS

Until recently, the Onda et al. (1968) model was considered the best parametric model to predict $K_L a$ (Roberts et al., 1985; Lamarche and Droste, 1989; Staudinger et al, 1990). The Onda model consists of three separate equations for the calculation of the local liquid and gas phase mass transfer coefficients, k_L and k_G , as well as the wetted specific interfacial surface area for mass transfer, a_w . The Onda model is given by the following equations:

$$k_L = 0.0051(\text{Re}_L)^{2/3}(\text{Sc}_L)^{-1/2}(\text{Er})^{-0.4}(\text{Sh}_L)^{-1/3} \quad (2)$$

$$\frac{k_G}{a_i D_G} = c (\text{Re}_G)^{0.7}(\text{Sc}_G)^{1/3}(\text{Er})^2 \quad (3)$$

$$a_w = a_i \left\{ 1 - \exp \left[-1.45(\text{Re}_L)^{0.1}(\text{Fr}_L)^{-0.05}(\text{We}_L)^{0.2}(\text{Mc})^{.75} \right] \right\} \quad (4)$$

in which, k_L = local liquid phase mass transfer coefficient (L/T); k_G = local gas phase mass transfer coefficient (L/T); a_w = wetted specific surface area of the packing (L^2/L^3); a_i = total specific surface area of the packing (L^2/L^3); L_f = liquid mass flux (M/L^2T); G_f = gas mass flux (M/L^2T); ρ_L = density of the liquid (M/L^3); ρ_G = density of the gas (M/L^3); D_L = liquid diffusion coefficient (L^2/T); D_G = gas diffusion coefficient (L^2/T); d_p = nominal packing diameter (L); g = gravitational constant (L/T^2); c = constant = 2 if $d_p < 15$ mm otherwise $c = 5.23$; μ_L = liquid dynamic viscosity (M/LT); μ_G = gas dynamic viscosity (M/LT); σ_c = surface tension of the packing material (M/L^2); and σ_L = surface tension of the liquid (M/L^2), and the following dimensionless numbers: $\text{Sc}_L = \mu_L/\rho_L D_L$ = liquid Schmidt number; $\text{Sc}_G = \mu_G/\rho_G D_G$ = gas Schmidt number; $\text{Mc} = \sigma_c/\sigma_L$ = wettability number; $\text{Re}_L = L_f/a_i \mu_L$ = liquid phase Reynolds number; $\text{Re}_G = G_f/a_i \mu_G$ = gas phase Reynolds number; $\text{Fr}_L = L_f^2 a_i / \rho_L^2 g$ = liquid phase Froude number; $\text{We}_L = L_f^2 / a_i \rho_L \sigma_L$ = liquid phase Weber number; and $\text{Sh}_L = \rho_L / \mu_L g$ = Liquid Sherwood number. M, L and T refer to mass, length and time units, respectively.

The two phase resistance theory postulates that the total resistance to interfacial mass transfer is equal to the sum of the individual liquid phase and gas phase resistances, therefore:

$$\frac{1}{K_L a} = \frac{1}{k_L a} + \frac{1}{H k_G a} \quad (5)$$

where $K_L a$ = the overall (liquid phase based) mass transfer coefficient; H is the Henry's Law constant expressed as the ratio of the VOC mass concentration in the gas phase to that in the liquid phase; and $a = a_w$.

The Onda model overestimates $K_L a$ by an average error of 30 to 40 percent for full-scale operations (Lenzo et al.; 1990, Staudinger et al., 1990; Djebbar and Narbaitz, 1995a; and Djebbar and Narbaitz, 1998). Several researchers attempted to improve the Onda model through simple modifications of the correlations (Gossett et al., 1985 and Djebbar and Narbaitz, 1995a). However, these attempts failed to be general because they did not address the fundamental problems of the Onda model (Djebbar and Narbaitz, 1998).

Building on the work of several researchers (Staudinger et al., 1990; Bravo et al., 1992; Dvorak et al., 1996), Djebbar and Narbaitz (1998) improved the Onda correlations using a newly compiled large database. The latter covers a wide range of operating conditions to avoid extrapolations, and includes data from several sources to minimize the impact of systematic errors. Their work was based on the assumption that the functional relationships of the Onda correlations are correct, but could be improved by the addition of two terms to address some of the deficiencies of the Onda model. The improved Onda model (Djebbar and Narbaitz, 1998) is given by the following equations:

$$\frac{k_L}{a_t D_L} = (0.15 \cdot 10^{-10}) (\text{Re}_L)^{0.65} (\text{Sc}_L)^{1.15} (\text{Sh}_L)^{1.8} (\text{Er})^{1.4} (\text{Ge})^{-0.6} \quad (6)$$

$$\frac{k_G}{a_t D_G} = 0.97 (\text{Re}_G)^{0.6} (\text{Sc}_G)^{1.5} (\text{Er})^{0.43} \quad (7)$$

$$a_w = a_t \left\{ 1 - \exp \left[-0.095 (\text{Re}_L)^{0.41} (\text{Re}_g)^{0.01} (\text{Fr}_L)^{-0.48} (\text{We}_L)^{0.38} (\text{Er})^{0.56} (\text{Mc})^{0.75} \right] \right\} \quad (8)$$

in which, Z = packed depth (L); $\text{Er} = 1/a_t d_p$ = packing efficiency number; $\text{Ge} = Z/d_p$ = geometry number.

The Djebbar and Narbaitz (1998) model is better than the Onda model, but it still has some shortcomings. For example, the improved Onda model was not able to simulate correctly mass transfer at high gas flow rate, liquid flow and packing diameter. Also, the improved Onda model was not able to simulate the observed sharp increase in the mass transfer coefficient, which is caused by the increase in the surface area at high gas flow rates. Figure 1, which confirms the

Bravo et al., (1992) findings, explains why models that are based on the Onda model form cannot predict the sharp increase in $K_L a$ at high gas loading rates. Both the Onda and the improved Onda models assume that the effective surface area value will not exceed the packing dry surface area value. The above indicated shortcomings of existing parametric models compounded with the limitations of the parametric approach triggered the search for an alternative approach using a nonparametric approach based on neural network technology (Djebbar and Narbaitz, 1995a, Narbaitz and Djebbar, 1996).

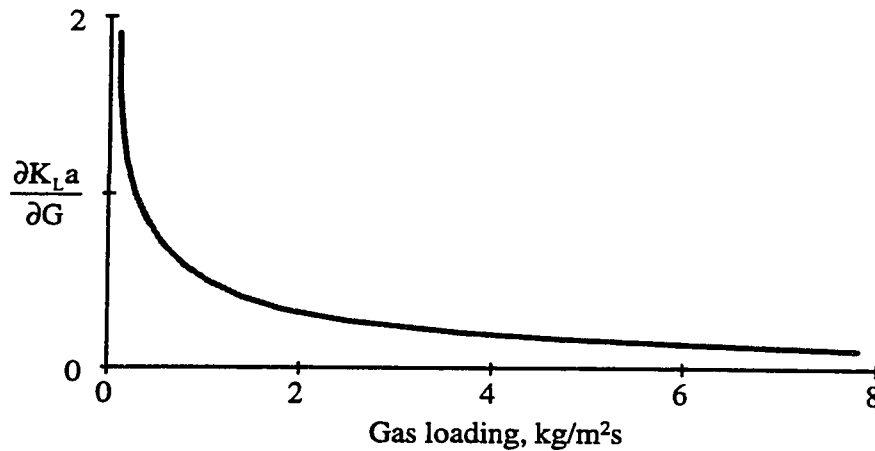


Figure 1. Example of the variation of the slope of Onda predicted $K_L a$ as a function of the gas loading rate.

NONPARAMETRIC APPROACH

In recent years neural networks (NNs) have shown exceptional performance as regression tools, especially when used for pattern recognition and function estimation. They are highly nonlinear, and can capture complex interactions among the input variables in a system without any prior knowledge about the nature of these interactions (Hammerstrom, 1993a; Basheer et al., 1996). The main advantage of NNs is that one does not have to explicitly assume a model form, which is a prerequisite in the parametric approach. Indeed, in NN a relationship of possibly complicated or unorthodox shape is generated by the data points themselves. In comparison to parametric methods, NNs tolerate imprecise or incomplete data, approximate results, and are less vulnerable to outliers (Hammerstrom, 1993a & b; Hayken, 1994; Zaabab et al., 1995). They are highly parallel, i.e., their numerous independent operations can be executed simultaneously. Although application of NN approach in civil engineering is limited and still in its infancy, it

produced very encouraging results (Thirumalaiah and Deo, 1998; French et al., 1992; Hsu et al., 1995; Basheer et al. 1996).

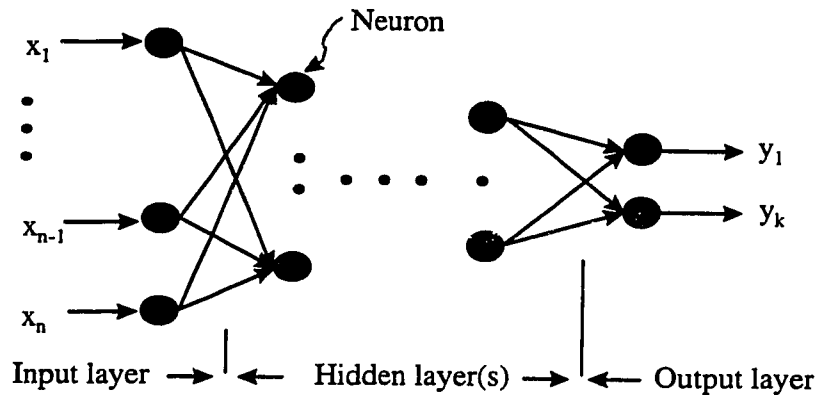


Figure 2. Fully connected feedforward multi-layer network with an input and an output layers and several hidden layers.

Research in NNs began in 1943 with the work of Mc Culloch and Pitts (1943), who demonstrated the capacity of NNs to calculate logic functions. But application of NNs really started in 1982 with the work of Hopfield (1982). NN can be defined as a highly parallel adaptive system capable of auto-improving by learning. It is inspired by the functioning mode of the animal brain in which a great number of neurons are interconnected by their synapses. By analogy, the artificial neuron is defined as the basic unit of the neural network. This neuron can receive one or more inputs, calculates the weighted sum and produces a unique output through a transfer function as Figure 2 and 3 show. Many transfer functions are available but the sigmoid function, given by the following equation, is the most common,

$$y = \frac{1}{1 + e^{-\alpha U}} \quad (9)$$

where y = the neuron output; α = multiplicative constant; and U = weighted sum of the neuron inputs. NN is an association of neurons; therefore, several types of network architectures are possible. However, the best performing are the multilayer networks (Figure 2), which are able to simulate nonlinear processes. The main principle of neural computing is the decomposition of the input-output relationship into series of linearly separable steps using hidden layers (Haykin, 1994).

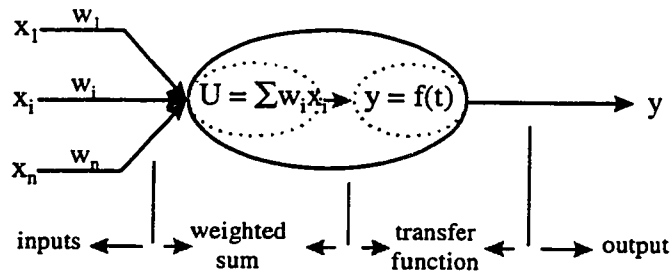
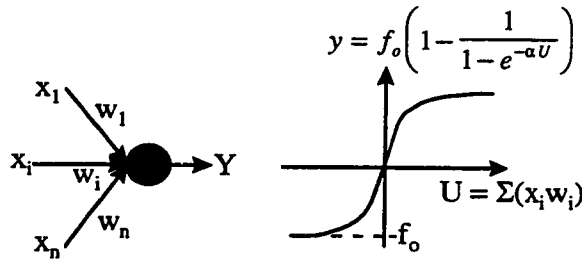
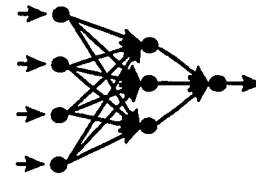


Figure 3. Architecture of a neuron.

- Data transformation: $x_i = f(x_i, x_{mean}, s)$

- Network architecture selection:

- Network training:



Find w_i by minimizing the error between observed and simulated $K_L a$.

Figure 4. Neural network development steps.

As Figure 4 shows, there are three distinct steps in developing a NN based solution. The first step is the data transformation or scaling. The second step is the network architecture definition, where the number of hidden layers, the number of neurons in each layer, and the connectivity between the neurons are set. In the third step, a learning algorithm is used to train the network to respond correctly to a given set of inputs.

SCALING OF THE DATA

The input node activities of the neural network should be small enough so that the sigmoidal hidden nodes are not saturated, i.e., their absolute values are not too large. It is also important that the absolute input values to the net are of the same order of magnitude. During training,

each weight is adjusted according to the overall error gradient, which is directly proportional to the magnitude of the input node. A very small input node will thus prevent the weight that connects it to the hidden layer from making a significant contribution to the derivative of the objective function and will slow down the training process (Djebbar and Narbaitz, 1995b). To overcome this potential problem, the data are usually scaled using linear, logarithmic, or normal transformations.

ARCHITECTURE SELECTION AND TRAINING

The exact number of hidden neurons and the connectivity between layers must be specified prior to the network training. The number of hidden neurons is usually determined via a trial and error procedure. The learning mechanism of NN is as follows (Rumelhart et al., 1986; Djebbar and Narbaitz, 1995b). First, the user defines the input variables, the output variables and the neurons in the predefined hidden layers. Then, the weights are assigned random initial values. At this stage, a set of inputs to the network produces a set of outputs that may be different from the observed values. It is necessary to change the weights at each connection so that the network outputs will coincide, as closely as possible, with the corresponding observed outputs. The observed errors on the output layer are used to determine the appropriate weight changes. This process of weights changes is called training, and may take a long time. Djebbar and Narbaitz (1995b) indicated that the main difficulties with this process are the choice of the network architecture and to a lesser degree the training algorithm. Various NN topologies have been proposed to date including Hopfield nets, Hamming nets, Carpenter/Grossberg classifiers, multilayer perceptrons, and Kohonen self-organizing feature maps (Haykin, 1994). Recent success in neural network research is mainly attributed to the achievements of multilayer perceptrons with backpropagation training algorithms. Rumelhart et al. (1986) presented a detailed description of back propagation algorithm. See also Djebbar and Narbaitz (1995b).

The network architecture and the learning algorithm (back-propagation) presented in Djebbar and Narbaitz (1995b) are merely representative. Not all of the details apply to all neural networks. Structural elements such as nodes, connections, layers, and weights are practically universal, but the arrangements between them vary. For example, some networks lack a hidden layer, and some have one or more hidden layers. Other variations include nodes that feed back to earlier nodes, connections that skip layers, and layers that are partly connected. There is no effective procedure that identifies the optimal architecture of the network prior to training.

However, an excessive number of hidden nodes may cause the network to memorize the training data. In such cases, the NN would not be able to interpolate effectively between adjacent training data points. Too few hidden nodes, on the other hand, will limit the network's ability to locate an adequate "relationship" between response and predictor variables. Various networks with different numbers of hidden nodes should be trained, and the network with the best performance on a test data set should be selected as the most adequate solution. Furthermore, nodes with very small relative weights usually indicate the small importance of the particular node compared to the other nodes.

NNs are usually slow and expensive to train. Nonetheless, once trained, running the network is fast. And although NNs may fail to find a satisfactory solution, this is a less common problem than with parametric regression. However, it can be hard to explain NN results, in that those results depend on thousands of calculations involving the input pattern and the connection weights. Unlike the parametric approach, the NN approach does not result in an explicit relationship between the independent and dependent variables. Showing how a given input yields a specific output may be harder than showing how a computer program works. This is because the values of the weights are themselves the result of a complex learning procedure. The above concerns are rather theoretical and NNs have been successfully applied in many fields (De Veaux et al., 1993; French et al., 1992; Hammerstrom, 1993a & b; Haykin, 1994).

Djebbar and Narbaitz (1995b) used NNs to estimate $K_L a$ in air stripping towers. However, the developed model was not able to perform well on the test data for three reasons. First, it used data from one source [i.e., part of Narbaitz et al. (1998) data] for training and validation. Subsequent testing of the network using Staudinger (1986) data produced errors in the order of 30 to 40%. Second, it used a limited number of variables which forced the network to memorize the training data rather than to search for the relationship between the variables. Finally, Djebbar and Narbaitz (1995b) used simple variables while transfer processes are usually analyzed using dimensionless numbers (Welty et al., 1976). Dimensional analysis simplifies modeling and experimental work by combining variables into a smaller number of dimensionless groups, guarantees the dimensional consistency of the resulting relationships, and transfers certain aspects of similarity between development data and application data (Welty et al., 1976). These shortcomings are addressed in the present study.

DESCRIPTION OF THE DATABASE

Experimental data in the public domain were surveyed and evaluated against certain criteria. These criteria include the following: (i) full scale operating conditions, such as packing of large diameters and large tower sizes; (ii) handling of end effects is described in detail; (iii) a high level of care is observed in sample collection, analysis, and the analysis method; and (iv) explicit description of the operating conditions, such as packing type and geometry, tower characteristics, liquid, gas and temperature values, and type and characteristics of the VOC(s) considered. This led to the development of the database, which is summarized in Tables 1, 2 and 3. The studies chosen from the literature encompass wide ranges of VOC air stripping operating conditions. These studies were conducted using modern, full-scale operating conditions. They include new types of packing media, optimum VOC air stripping factors in the range of 2 to 7, typical liquid loading rates of 2 to 43 kg/m²s, Henry's Law constants between 0.02 and 1.4 atm. m³ liquid/m³ air, gas flow rates between 0.06 and 5.7 kg/m²s, with an air to water ratios between 2 and 500, total packing depths between 1.2 and 5.2 m, liquid phase temperature between 7 and 30°C, and packing nominal diameters mainly between 2.54 and 9.4 cm. This database is the most comprehensive gathered to date. It originates from 10 different literature sources with a total of 1252 data points. It is about three times the size of the Onda et al. (1968) database. Table 1 lists the studies used to build the database and the main characteristics of their respective experimental setups. Table 2 contains the packing used in this database with their main characteristics. Finally, Table 3 contains the VOCs used in this database with their main characteristics. As Table 2 indicates, the database contains air stripping results using structured packings.

To interpret the study results adequately, certain physical properties are required, for instance, the liquid density, molecular diffusion coefficients, Henry's Law constants, and critical surface tension. Great care was taken in determining these physical properties because they considerably affect the resulting mass transfer coefficient.

Table 1 Summary of pilot-scale studies selected for the test database (after Djebbar and Narbaitz, 1998).

Study	Number of data points	Tower		Loading rates		Air-to-water ratio
		height (m)	diameter (cm)	Air (kg/m ² s)	Water (kg/m ² s)	
Gossett et al. (1985)	271	2.44	44.5	0.06-1	10-23	10-170
Gross & Termaath (1985)	54	2.4-1.2	19	0.4-0.4	14.5	37.8
Raczko et al. (1985)	16	3.05	30.5	0.3-1.2	11-31	7-103
Hess et al. (1983)	59	3.05	30.5	0.2-0.9	6-43	40-160
Cline et al. (1985)	15	3.05	30.5	0.1-0.7	8.6-24	18-85
Umphres et al. (1982)	12	2.34	30.5	0.3-1.3	2.6-11	8
Narbaitz et al. (1998)	698	4.6	76.2	0.15-1.3	5.5-27.5	8.5-42
Lang (1991)	67	2.7-5.2	61, 91.5	0.6-4.5	2-24	2.5-20
Rukovena (1987)	54	3.05-5.2	43, 89	0.2-5.6	4.3-28.5	1-80
Michael et al. (1991)	6	1.22	61	0.3-0.8	6.5	8-27

Table 2 Names and main characteristics of packings (after Djebbar and Narbaitz, 1998).

Packing	Diameter (cm)	Surface area (m ⁻¹)
Random packing		
Rashig Rings	1.3	400
Ceramic Saddles	1.3, 2.5	466, 259
Pall Rings	1.6, 2.5, 5	341, 220, 108
Tellerettes	2.5, 5	180, 125
Norpac	3.8, 5	145, 100
Hi-Flow Rings	5	97
Flexiring	5	115
Tripac	5	157
Cascade Minirings	5, 7.6	210, 141
Flexissaddles	7.6	88.6
LANPAC TM	8.9	137
Snowflakes	9.4	91.8
Structured packing		
Munters	1.3	420
Flexipac	2.5	131

Table 3 List of VOCs used in this study and their characteristics (Haarhoff and Cleasby, 1990).

Compound name	Chemical formula	Henry's Law const. at 20°C (atm. m ³ liquid/m ³ air)
Dichloromethane	CH ₂ Cl ₂	0.0725
Bromoform	CHBr ₃	0.028
Chloroform	CHCl ₃	0.11677
Bromodichloromethane	CHCl ₂ Br	0.095
Dibromochloromethane	CHClBr ₂	0.036
Carbon Tetrachloride	CCl ₄	0.985
Chloroethane	C ₂ H ₅ Cl	0.3968
1,1-Dichloroethane	C ₂ H ₄ Cl ₂	0.182
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	0.059
1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	0.561
1,1,2,2-Tetrachloroethane	C ₂ H ₂ Cl ₄	0.016
Vinyl chloride	C ₂ H ₃ Cl	0.923
cis-1,2-Dichloroethylene	C ₂ H ₂ Cl ₂	0.125
Trichloroethylene	C ₂ HCl ₃	0.302
Tetrachloroethylene	C ₂ Cl ₄	0.557
1,2-Dichloropropane	C ₃ H ₆ Cl ₂	0.096
Benzene	C ₆ H ₆	0.23
Chlorobenzene	C ₆ H ₅ Cl	0.16
m-Dichlorobenzene	C ₆ H ₄ Cl ₂	0.15
Toluene	C ₆ H ₅ CH ₃	0.19
m-Xylene	CH ₃ C ₆ H ₄ CH ₃	0.45
Ethylbenzene	C ₈ H ₁₀	0.27

Henry's Law constant values were obtained from experimental studies such as Haarhoff and Cleasby (1990), Gossett (1987), and Lamarche and Droste (1989). The liquid and gas phases diffusion values were determined using the diffusion values at 20°C from Hayduk and Laudie (1974) and Lyman et al. (1990), respectively. These values were then corrected for the liquid temperature (Treybal, 1980). Values of 0.75 and 0.033 N/m were used for the critical surface tensions of water and plastic packing, respectively (Dvorak et al., 1996).

Observed mass transfer coefficients were estimated using carefully determined concentrations. The concentrations used are those at the top and bottom of the packings or those corrected for end effects. Excluding end effects in the evaluation of mass transfer correlations is a common practice (Roberts et al., 1985; Lamarche and Droste, 1989). By excluding end effects, the design based on these data adds a safety margin because additional removal will take place at the top and bottom of the packing media. Observed mass transfer coefficients are determined using the generalized equation which accepts influent air with a concentration greater than zero (Djebbar and Narbaitz, 1995a):

$$z = \left[\frac{L}{K_L a} \right] * \left[\frac{R}{R-1} \ln \left\{ \frac{c_i (1-1/R) + c_o / R}{c_{i+1} (1+1/R) + c_o / R} \right\} \right] = [\text{HTU}] * [\text{NTU}] \quad (10)$$

where $R = \frac{H G}{P_t L}$ = the stripping factor (dimensionless); HTU = the height of a transfer unit (m);

NTU = the number of transfer units (dimensionless); c_o = VOC concentration in the effluent liquid at depth Z , the bottom of the packing media in Figure 5 (kg/m³); H = the Henry's Law constant (atm. m³ liquid/m³ air); P_t = the total operating pressure (atm); and L = the liquid volumetric flow rate per unit cross sectional area (m³/m² s), G = the volumetric gas flow rate per unit cross sectional area (m³/m² s), and c_i and c_{i+1} = the VOC concentrations in the liquid phase at the top and bottom of packed depth z , respectively (Figure 5).

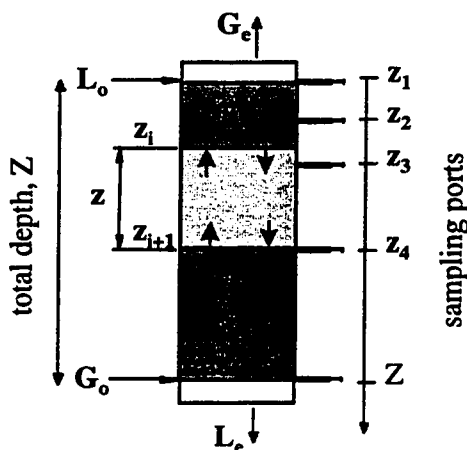


Figure 5. Definition of tower parameters used in the analysis.

METHOD OF ANALYSIS

A FORTRAN program was developed to conduct the NN analysis based on the algorithm presented in Djebbar and Narbaitz (1995b). For ease of direct comparison, this study used the same data division used in Djebbar and Narbaitz (1998). The data were divided randomly into two parts. The first 500 data points that constitute the developmental data set was used to determine the best network architecture and the optimum values of the weighting factors. A

second data set, consisting of 578 data points, was used to validate the proposed model and to compare its performance with those of the Onda and improved Onda models.

The evaluation of results was conducted using basic statistical tools. The absolute average error, AAE, is given by:

$$AAE = \frac{1}{n} \sum_{i=1}^n \frac{|(K_L a)_{exp} - (K_L a)_{pre}|}{(K_L a)_{exp}} \quad (11)$$

and the average algebraic error, AGE, is given by:

$$AGE = \frac{1}{n} \sum_{i=1}^n \frac{(K_L a)_{exp} - (K_L a)_{pre}}{(K_L a)_{exp}} \quad (12)$$

where n = the number of data points; and, $(K_L a)_{exp}$ and $(K_L a)_{pre}$ = the experimental and the predicted mass transfer coefficients, respectively. AAE is a measure of average absolute deviation, while AGE measures the overall over- or under-estimation. Roberts et al. (1985) suggested that the standard error of estimates of $K_L a$ should be based on its logarithm transform, i.e.;

$$SEE = \left\{ \frac{1}{n} \sum_{i=1}^n (\text{Log } (K_L a)_{exp} - \text{Log } (K_L a)_{pre})^2 \right\}^{0.5} \quad (13)$$

Finally, the interval limited by one standard deviation defines the expected 68% confidence level and is given by:

$$F = 10^{SEE} \quad (14)$$

RESULTS AND ANALYSIS

The initial step in the analysis investigates the required input to the network. Appendix A42 gives a general approach to network selection and training along with an example of training session results. Experience learned in previous work using the parametric and nonparametric approaches (Djebbar and Narbaitz, 1995b, 1998, Narbaitz and Djebbar, 1996) was used to select the input variables. Several training runs were conducted using different numbers and combinations of variables. The best input representation consists of eight dimensionless numbers. These are liquid and gas phases Reynolds numbers, liquid and gas phases Schmidt numbers, Froude number, Weber number, packing efficiency number, and the geometry number,

1994). Therefore, the symmetric function was used in the present study and the algorithm version described in Djebbar and Narbaitz (1995b) was modified accordingly.

The value of α controls the slope of the linear part of the sigmoid function. α should be chosen such that most of the input values, or the transformed input values, to the network fall within the “linear” range of the transfer function $f(t)$, and not in the saturation zone. This suggests that the range of the operating values of the variables must be known. The proposed transformation, Equation (16), is not explicit about these ranges. If the inputs are in the saturation range for given values of α and f_0 , the outputs will saturate and will not cover the entire range of observed $K_L a$ values. After a series of numerical experiments, values of $f_0 = 7.5$ and $\alpha = 0.01$ were found to yield the best outcomes, resulting in the following transfer function equation,

$$y = 7.5 \left(\frac{1}{1 - e^{-0.01z}} \right) + 3.5 \quad (17)$$

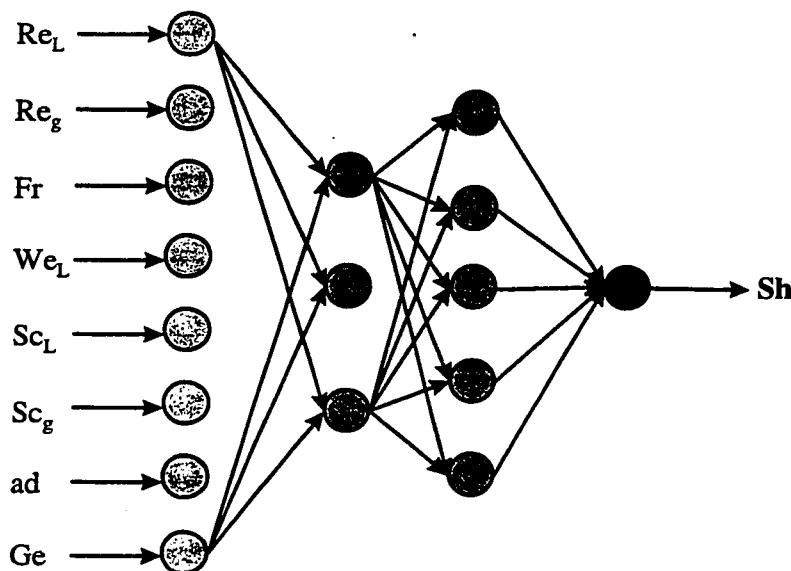


Figure 6. Architecture of the selected network; two hidden layers with three and five neurons, respectively.

The choice of the transfer function was not completely independent from the choice of the network architecture, and, as indicated previously, there are no specific guidelines that regulates the selection of the network architecture. However, after a series of simulations, a scheme of two hidden layers with three and five neurons each was selected (Figure 6). The training of the

network was conducted on a Pentium Pro, 300 MHz IBM compatible PC. A typical training run took about 24 hours, after which the errors became practically constant. However, running the network solution is very fast, typically less than a second.

Figure 7 shows the results of the goodness of fit tests for the 500 data points that constitute the training data set. The NN model produced an average error of 18%, with 68% of the data within a band limited by a factor of 1.25 from the best fit line. The training data set as a whole is slightly overestimated with an average algebraic error of 4%. These results are better than those of the developmental stage of the previous parametric models. For example, the Onda model (Onda et al., 1968) and the improved Onda model (Djebbar and Narbaitz, 1998) had an AAE of 20% and 22.5%, respectively.

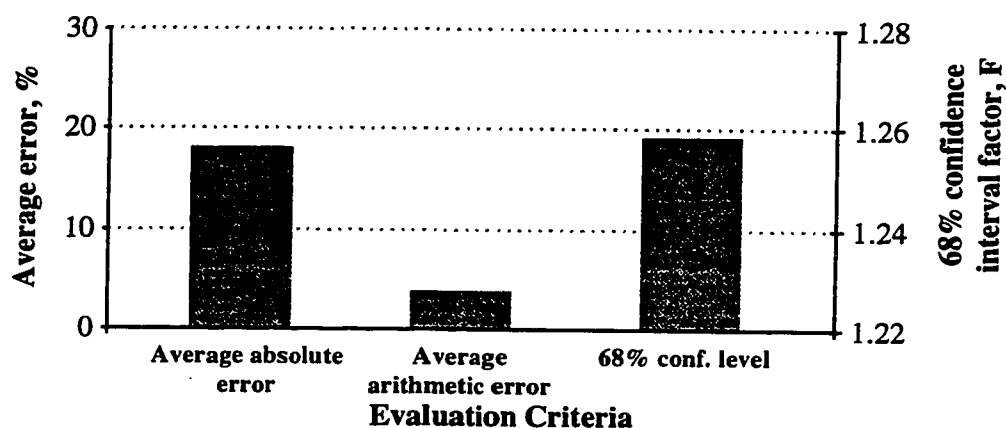


Figure 7. Results of the neural network using the developmental data base.

The second part of the database is used to validate the developed model. Figure 8 compares the results of the three models: the Onda, the improved Onda, and the NN models. The NN predictions are superior to those of the Onda and the improved Onda models. The improved Onda and NN models produced average arithmetic errors of +0.7% and -3%, and the percentages of data overestimated are 44 and 46%, respectively. The average error was 30% for the Onda model, 22% for the improved Onda model and 17.5% for the NN model (Figure 8). This NN model reduced the AAE by more than 40% compared to the Onda model. The large error of the Onda model is caused by the overestimation of K_{La} in 80% of the cases, with an average arithmetic error of +23% (Figure 8). 68% of the validation data is within a band around the best fit line, which is limited by a factor of 1.27 for the NN model, 1.32 for the improved model, and

1.39 for the Onda model (Figure 8). Therefore, for the same level of risk, the NN based design will require a smaller safety factor than the parametric based designs, which will have cost implications.

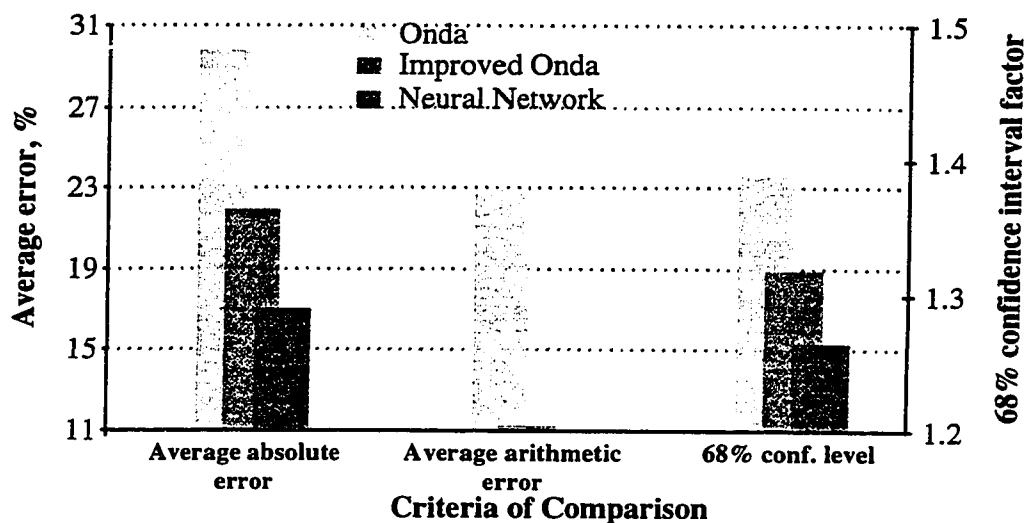


Figure 8. Average errors and F factor for the validation data set.

Figure 9 compares the errors in predicting data grouped by source (author). One can notice the large variation in errors, from one author to another, in the Onda model predictions. This variation is much smaller in the improved Onda model, and is further reduced by the NN model. It is important here to recall the impact of the errors in the variables on the observed K_{La} . Djebbar and Narbaitz (1995a) estimated the impact of these errors to be in the order of 10 to 15%. Also, Djebbar and Narbaitz (1998) indicated that the error inconsistency from one author to another could be due to errors in chemical analysis and due to operating problems, such as end effects, channeling, and liquid distribution system. Therefore, the error in different data sources will always exist, and is not expected to be the same. Consequently, the source of the data will have an impact on the results. For example the $L_r = 23.5 \text{ kg/m}^2\text{s}$ data in Figure 10 is from the Narbaitz et al. (1998), i.e. from one data source only, whereas the $L_r = 28.6 \text{ kg/m}^2\text{s}$ data is from Narbaitz et al. (1998) and Lang (1991).

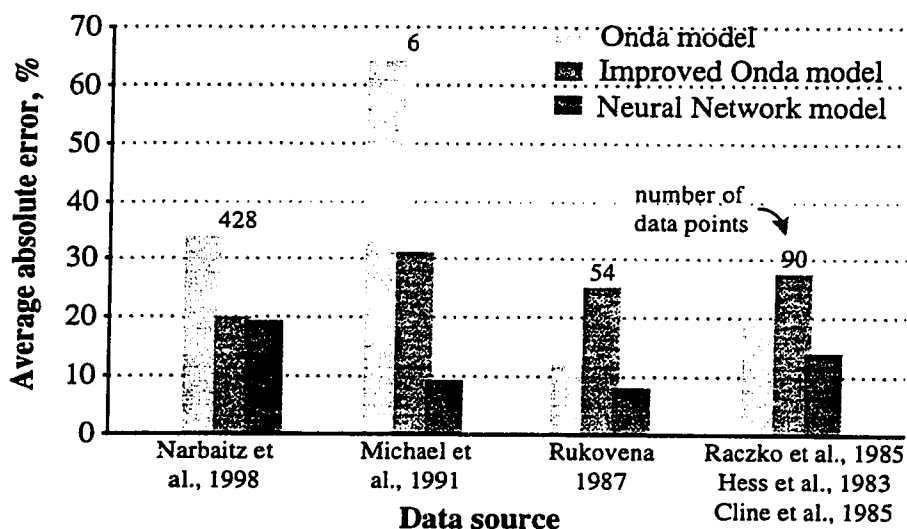


Figure 9. Average absolute error for individual data sources of the validation data set.

Figure 10 compares the error in predicting K_{La} as a function of the liquid flow rate. As the flow rate increases, the error in the Onda predictions tends to decrease. This may be due to inaccuracy in simulating liquid flow effect on K_{La} by the Onda model (Djebbar and Narbaitz, 1998). The improved Onda and NN models resulted in lower errors, but also tend to improve with increasing liquid loading.

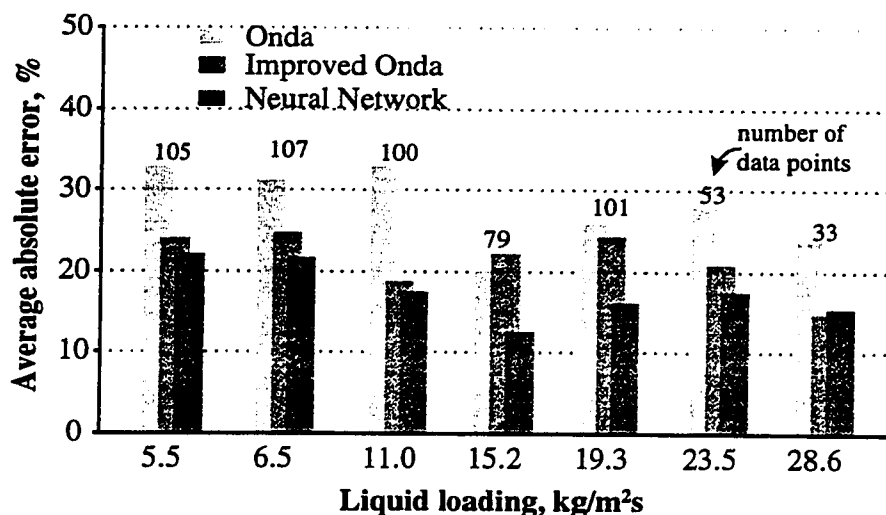


Figure 10. Average absolute error of the Onda and improved model as a function of the liquid loading for the validation data set.

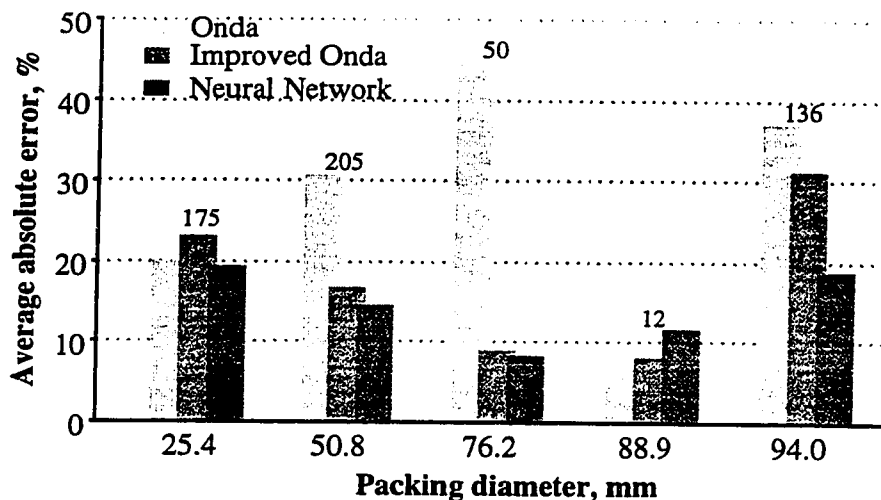


Figure 11. Average absolute error of the Onda and improved model as a function of the packing diameter for the validation data set.

Figure 11 shows the variation of the error with the packing diameter. The Onda deviation increases with the packing diameter, while both the improved Onda and NN models show U-shaped trends. However the U-shape is less apparent in the NN case. The U-shaped trend may be misleading for two reasons. First, some packing presented in Figure 11 belong to one data source only, and therefore it will certainly carry with it errors specific to the source of the data, as discussed earlier. Second, as found by Djebbar and Narbaitz (1998), the packing diameter is not a good indicator of the transfer characteristics. The error in simulating the transfer characteristics may seem correlated with the change in the packing diameter. However, the transfer characteristics are not modeled correctly by the values of the packing diameter used in this analysis. Second, some of the packing diameters shown in Figure 11 represent data of only one packing type, while others represent more than one packing and are from different data sources. So the ordinate involves changes in the packing particle's geometry, diameter as well as the data source.

This points to the need to look for an alternative variable that reflects better the effect of the geometry on the transfer characteristics. A possible alternative variable would be the pressure drop. Pressure drop is the loss of energy due to the packing particles arrangement, the air path formation, and the packing's surface characteristics. The pressure drop is expected to be closely correlated to the geometry of the packing and its dimensions. The authors are not aware of any work that relates modern packing performance to air pressure losses through the packings.

Pressure drop data are usually lacking and are only considered in connection with the operating cost of blower and its optimization, and not in terms of its relation to the transfer characteristics.

Figures 12 to 15 show the improvement in the prediction results produced by the NN model, compared to previous models. The following sections investigate the effect of liquid flow, gas flow, and packing depth and compare them to the established practice and theory.

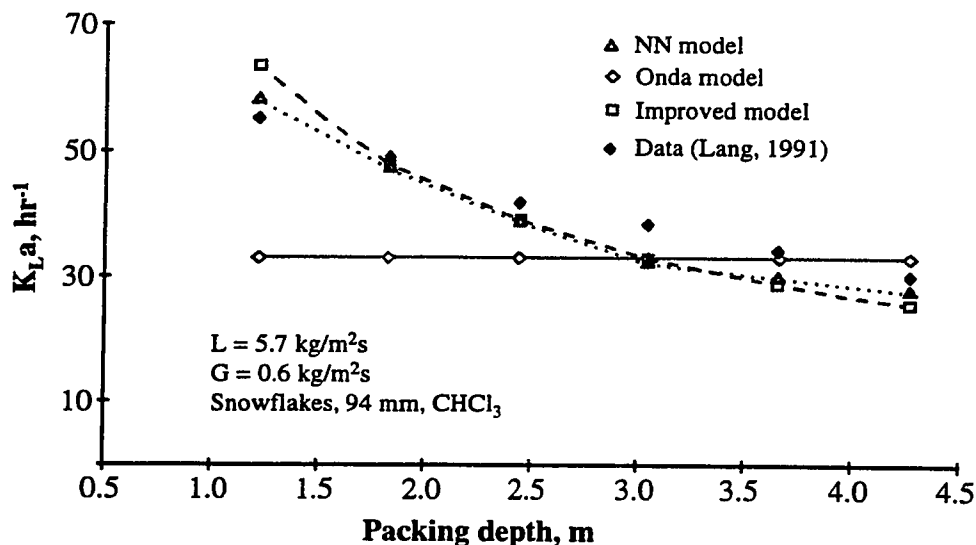


Figure 12. Effect of packing depth on simulated K_La .

Mass transfer theory in packed towers assumes that K_La is independent of the packing depth. However, previous experimental results contradict this assumption (Djebbar and Narbaitz, 1995a, Harriott, 1989). Figure 12 shows the variation of K_La with the packing depth for the specified conditions. The Onda model is independent of the packed depth and therefore it predicts a constant value for different packing depths, assuming that all other variables are constant. The improved Onda estimates change with the packing depth but they tend to overestimate K_La in short columns. The NN model, on the other hand, closely predicts observed data. Notice that the absolute value of the slope of the improved Onda curve is higher than that of the NN curve. There is no theoretical argument that supports one curve over the other. However, the NN curve is more plausible for three reasons. First, in general NN results simulate more closely observed data. Second, the effect of the packing depth is expected to level off as the column becomes taller, as shown by the NN curve. However, contrary to what is intuitively

expected, the improved Onda model seems to predict smaller and smaller values as the packing depth increases. Finally, the improved Onda model predicts very high K_{La} values for short columns, which is not supported by observations.

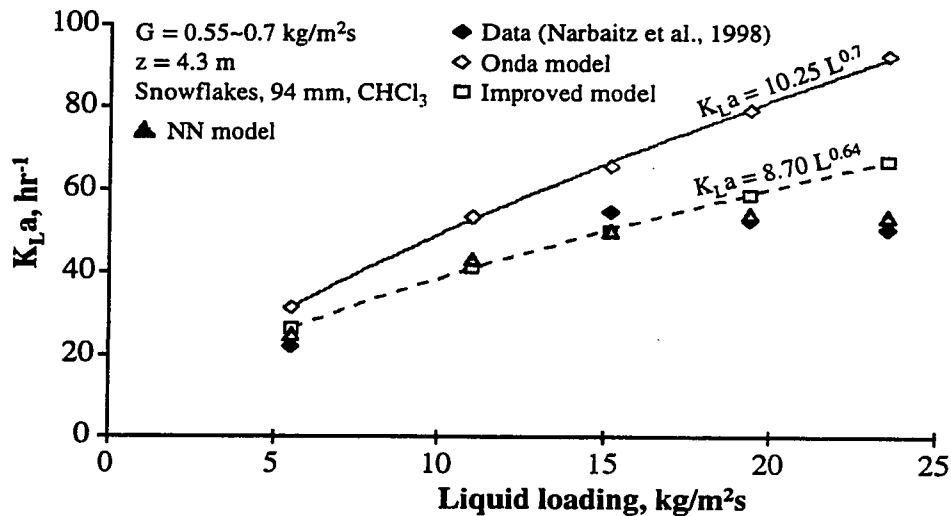


Figure 13. Effect of liquid flow on K_{La} .

The second variable which was assessed in this study is the liquid loading. Figure 13 is a plot of simulated and observed K_{La} as a function of liquid loading for the indicated conditions. Relatively, the three models produce good results at low liquid loadings. At high liquid loading, both the Onda and improved Onda predict higher K_{La} values than the observed data. The points associated with the Onda and improved Onda models were regressed and plotted as dashed lines (Figure 13). The following equation was used for the regression,

$$K_{La} = b_o L_f^{b_1} \quad (18)$$

where L_f = the liquid loading and b_o , b_1 = regression parameters. As shown in Figure 13, the Onda and improved Onda models predictions were described well over the entire range by equation (18) type expression. Davidson's (1959) comparison of theory with experimental data indicated that the liquid flow rate exponent, b_1 , should be appreciably less than 2/3. Streamline theory (laminar flow conditions) in conjunction with the penetration model shows that the liquid phase K_{La} should be proportional to the liquid flow rate to the 1/3 power (Vivian and Peaceman, 1956). However, experimental data obtained by Vivian and King (1964) and Vivian and Peaceman (1956) suggested that K_{La} should be proportional to the Reynolds number (and thus to

L_f) to the power of approximately 0.4. The set of curves generated by NN (Figure 13) can not be approximated well using only one equation. Most importantly, the NN solution yielded two different values for b_1 : For liquid loading less than approximately $18 \text{ kg/m}^2\text{s}$, b_1 is equal to 0.82. However, for higher liquid loading rates, b_1 is equal to 0.4. Therefore, the NN differentiates between two regions, which may be an indication of a change in the liquid dynamics. Bravo et al. (1992) have shown that the relationship between the mass transfer coefficients and the operating variables changes with changing operating conditions, such as different flowrates or packing material. This means that the values of the exponents in parametric correlations should change accordingly. This important fact is confirmed by our NN results.

Also, it is expected that the increase in $K_L a$ when the liquid flow increases should level off, and may even decrease for two reasons. First, when the liquid flow increases at low flow rates, the surface area that is wetted increases while the flow depth over the packing surfaces remains almost constant (Treybal, 1980). When the liquid loading approaches the loading region (Treybal, 1980), the flow depth increases, the mixing efficiency at the packing junction decreases, the dead zones in packing junctions increase, and the mass transfer coefficient is expected to level off. When approaching flooding condition, $K_L a$ may even decrease. This is predicted by the NN solution. On the other hand, neither the Onda nor the improved Onda models (Figure 13) predict this interesting behavior. In fact, the Onda and improved Onda models predict a continual increase in mass transfer coefficient, which is not logical at all.

Using the same approach, the effect of gas loading rate was also assessed. Figure 14 shows a comparison between observed and predicted $K_L a$ when only gas flow changes. The left side of the plot shows little difference between the three models. The right side, however, shows a clear difference between the three models. Both the Onda and improved Onda models show that $K_L a$ is practically independent of the gas loading. Dvorak et al. (1996) found that $K_L a$ is more sensitive to gas velocity than Onda predicts. As the gas loading increases, at high gas flow rates, mass transfer tends to be underestimated by the Onda model. At high gas flow rates, the Onda and the improved Onda models predict that the liquid film resistance accounts for nearly all mass transfer resistance. The Dvorak et al. experimental data contradict this assumption, and so do the data in this research, as Figure 14 shows.

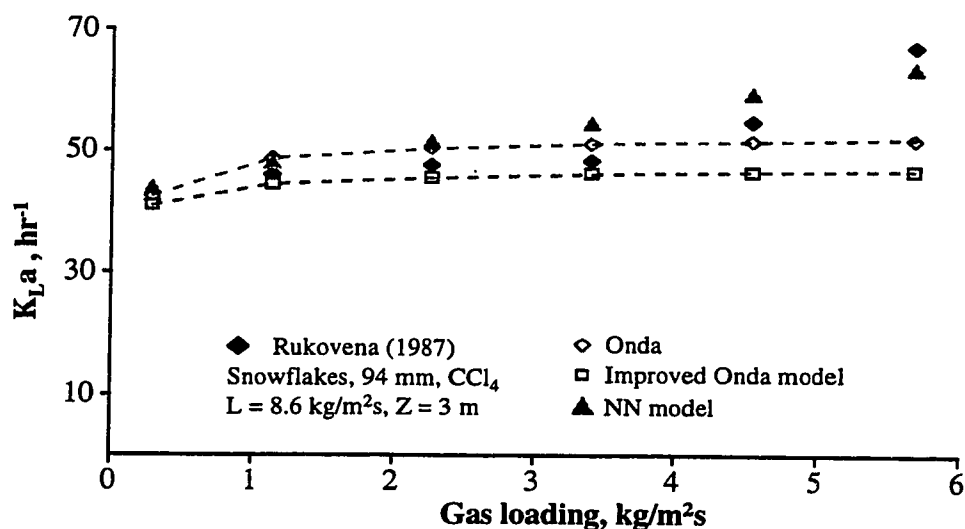


Figure 14. Effect of gas loading rate on simulated K_{La} .

Dvorak et al. (1996) attributed the underestimation of K_{La} to an error in Onda's specific wetted surface area equation. Several studies indicated that the specific surface area can be larger than the packing dry surface area, which can not be obtained using either the Onda or the improved Onda equations for specific surface area. Consequently, as Figure 14 shows, both Onda and improved Onda models underestimate K_{La} at high gas loading rates. Dvorak et al. (1996) found that as gas loading decreases below $1 \text{ kg/m}^2\text{s}$, mass transfer tended to be underestimated by the Onda model. Gas-phase resistance is relatively large at low gas flow rates. Several studies (Gossett et al, 1985; Roberts et al., 1985; Little and Sellek, 1991) indicated that the Onda correlations underestimate the gas film resistance to mass transfer at low gas loading rates (Dvorak et al., 1996). To overcome this problem, Dvorak et al. (1996) suggested the change of front end coefficient as well as the exponent of the gas phase Reynolds number. When these changes were implemented in the improved Onda correlations, they did not substantially improve the predictions.

The NN model succeeded in predicting K_{La} at both low and high gas flow rates. This suggests that the NN model simulates well the effect of the gas flow rate compared to both the Onda and the improved Onda models. Observed data show a sharp increase in K_{La} at high gas loading rates, which occurs around a gas loading rate of $3.5 \text{ kg/m}^2\text{s}$.

Finally a comparison using small and structured packing data was conducted. There are two packings only in the structured packing data set. Figure 15 shows the results based on the average absolute error. The structured packing diameter is smaller or equal than 2.5 cm. Therefore, they can be considered as small packing data, where the Onda model is considered reliable. The three models performed comparatively and equally well with an AAE smaller than 25% for the three models.

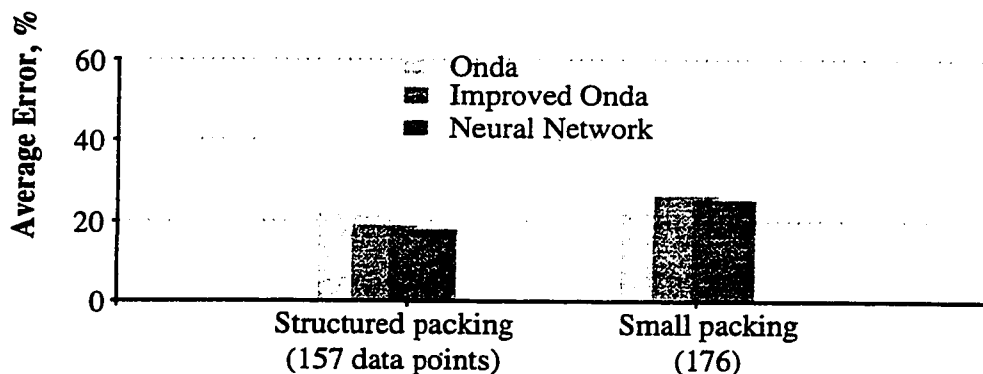


Figure 15. Simulation results using Cummins data, small and structured packing data.

The results obtained in this study shows the powerfulness and superiority of NNs over traditional modeling techniques. This superiority is reflected qualitatively, i.e., in the nature of the predictions, and quantitatively, i.e., in the quality of fit. Recall that NNs are nonparametric and therefore they are not confined to follow pre-specific relationships.

CONCLUSION

This paper presents a nontraditional approach to the analysis of the mass transfer coefficient in air stripping packed towers based on NNs technology. As a first step, architecture selection and weights optimization of the NN model were performed using a large, new set of experimental data. Eight key dimensionless numbers were used in the model development namely: Reynolds liquid and gas, Schmidt liquid and gas, Froude, Weber, Geometry, and Efficiency numbers.

In the validation step, the NN model had an error of 17.5% which represents more than a 40% improvement over the Onda model predictions and more than a 20% improvement over the

improved model. The NN model addressed many of the shortcomings of both the Onda and improved models. The average absolute error for the validation, as well as for the development data, was found to be less than 19% with 68% of the data within a factor of 1.27 from the best fit line. The same parameters are 24% and 1.3 for the improved model and 29% and 1.39 for Onda model.

The NN models K_{La} using functions of L_f raised to different exponents as opposed to the constant exponent of current parametric models. It was able to simulate the sudden increase in K_{La} at high gas loading rates. Also, it simulates more realistically the effect of the packing depth.

However, the effect of the packing diameter, if any, is still not well modeled. This shortcoming is not due to the estimation method, but rather it is due to the lack of a variable that represents the geometry more accurately. An alternative approach would be to use the pressure drop characteristics or the liquid flow depth over the packing surface, which need further investigation.

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CHAPTER 8

CONCLUSION AND RECOMMENDATIONS

8.1 MAJOR CONCLUSIONS

1. The database assembled for this study is both comprehensive and representative of modern applications of air stripping towers. The database originates from 12 different studies, tested 19 modern packing types, and investigated the removal of 22 compounds of interest to ground water remediation. Great care was taken in estimating the physical, chemical, and operating characteristics of the data. This database can be used for further air stripping related studies and applications.
2. The Onda model form has been found to have some limitations and shortcomings including:
 - (i) The overestimation of K_{La} by 30 to 40% for large size packings used in current full-scale air stripping applications.
 - (ii) This overestimation of K_{La} increases with increasing packing diameter.
 - (iii) The experimental mass transfer coefficient K_{La} decreased with the packing depth.
 - (iv) Observed increases or decreases in K_{La} in the upper part of the column is related to the adjustment of the wetted packing surface area associated with the shift from the liquid distribution pattern of the distributor to the natural flow distribution pattern of the packing. There is no simple and reliable method to account for this phenomenon.

- (v) Typical errors in the variables explained only part of the total observed deviation in the Onda predictions. The impact of typical variables' errors on the Onda predictions are in the order of 10%. A large part of the deviation in the Onda predictions is attributed to the lack of fit of the Onda model itself.
3. The evaluation of the Onda model showed that not all the observed deviation between measured and simulated K_La values resulted from deficiencies in this model. Part of the observed deviation may be caused by column operational problems and experimental errors. These problems will always exist, to a certain extent, in any operational tower. Their relative effect on the measured mass transfer coefficient can be high (up to $\pm 50\%$ of the theoretical value). However, their effect can be minimized and confined to a negligible amount only through sound design and careful operation, as described in this thesis.
 4. The corrections of the Onda estimates by Djebbar and Narbaitz (1995) and Gossett et al. (1985) did not address the fundamental limitations of the model. Therefore, they should be used only for conditions that are similar to their respective developmental data.
 5. Based on the parametric approach, new correlations were developed using the new database. These new correlations used the Onda correlations functional forms and addressed several of the shortcomings of the Onda correlations, such as packing depth, increase in error with increasing packing diameter, and the tendency to overestimate K_La . The average error in the new model predictions is 20% smaller than that of the Onda model's.
 6. Some shortcomings of the improved Onda correlations remain. These particularly include the effect of high gas flow rate and the packing diameter. The packing diameter was not found to be a strong indicator of the transfer characteristics as previously thought. This may be attributed to the form of the correlations and/or the packing diameter definition. Different packing diameter definitions were tested, but none of them produced particularly better results.
 7. The neural network solution produced better results than the Onda and the improved Onda models. It simulates correctly the effect of gas loading while accounting for the effects of liquid flow rate and packing depth more reasonably than existing parametric methods. The

average absolute error for the validation, as well as for the development data, was less than 19% with 68% of the data within a factor of 1.27 from the best fit line. The same parameters are 24% and 1.3 for the improved model and 29% and 1.39 for Onda model.

8. The neural network models K_{La} using functions of L_f raised to different exponents as opposed to the constant exponent of current parametric models. It was able to simulate the sudden increase in K_{La} at high gas loading rates. Also, it simulates more realistically the effect of the packing depth.
9. The effect of the packing geometry on mass transfer is still not well modeled even by NN. This shortcoming is not due to the estimation method. It is, rather, due to the absence of a variable that represents the geometry more accurately.

8.2 RECOMMENDATIONS FOR FURTHER INVESTIGATIONS

In light of the findings of this study, the author recommends the followings:

1. The development of a parametric model for K_{La} based on synthetic data generated by the neural network solution should be investigated. A promising approach would be to:
 - use the k_L and k_g correlation forms of the improved Onda model.
 - change the Onda surface area correlation so that it produces surface area values that are larger than the dry surface area value.
 - in addition to existing experimental data, use the neural network model to generate synthetic data to estimate the parameters of the correlations.
2. The neural network model could be used to investigate individual components of the mass transfer characteristics. This, however, needs experimental data on the individual components of the transfer components, which are only presently available for laboratory scale data that use traditional small packings.
3. The liquid distribution affects the transfer characteristics in packed towers especially at the upper part of the column. Its inclusion in the correlations proved to be difficult and complex. However, its drawback can be avoided by using a good liquid distribution system whose distribution quality is at least as good as that of the packing.
4. A flow depth characterizing variable should be considered to estimate the Reynolds number instead of the constant dry surface area.

5. The pressure drop may be a strong indicator of the transfer characteristics. Its use to estimate mass transfer characteristics should be investigated.

APPENDIXES

- Appendix A1** Chemical characteristics of volatile compounds of interest.
- Appendix A2** Packing characteristics.
- Appendix A3** "NON PARAMETRIC MODELING OF MASS TRANSFER COEFFICIENTS FOR AIR STRIPPING TOWERS." Published in the CSCE Journal.
- Appendix A4** "Neural Network Estimation of Air Stripping Mass Transfer Coefficients." Presented at the 1995 WEFTEC, Miami Beach.
- Appendix A5** Data Base.
- Appendix A6** Neural Network FORTRAN Program.

APPENDIX A1

Table A.1 Packing characteristics.

ID	Name	Material of		Diameter	Surface	Area	Source
		construction	mm				
1	Rashig rings	Ceramic	6	787	1		
2			12.7	400	1		
3			16	328	1		
4			19.1	262	1		
5			25.4	190	1		
6			32	148	1		
7			38.1	125	1		
8			50.8	92	1		
9			76.2	62	1		
10		metal 0.8mm	6	774	1		
11			12.7	420	1		
12			19.1	274	1		
13			25.4	206	1		
14		metal 1.6mm	12.7	387	1		
15			19.1	236	1		
16			25.4	186	1		
17			32	162	1		
18			38.1	135	1		
19			50.8	103	1		
20			76.2	68	1		
21	Pall rings	Plastic	16	341	2		
22			25.4	210	2		
23			38.1	123	2		
24			50.8	108	2		
25			76.2	85	2		
26			88.9	79	2		
27		metal	16	341	2		
28			25.4	206	2		
29			38.1	128	2		
30			50.8	102	2		
31		Ceramic	25.4	207	2		
32			38.1	154	2		
33			50.8	125	2		

Table A.1 Packing characteristics.

ID	Name	Material of		Diameter	Surface	Area	Source
		construction	mm				
34	Flexirings	Plastic	16	345	3		
35			25.4	213	3		
36			38.1	131	3		
37			50.8	115	3		
38			88.9	92	3		
39	Cascade Mini-Rings	Plastic	50.8	210	5		
40			76.2	141.1	5		
41	Ballast rings	Plastic	25.4	213	2		
42			38.1	131	2		
43			50.8	105	2		
44			88.9	85	2		
45	Bundle rings	Ceramic	25.4	300	7		
46			38.1	280	7		
47	Tripack	Plastic	25.4	279	7		
48			50.8	148	7		
49			88.9	124.7	7		
50	Nor-Pac	Plastic	15.9	331.4	7		
51			25.4	180.5	7		
52			38.1	144.4	7		
53			50.8	102	7		
53	Flexisaddles	plastic	25.4	207	3		
54			76.2	88.6	3		
55	Berl Saddles	Ceramic	6	899	6		
56			12.7	466	6		
57			19.1	269	6		
58			25.4	259	6		
59			38.1	177	6		
60			50.8	121	6		
61	Intalox Saddles	Ceramic	6	984	2		
62			12.7	623	2		
63			19.1	335	2		
64			25.4	256	2		
67			76.2	92	2		

Table A.1 Packing characteristics.

ID	Name	Material of construction		Diameter mm	Surface Area m ² /m ³	Source
68		Plastic		25.4	207	2
69				50.8	108	2
70				76.2	89	2
71	Super Intalox Saddles	Ceramic		25.4	253	2
72				50.8	105	2
73		Plastic		25.4	207	2
74				50.8	108	2
75				76.2	89	2
76	Novalox Saddles	Plastic		25.4	256	6
77				38.1	256	6
78				50.8	121	6
79				76.2	105	6
80		Ceramic		25.4	256	6
81				38.1	200	6
82				50.8	121	6
83				76.2	92	6
84	High-Flow	Ceramic		25.4	285	6
85				38.1	140	6
86				50.8	97	6
87				76.2	61	6
88		Plastic		50.8	110	6
88	Snowflakes	Plastic		94	91.8	2
89	Tellerettes	Plastic		25.4	180	2
90				50.8	125	2
91				67.2	112	2
92	Munters 6560	Plastic		15	419.8	9
93	12560			25.4	227	9
94	Flexipac #2	Plastic		22.2	246	4
95	#3			26.9	131.18	4
96	Kompac	Plastic		50.8	102	
97	Surfpac X-Flo 30	Plastic		31.5	98.5	

Table A.1 Packing characteristics.

ID	Name	Material of construction		Diameter mm	Surface Area m ² /m ³	Source
98	IMPAC	Plastic		83.82	213	8
99				139.7	108	8
100	LANPAC	Plastic		58.42	223	8
101				88.9	147.5	8
1.	Perry and Chilton (1973)			5. Glitish Bulletin 345		8. Lanec Products, Inc.
2.	Single, R.F. (1987)			6. Rauschert Industries Inc. 1994		9. Munters Inc.
3.	Koch Bulletin KRP-2, 1987.			7. Jaeger Product Bulletin 600		
4.	Koch Bulletin KRP-4, 1987.					

APPENDIX A2

Table A.2 Chemical characteristics of volatile compounds of interest.

ID	Compound Name	Chemical Formula	Diffusion (m ² /s)		H ₂₀ m ³ liq./m ³ gas	A Equ. 2.2	Source of H ₂₀
			Gas E-10 (5)	Water E-6 (6)			
1	Carbondioxide	CO ₂	17.7	16.6	1.1286	2070	3
2	Oxygen	O ₂	21.2	19.2	30	1450	2
3	Amonia	NH ₃	13.07	21.6	0.000568	3754	3
4	Chloromethane	CH ₃ Cl	13.2	13.6	0.2787	4215	1
5	Bromomethane	CH ₃ Br	12.8	12	0.56	4375	1
6	Dichloromethane	CH ₂ Cl ₂	10.7	10.6	0.0725	3817	1
7	Chloroform	CHCl ₃	9.23	9.18	0.11677	4612	1
8	Bromoform	CHBr ₃	8.83	8.08	0.028	4399	1
9	Bromodichloromethane	CHCl ₂ Br	9.09	8.72	0.095	4375	1
10	Chlorodibromomethane	CHBr ₂ Cl	8.96	8.37	0.036	4375	1
11	Carbontetrachloride	CCl ₄	8.18	8.22	0.98558	4411	1
12	Dichlorodifluoromethane	CCl ₂ F ₂	9.94	10.2	11	3224	1
13	Fluorotrichloromethane	CCl ₃ F	8.94	9.08	4.6	4375	1
14	Chloroethane	C ₂ H ₅ Cl	10.6	11.2	0.3968	3120	1
15	1,1-Dichloroethane	C ₂ H ₄ Cl ₂	9.1	9.33	0.182385	4128	1
16	1,2-Dichloroethane	C ₂ H ₄ Cl ₂	9.15	9.19	0.059	3620	1
17	1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	8.13	8.28	0.56059	4133	1
18	1,1,2-Trichloroethane	C ₂ H ₃ Cl ₃	8.13	8.11	0.049	4375	1
19	1,1,1,2-Tetrachloroethane	C ₂ H ₂ Cl ₄	7.36	7.37	0.016	4375	1
20	1,1,2,2-Tetrachloroethane	C ₂ H ₂ Cl ₄	7.36	7.32	0.016	4375	1
21	Chloroethylene	C ₂ H ₃ Cl	11.3	11.9	0.92315	3286	1
22	1,1-Dichloroethylene	C ₂ H ₂ Cl ₂	9.61	9.77	0.87599	3729	1
23	Trans-1,2-Dichloroethylene	C ₂ H ₂ Cl ₂	8.61	8.71	0.32	4182	1
24	Cis-1,2-Dichloroethylene	C ₂ H ₂ Cl ₂	9.61	9.64	0.12515	4192	1
25	Ethylenedibromide	C ₂ H ₂ Br ₂	8.89	8.32	0.028	4375	1
26	Trichloroethylene	C ₂ HCl ₃	8.45	8.46	0.30192	4780	1
27	Tetracloroethylene	C ₂ Cl ₄	7.61	7.59	0.5571	4918	1
28	1,2-Dichloropropane	C ₃ H ₆ Cl ₂	8.07	8.27	0.096	4375	1
29	1,3-Dichloropropane	C ₃ H ₆ Cl ₂	8.07	8.27	43	3917	1
30	1,2-Dichloropropane	C ₃ H ₆ Cl ₂	8.07	8.27	15.53	3477	1
31	1,2-Dibromo-3-chloropropane	C ₃ H ₅ Br ₂ Cl	7.17	6.87	0.013	4375	1
32	Cis-1,3-Dichloro-1-propylene	C ₃ H ₄ Cl ₂	8.39	8.47	0.056	4375	1
33	Trans-1,3-Dichloro-1-propylene	C ₃ H ₄ Cl ₂	8.39	8.44	0.054	4375	1
34	1-Chlorobutane	C ₄ H ₉ Cl	-	-	0.565	3482	4
35	2-Chlorobutane	C ₄ H ₉ Cl	-	-	0.77	4499	4
36	1,4-Dichlorobutane	C ₄ H ₈ Cl ₂	-	-	0.017	3128	4
37	1-Chloropentane	C ₅ H ₁₁ Cl	-	-	0.749	4727	4
38	1,5-Dichloropentane	C ₅ H ₁₀ Cl ₂	-	-	0.211	1597	4
39	1-Chlorohexane	C ₆ H ₁₃ Cl	-	-	0.775	4459	4
40	Benzene	C ₆ H ₆	9.02	9.37	0.23	3680	1
41	Bromobenzene	C ₆ H ₅ Br	7.93	7.71	0.057	4375	1
42	Chlorobenzene	C ₆ H ₅ Cl	7.48	7.7	0.16	4375	1
43	o-DiChlorobenzene	C ₆ H ₄ Cl ₂	7.29	7.22	0.08	4375	1
44	m-Dichlorobenzene	C ₆ H ₄ Cl ₂	7.29	7.24	0.15	4375	1
45	p-Dichlorobenzene	C ₆ H ₄ Cl ₂	7.29	7.24	0.12	4375	1
46	1,2,4-Trichlorobenzene	C ₆ H ₃ Br ₃	6.71	6.6	0.096	4375	1
47	2,4-Dinitrotoluene	C ₆ H ₈ N ₂ CH ₃	6.48	6.22	0.00021	4375	1
48	Toluene	C ₆ H ₅ .CH ₃	7.98	8.31	0.19	8100	1
49	Ethylbenzene	C ₈ H ₈	7.21	7.53	0.27	4375	1
50	o-Xylene	C ₈ H ₁₀	7.21	7.5	0.33	4375	1
51	m-Xylene	CH ₃ C ₆ H ₄ CH ₃	7.21	7.52	0.45	4375	1
52	p-Xylene	C ₈ H ₁₀	7.21	7.52	0.29	4375	1

1 Haarhoff and Cleasby (1990)

2 Roberts et al (1985)

3 Treybal (1983)

4 Leighon and Calo (1981)

5 Layman et al. (1990)

6 Hayduk and Laudie (1974)

APPENDIX A3

"NON PARAMETRIC MODELING OF MASS TRANSFER COEFFICIENTS FOR AIR STRIPPING TOWERS"

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Nonparametric modeling of mass transfer coefficients for air stripping packed towers¹

Roberto M. Narbaitz and Yassine Djebbar

Abstract: Existing parametric correlations have been found to have difficulties in predicting the removal of trace levels of volatile organic chemicals by modern air stripping towers. In this study, a new approach using a nonparametric kernel regression method was used to predict the mass transfer coefficient, $K_L a$, of air stripping towers. Although only four variables were used, the predictions are already improved more than 50% as compared with Onda correlation, the best existing parametric correlation. The proposed technique shows a dependency of $K_L a$ on the liquid flow rate which is in good agreement with established theory. Previous parametric approaches were unable to model this relationship correctly.

Key words: mass transfer coefficient, air stripping tower, volatile organic compound, nonparametric kernel regression.

Résumé : Les recherches antérieures ont montré que les corrélations paramétriques ont des difficultés à prédire l'enlèvement des composés organiques volatils par les tours modernes d'épuration à l'air. Dans cette étude, une nouvelle approche utilisant la régression non paramétrique avec noyau est employée pour prédire le coefficient de transfert de matière, $K_L a$, dans ces tours. Quoique quatre variables seulement aient été utilisées, les prédictions sont déjà améliorées de plus de 50% comparé à la corrélation d'Onda, la meilleure corrélation paramétrique. La technique proposée montre une dépendance de $K_L a$ vis-à-vis du débit d'eau qui coïncide avec la théorie établie. L'approche paramétrique, par contre, ne peut pas simuler correctement cette dépendance.

Mots clés : coefficient de transfert de matière, tour d'épuration à l'air, composé organique volatil, régression non paramétrique par noyau.

Introduction

Groundwater contamination by trace levels of volatile organic compounds (VOCs) has emerged as a major water quality issue. Most VOCs are not removed by conventional water treatment operations. In the amendment to the Safe Drinking Water Act in 1986, the United States Environmental Protection Agency recognized air stripping as a best available technology for VOC treatment. The most important parameter in the design of an air stripping tower is the overall liquid phase mass transfer coefficient, $K_L a$. Engineers often calculate $K_L a$ using a mass transfer correlation because they are easy to use and avoid costly pilot-scale tests.

Tens of mathematical parametric correlations have been developed to predict $K_L a$ for packed towers. Among these models, there is agreement in the recent literature that the Onda model (1968) is the best $K_L a$ correlation for air strip-

ping applications (Staudinger et al. 1990; Roberts et al. 1985; Lamarche and Droste 1989). The literature also shows that this model yields satisfactory results for lab data. However, 30–50% deviations from predictions are often reported in full-scale applications (Lenzo et al. 1990; Staudinger et al. 1990; Djebbar and Narbaitz 1995). The lack of good predictive ability is due to (i) the extrapolative nature of the predictions; (ii) the limited operating conditions in the data bases used to develop the correlations; (iii) the parametric regression techniques used to generate these models; and (iv) the changing nature of mass transfer relationships from one set of operating conditions to another, which are not well understood and are poorly mimicked by current parametric models (Djebbar and Narbaitz 1995; Bravo et al. 1992).

Recent developments in statistical theory have provided a new modeling approach, the nonparametric regression, using nonparametric function estimation. The advantage of nonparametric regression, compared with parametric regression, is the avoidance of model form selection. This method has been successfully applied in other domains such as geology, hydrology, process control, and market forecasting (e.g., Wen and Kung 1993; French et al. 1992; Härdle 1989; Adamowski 1985).

The objective of this study is to develop a method to predict $K_L a$, which overcomes the shortcomings of existing approaches, by modeling a large new pilot-scale air stripping data base via a nonparametric estimation technique. The results of this new approach will be compared with the Onda model predictions.

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Parametric versus nonparametric approaches

Parametric models are the most commonly used way to describe treatment processes. They predict performance (dependent variables) as a mathematical function of a set of design variables (independent variables) and a set of constants (parameters), for example,

$$[1] \quad y = g(x_i) = \alpha x_1^\beta x_2^\gamma \dots$$

where y is the dependent variable being predicted; x_1 and x_2 are the independent variables; and α , β , and γ are the parameters. The parameters are usually determined by parameter estimation methods such as least squares, which have certain limitations and require large sets of accurate data to yield satisfactory results. For the optimal properties of the least squares estimates to be valid in the parametric approach, it is essential that the following assumptions hold: (i) the values of the operating variables are known exactly; (ii) the model form is known; (iii) the errors and the observed responses at each set of operating conditions have the same variance; (iv) the errors (and the observed values of the responses) are not correlated and thus are statistically independent; and (v) the errors are identically and normally distributed with zero mean and variance σ^2 . It is obvious that the above assumptions are rarely satisfied. A key assumption of parametric modeling is that the model form, i.e., a mathematical expression to describe g in [1], is known. However, this form is often unknown and always, to some extent, subjectively assumed (Adamowski 1985; Silverman 1986). Once regressed, these models can be readily applied using a simple calculator. It is also important to add that the smoothing process in parametric regression considers the entire data, which makes it vulnerable to deviations due to outliers. An alternative method that overcomes some of the difficulties encountered with the parametric regression approach is nonparametric regression.

Nonparametric regression involves nonparametric density estimation. Nonparametric density estimation was first proposed by Fix and Hodges (1951) as a way of freeing discriminate analysis from rigid distributional assumptions, such as those of the least squares method. The main advantage of these techniques is the avoidance of model form selection. Indeed, in nonparametric estimation, there is no need to assume a relationship of prespecified form, since a relationship of possibly complicated or unorthodox shape is generated by the data points themselves. Although it will be assumed that the distribution has a probability density f , the data will be allowed to "speak for themselves" in determining the estimate of f , more than would be the case if f was constrained to fall in a given parametric family. The most popular and commonly used nonparametric method is the Kernel function technique (Härdle 1989). The Kernel function is an assumed probability distribution function (pdf) defined by its shape, such as the normal pdf or the rectangular pdf, and by its window width. The window widths are a range of values of the independent variables that define the narrow regions over which the smoothing is conducted. This means that the smoothing is local. This is a more reasonable approach than parametric methods where fitting involves the entire data set, even though it may have widely different

behavior over different regions. To model this type of behavior, Bravo et al. (1992) even suggested that the parameters of existing correlations need to be adjusted from one operating region to another. Thus, nonparametric techniques appear to be well suited for the analysis of air stripping $K_L a$ data.

Similar to parametric regression, nonparametric regression suffers from a drawback when used for extrapolation. By its nature, nonparametric methods do not necessarily yield accurate predictions beyond the values of the observed data (Adamowski and Feluch 1990). However, in many engineering applications, extrapolation is much less of concern because experiments are usually designed to cover application ranges.

Onda model

All existing mass transfer prediction models are parametric. These models have been discussed in Djebbar and Narbaiz (1995), Au-Yeung and Ponter (1983), Staudinger et al. (1990), etc. As indicated earlier, the Onda model (Onda et al. 1968) is considered to be the best correlation. The Onda model consists of three separate equations for the calculation of the individual liquid and gas phase mass transfer coefficients, k_L and k_G , as well as the wetted specific interfacial surface area for mass transfer, a_w . These equations are

$$[2] \quad k_L = 0.0051(L_T/a_w \mu_L)^{2/3} (\mu_L/\rho_L D_L)^{-1/2} (a_t d_p)^{0.4} \times (\rho_L/\mu_L g)^{-1/3}$$

$$[3] \quad k_G = c a_t D_G (G/a_w \mu_G)^{0.7} (\mu_G/\rho_G D_G)^{1/3} (a_t d_p)^{-2}$$

$$[4] \quad a_w = a_t \{1 - \exp[-1.45(\sigma_C/\sigma_L)^{0.75} (\text{Re}_L)^{0.1} (\text{Fr}_L)^{-0.05} \times (\text{We}_L)^{0.2}]\}$$

in which k_L is the chemical-specific liquid phase mass transfer coefficient (L/T); k_G is the chemical-specific gas phase mass transfer coefficient (L/T); a_w is the wetted specific surface area of the packing (L²/L³); a_t is the total specific surface area of packing (L²/L³); L_T is the liquid mass flux (M/L²T); G is the gas mass flux (M/L²T); ρ_L is the density of the liquid (M/L³); ρ_G is the density of the gas (M/L³); D_L is the liquid diffusion coefficient (L²/T); D_G is the gas diffusion coefficient (L²/T); d_p is the nominal packing diameter (L); g is the gravitational constant (L/T²); c is a constant, $c = 2$ if $d_p < 15$ mm, otherwise $c = 5.23$; σ_C is the surface tension of packing material (M/T²); σ_L is the surface tension of liquid (M/T²); $\text{Re}_L = L_T/a_w \mu_L$ is the liquid phase Reynolds number (dimensionless); $\text{Fr}_L = L_T^2/a_w \rho_L^2 g$ is the liquid phase Froude number (dimensionless); $\text{We}_L = L_T^2/a_w \rho_L \sigma_L$ is the liquid phase Weber number (dimensionless); μ_L is the liquid viscosity (M/LT); and μ_G is the gas viscosity (M/LT). M , L , and T refer to mass, length, and time units, respectively.

The two-phase resistance theory postulates that the total resistance to interfacial mass transfer is equal to the sum of the individual liquid phase and gas phase resistances, therefore

$$[5] \quad \frac{1}{K_L a} = \frac{1}{k_L a} + \frac{1}{H_c k_G a}$$

where $K_1 a$ is the overall (liquid phase based) mass transfer coefficient; H_c is the Henry's constant expressed as the ratio of the mass concentration in the gas phase to that in the liquid phase; and $a = a_w$ in [4].

Nonparametric kernel regression approach

The value of a dependent variable y at a given value of the independent variable x can be estimated through a weighted average around x , that is,

$$[6] \quad E(y|x) = m(x) = \frac{1}{k} \sum_{i=1}^k w_i(x) y_i$$

where $m(x)$ is the expected value of the dependent variable y at x ; k is the number of neighboring observations; y_i is the observation at x_i ; and w_i is weight (Fig. 1). The basic idea of the local average $m(x)$ is equivalent to the procedure of finding a local weighted least squares estimate (Härdle 1989):

$$[7] \quad \min_{\xi} \left\{ \frac{1}{k} \sum_{i=1}^k w_i(x) (y_i - \xi)^2 \right\} = \frac{1}{k} \sum_{i=1}^k w_i(x) (y_i - m(x))^2$$

As such, this estimate ($m(x)$) takes advantage of the fact that more information about $m(x)$ is contained in the surrounding of x rather than in points far away from x . Therefore more weight is given to the information contained in the neighborhood of x and less weight is given to the information contained in points far from x . In parametric estimation, equal weight is given to the information in all points, even though the process behavior within the neighborhood of x is likely to be different from the process behavior in points far from x .

In nonparametric regression, the value of the predicted variable $m(x)$, which is a function of the independent variables, x , can be established as the ratio of two probability density functions (Härdle 1989):

$$[8] \quad m(x) = E(y|X = x) = \frac{\int y f(x, y) dy}{f_x(x)}$$

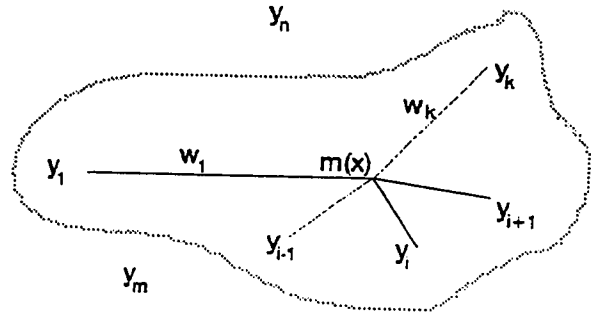
where $f(x, y)$ is the joint density function of x and y ; $f_x(x)$ is the marginal density function of x ; and $E(y|X = x)$ is the optimal estimate from regressing y on x . By analogy to [6] and [7], the weight is approximated by $w(x) = f(x, y)/f_x(x)$. The probability distribution functions, $f(x, y)$ and $f_x(x)$, can be estimated with nonparametric frequency techniques (Muller 1988; Rao 1983) using the kernel function. For the multivariate function ($f(x) = f(x_1, x_2, \dots, x_p)$), in the discrete form where the same type of distribution (i.e., the kernel) is assumed for all of the variables, the estimates $\hat{f}_x(x)$ and $\hat{f}(x, y)$ of $f_x(x)$ and $f(x, y)$ respectively are given by

$$[9] \quad \hat{f}_x(x) = \frac{1}{n} \sum_{i=1}^n \left[\prod_{o=1}^p \frac{1}{h_o} K\left(\frac{x_o - x_{oi}}{h_o}\right) \right]$$

$$[10] \quad \hat{f}(x, y) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h_y} K\left(\frac{y - y_i}{h_y}\right) \left[\prod_{o=1}^p \frac{1}{h_o} K\left(\frac{x_o - x_{oi}}{h_o}\right) \right]$$

In these equations, i and o are the data and the variable counters going up to n and p , respectively; h is the window width that defines the neighborhood, also called the smoothing

Fig. 1. Weighted average estimation of a dependent variable, y , at x .



parameter; and $K(t)$ is the kernel function. A fixed window width is used for each variable. However, h changes from one variable to another. According to Härdle (1989), the kernel $K(t)$ must satisfy the following conditions:

$$\int K(t) dt = 1$$

$$[11] \quad \int t K(t) dt = 0$$

$$\int t^2 K(t) dt = c \neq 0$$

where c is the kernel variance. Incorporating [9] and [10] into [8], the optimal estimate from a regression of y on X is given by (Muller 1988)

$$[12] \quad E(y|X = x) = \frac{\sum_{i=1}^n y_i \prod_{o=1}^p \frac{1}{h_o} K\left(\frac{x_o - x_{oi}}{h_o}\right)}{\sum_{i=1}^n \prod_{o=1}^p \frac{1}{h_o} K\left(\frac{x_o - x_{oi}}{h_o}\right)}$$

The goodness-of-fit of the nonparametric regression curve is usually measured by the mean integrated squares error, MISE, defined by the following equation (Härdle 1989):

$$[13] \quad \text{MISE}(\hat{f}) = E \int [\hat{f}(x) - f(x)]^2 dx = \int [E\hat{f}(x) - f(x)]^2 dx + \int \text{Var} \hat{f}(x) dx$$

where the integrand in the first integral corresponds to squared bias, and that in the second integral is the variance at x . Härdle (1989) found that the squared bias and the variance are related to h as follows:

$$[14] \quad \begin{aligned} \text{squared bias} &\propto \text{function}(h^4) \\ \text{variance at } x &\propto \text{function}\left(\frac{1}{h}\right) \end{aligned}$$

Hence, if we attempt to eliminate the bias by using a very small value of h , the integrated variance will become large and vice versa. Also, if h is chosen too large, the bimodal nature of the distribution will be obscured; whereas if h is chosen too small, the spurious fine structure of the estimated curve becomes visible. As the window width h decreases, the estimated curve tends to follow the developmental data points rather than to estimate the real function f . At this point the

solution is rather a "memorization" of the developmental data set. Whatever method of density estimation is being used for the kernel (i.e., normal, rectangular, etc.), the choice of the smoothing parameter implies a trade-off between random error and systematic error. The spread of the kernel function, defined by the smoothing parameter h , must be calibrated based on the entire dataset. Silverman (1986) showed on the basis of MISE that changing the kernel function has very little impact, and it is only the window width, h , that will determine the quality of the fit. For the purpose of this study, the normal probability distribution function is chosen as the kernel function, i.e.,

$$[15] \quad K(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

This function is unbounded and has a tail which does not die off quickly. Bounded kernels (e.g., rectangular) have a bounded extrapolation range. Unbounded kernels can somewhat improve the extrapolation (Adamowski and Feluch 1991). Several procedures can be used to determine the optimal window widths, h , that minimize the MISE. According to Scott and Terrel (1987), the least squares cross validation technique gives consistent and asymptotically optimal density estimates. Because the MISE is a function of the unknown function f ([13]), Rudemo (1982) showed that minimizing MISE parallels minimizing the following expression:

$$[16a] \quad S = \text{MISE} - \int_{-\infty}^{+\infty} f^2(x) dx$$

$$= \int f^2(x) dx - \frac{2}{n(n-1)} \sum_{i,j=1}^n \prod_{o=1}^p \frac{1}{h_o} K\left(\frac{X_o^i - X_o^j}{h}\right)$$

If the normal density is used for the kernel, the expression of S becomes (Adamowski and Feluch 1991):

$$[16b] \quad S = \frac{1}{np^{2/2} \prod_{o=1}^p h_o} \left\{ 1 + \sum_{i,j=1}^n \prod_{o=1}^p \left[\frac{2}{n} \exp\left(-\frac{\sum_{o=1}^p \left(\frac{X_o^i - X_o^j}{h}\right)^2}{4}\right) - \frac{2^{2+\frac{p}{2}}}{n-1} \exp\left(-\frac{\sum_{o=1}^p \left(\frac{X_o^i - X_o^j}{h}\right)^2}{4}\right) \right] \right\}$$

The minimum value of S is obtained by equating to zero the derivative of S with respect to h_1 , that is,

$$[17] \quad \frac{\partial S}{\partial h_o} = -\frac{n}{2} + \frac{1}{2} \sum_{i,j=1}^n \prod_{o=1}^p \exp\left(-\frac{1}{4} \left(\frac{X_o^i - X_o^j}{h_o}\right)^2\right) \times \left[\left(1 - \frac{4n}{n-1} 2^{\frac{p}{2}}\right) \exp\left(-\frac{1}{4} \left(\frac{X_o^i - X_o^j}{h_o}\right)^2\right) \times \left(\frac{X_o^i - X_o^j}{h_o} - 1\right) \left(\frac{X_o^i - X_o^j}{h_o} + 1\right) - 1 \right] = 0$$

For the p independent variables, there is a set of p nonlinear equations analogous to [17]. These equations are solved for

Fig. 2. Definition of tower parameters used in the analysis.

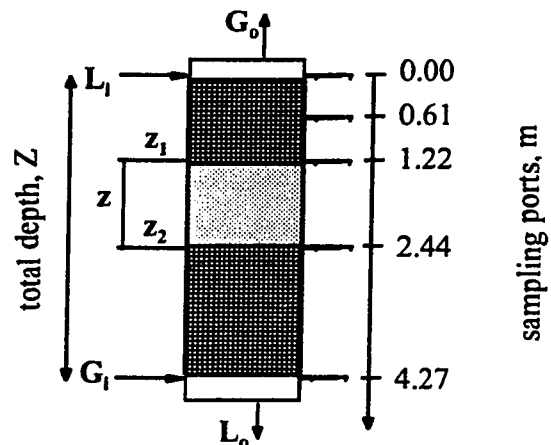


Table 1. Characteristics of the packing material found in the data base of Narbaitz et al. (1990).

Packing name	Company	Diameter (cm (in.))	Surface area (m ² /m ³)
Cascade Miniring #2	Glitsch Inc.	7.62 (3)	150.86
Flexiring #2	Koch	5.08 (2)	114.78
Flexisaddle #3	Koch	7.62 (3)	88.55
Tripack #1	Jeager Inc.	5.08 (2)	157.42
Nor-Pac #3	NSW	3.80 (1.5)	100.03
Nor-Pac #4	NSW	5.08 (2)	145.00
Snowflakes	Glitsch Inc.	9.40 (3.7)	91.83

the optimal values of h by the iterative cross validation technique (Rudemo 1982).

Description of the data base

Experimental data in the public domain are abundant; however, acceptable quality data that are representative of real world applications are not. A new data base has been developed by Narbaitz et al. (1990) in a large pilot-scale study using several modern large diameter packings and numerous full-scale operating conditions. A schematic representation of the air stripping tower is shown in Fig. 2. It consists of a 0.76 m (30 in.) diameter tower, with a total height of 8.84 m (29 ft) and filled with 4.57 m (15 ft) of packing. This tower can treat up to 760 L/min (200 gpm). It has five sampling ports within the packing located at 0.0, 0.61, 1.22, 2.44, and 4.27 m (0, 2, 4, 8, and 14 ft) from the top of the packed zone, respectively. To break any wall flow, the column is equipped at 1.22 m (4 ft) intervals with aluminum redistributor rings that extend 7.62 cm (3 in.) inwards from the column wall. The characteristics of the packings tested are summarized in Table 1. The VOCs were studied in three multicomponent mixtures (Table 2) consisting of approximately 100 µg/L of each VOC. At these low solute concentrations, the Henry's law constant is not affected by the presence of other compounds, as reported by Munz and Roberts (1987) and Mackay and Shiu (1981). Table 2 lists the Henry's law constants and the dif-

Table 2. Characteristics of the chemical compounds found in the data base of Narbaitz et al. (1990).

Group	Compound name	Formula	Diffusion (m ² /s)		<i>H</i> (20°C) (dimensionless)
			Gas (× 10 ⁶)	Water (× 10 ¹⁰)	
GI	Chloroform	CHCl ₃	9.23	9.18	0.117
	1,1,1-trichloroethane	C ₂ H ₃ Cl ₃	8.13	8.28	0.561
	Carbon tetrachloride	CCl ₄	8.18	8.22	0.986
	Trichloroethylene	C ₂ HCl ₃	8.45	8.46	0.302
	Tetrachloroethylene	C ₂ Cl ₄	7.61	7.59	0.557
GII	Chloroform	CHCl ₃	9.23	9.18	0.117
	Bromodichloromethane	CHCl ₂ Br	9.09	8.72	0.095
	Chlorodibromomethane	CHBr ₂ Cl	8.96	8.37	0.036
	Bromoform	CHBr ₃	8.83	8.08	0.028
GIII	Toluene	C ₆ H ₅ CH ₃	7.98	8.31	0.190
	Chlorobenzene	C ₆ H ₅ Cl	7.48	7.70	0.160
	M-xylene	C ₈ H ₁₀	7.21	7.52	0.450
	M-dichlorobenzene	C ₆ H ₄ Cl ₂	7.29	7.24	0.150

fusion coefficients of the VOCs considered, as reported by Gossett (1987) and Haarhoff and Cleasby (1990). The operating ranges of liquid flow, air to water ratio, and temperature are presented in Table 3.

The stripping factor *R* (dimensionless) is given by

$$[18] \quad R = \frac{HG}{P_t L_f}$$

where *H* is the Henry's law coefficient on a volume to volume basis (L/atm), and *P_t* is the total operating pressure (atm). In these experiments the minimum stripping factor was 3, well above the critical value of 1. This is the lowest value of *R* for which complete VOC removal is possible, as it is not limited by equilibrium (Kavanaugh and Trussell 1980).

More details about this data base can be found in Narbaitz et al. (1990). The overall experimental *K_La* values were obtained based on the values of the concentration in the five sampling points. These concentrations are strictly within the packing media, so they are free of end effects. Thus, the Narbaitz et al. data base has a particular advantage over the previous ones, in that the data are used directly in the analysis without correcting for end effects. The experimental *K_La* is calculated by the following equation (Djebbar and Narbaitz 1995):

$$[19] \quad K_L a = \left(\frac{L_f}{z \rho_L} \right) \left[\frac{R}{R-1} \ln \frac{c_1(1-1/R) + c_0/R}{c_2(1-1/R) + c_0/R} \right]$$

where *c₀* is the liquid effluent VOC concentration at depth *Z*, the bottom of the packing media (Fig. 1) (M/L³); *c₁* and *c₂* are the VOC concentrations in the liquid at the depths *z₁* and *z₂*, respectively (M/L³); and *z* = *z₂* - *z₁* (Fig. 1).

Method of analysis

A FORTRAN program was developed to conduct the nonparametric regression. Each packing data were divided randomly into two groups of two thirds and one third each. Then, the two-third and the one-third groups of all packings are merged

Table 3. Operating ranges of liquid flow, air to water ratio, and water temperature.

Variable	Operating range
Liquid flow, kg/(m ² ·s)	5.6–41.0
Air to water ratio	25–100
Water temperature, °C	23–28

into two large separate groups. One group containing two thirds of the total 538 data points was used to determine the optimum values of the smoothing factors by the cross validation technique (Rudemo 1982; Adamowski and Feluch 1991). As in nonlinear parametric regression, wrong initial guesses, local minima, and nonconvergence can be encountered. Remedial actions are similar to those employed for nonlinear parametric regression, such as changing the initial guesses. It is to be noted that with a 486, 33-MHz IBM compatible PC, each run of the development stage took on average 24 h. However, once the optimum smoothing variables were obtained, the predictions were obtained in less than 6 s.

The remaining one third of the data were used to validate the proposed prediction tool and to capture it with the Onda model predictions. Some of these data were outside the ranges of the training data. The evaluation of the Onda correlation was conducted using basic statistical tools. The absolute average error, AAE, is given by

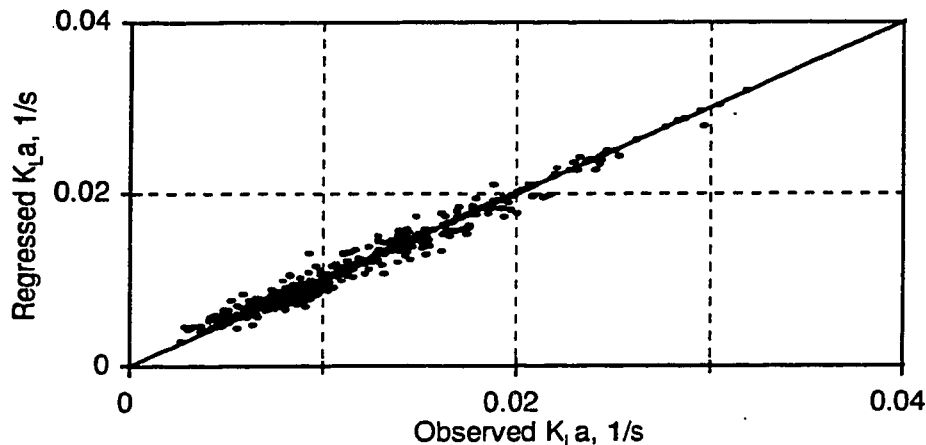
$$[20] \quad AAE = \frac{1}{n} \sum_{i=1}^n \frac{|(K_L a)_{exp} - (K_L a)_{pre}|}{(K_L a)_{exp}}$$

and the average algebraic error, AGE, is given by

$$[21] \quad AGE = \frac{1}{n} \sum_{i=1}^n \frac{(K_L a)_{exp} - (K_L a)_{pre}}{(K_L a)_{exp}}$$

where *n* is the number of data points; and (*K_La*)_{exp} and (*K_La*)_{pre} are the experimental and the predicted mass trans-

Fig. 3. NKR simulations of $K_L a$ versus observed $K_L a$ for the data used in the model development.



fer coefficients, respectively. AAE is a measure of average absolute deviation, and AGE is a measure of the overall overestimation or underestimation.

Results and discussion

Djebbar and Narbaitz (1995) enumerated the important variables in air stripping. They include liquid and gas flows, Henry's law constant, packing diameter, packing surface area, VOC diffusivities, physicochemical characteristics of the fluids, etc. Silverman (1986) has shown that the required sample size, for a given MISE, increases substantially as the number of independent variables increases. For the number of data points available for the development stage (two thirds of the Narbaitz et al. data base), Silverman suggests that only four variables can be used. The four variables selected were liquid and gas flow rates, packing surface area, and Henry's law constant. They were chosen because they are important and they showed the widest range of values within the data base.

Results of the developmental stage are plotted in Fig. 3 as the nonparametric kernel regression (NKR)-simulated $K_L a$ versus the observed $K_L a$. The diagonal line indicates the situation where the simulations are perfect and the magnitude of the deviations from this line is a direct indication of the quality of the simulations. This figure shows a high correlation between the observed and simulated $K_L a$ values. The average error (AAE) is 5.9%. This result is superior to previous parametric correlations at the developmental stage. Even though the Onda model involves 10 variables, it resulted in a 20% deviation between predicted and experimental data for its own developmental data set. The experimental error reported in the literature is expected to be between 8% and 12% (Lenzo et al. 1990). The lower value of deviation obtained with the nonparametric regression may be due to "memorization" of the data by the NKR method. As explained earlier, memorization occurs when the window width is very small. However, the extensive precautions taken in conducting these experiments may also explain this small average deviation. Confidence in the NKR solution, however, is gained only by testing its ability to predict data

that are not used in the solution development.

Results of the validation stage using the remaining one third of the data are plotted as the predicted $K_L a$ versus the observed $K_L a$ for the NKR method and the Onda model in Figs. 4 and 5, respectively. Visual inspection of these figures shows a larger spread in the Onda predictions compared with the NKR predictions. Also, most of the data in the Onda predictions are overestimated, and the NKR predictions are more or less evenly distributed around the diagonal line. The average error was 14.9% and 31.3% for the NKR and Onda predictions, respectively (Fig. 6). This represents a 50% improvement compared to the Onda correlation. The Onda model overestimated the observed $K_L a$ in 84% of the data by an average error of 33.3%, whereas just 32% of the data are overestimated by the nonparametric method and the average overestimation is only 13%. Figures 7, 8, and 9 show the variation of the error in both the parametric and Onda predictions as a function of three variables: packing diameter, liquid flow, and packing type, respectively. No significant trends are detectable in the NKR results and the simulations are consistent in Figs. 8 and 9. In Fig. 9, however, the Onda predictions had a lower average error than the NKR predictions for the 50.8 mm (2 in.) Flexirings. This may be due to the geometry of this packing which resembles more those used to calibrate the Onda model. The only type of packing used by both studies are saddles; however, the saddles used by Narbaitz et al. (1990) were much larger than those used by Onda and coworkers. The poor Onda predictions for this type of packing are probably due to the size difference.

The Onda predictions tend to be functions of the packing diameter, as found by Djebbar and Narbaitz (1995). The NKR predictions in Fig. 7 seem to show a slight trend with respect to the packing diameter. This may be because the packing surface area does not completely characterize the packing geometries. Therefore including an additional packing characterizing variable, such as the packing diameter, is a topic to be further investigated. The reliability of the NKR techniques is sensitive to the number of data points and the number of independent variables considered (Silverman 1986). As the number of points within this data base was less than that recommended for NKR applications with five independ-

Fig. 4. NKR predicted $K_L a$ versus observed $K_L a$ for the validation data.

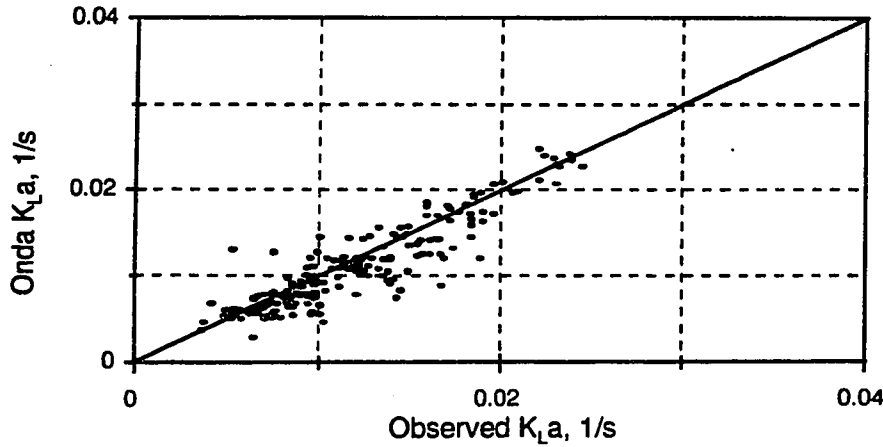


Fig. 5. Onda $K_L a$ predictions versus observed $K_L a$ for the validation data.

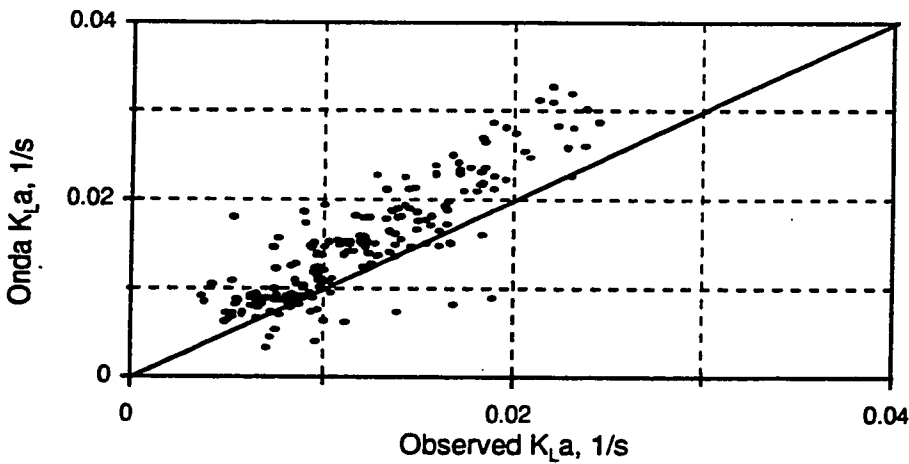
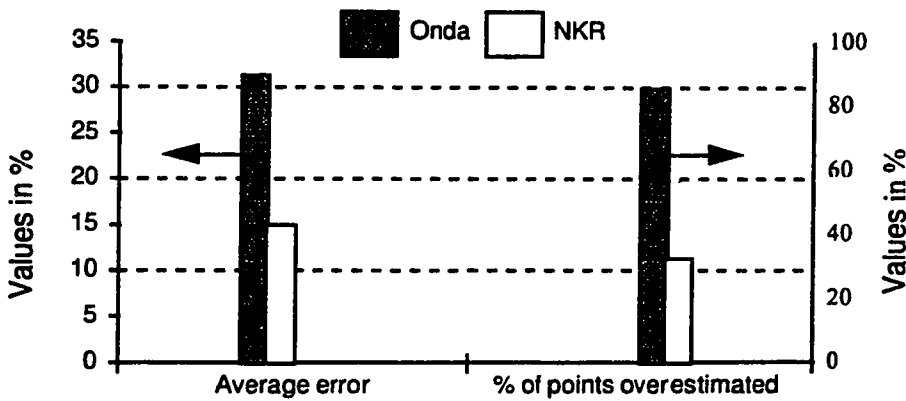


Fig. 6. Comparison between the Onda correlation and the NKR for the validation data.



ent variables, the NKR method was not applied with packing diameter as a fifth variable. An expanded data base is being assembled to further assess this.

It is important to keep in mind the limitations of this study. This study is based on a single source of data (Narbaitz et al.

1990). In addition, the water temperatures only range from 23°C to 28°C. This is important because the Henry's law constant, which is critical, is a function of water temperature. Air temperature varied over a wider range, but Dyksen et al. (1982) showed that it does not have a significant impact

Fig. 7. Average error in the NKR and the Onda predictions versus packing diameter, for the validation data.

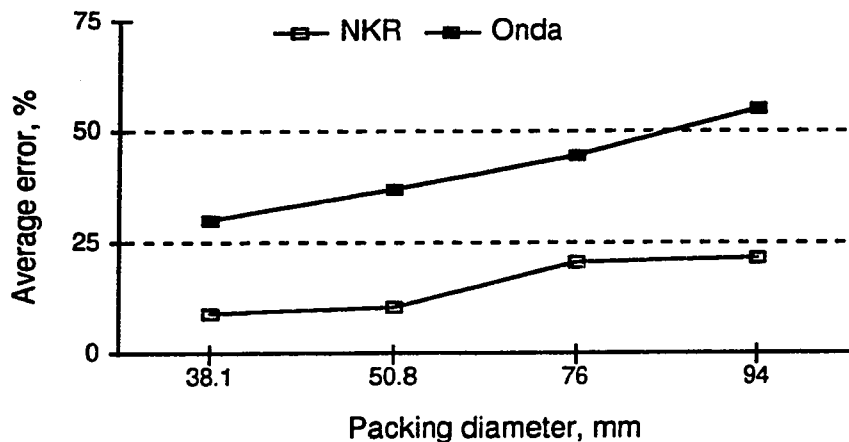


Fig. 8. Average error in the NKR and the Onda predictions versus liquid flow rate, for the validation data.

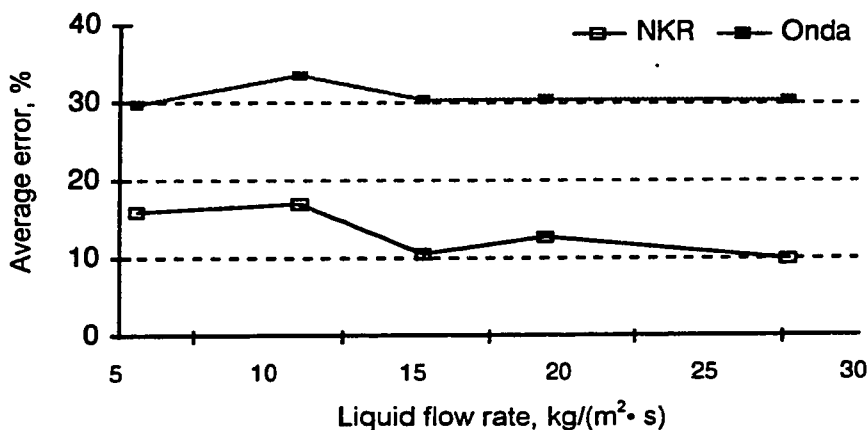


Fig. 9. Average error in the NKR and the Onda predictions for several packing types, for the validation data.

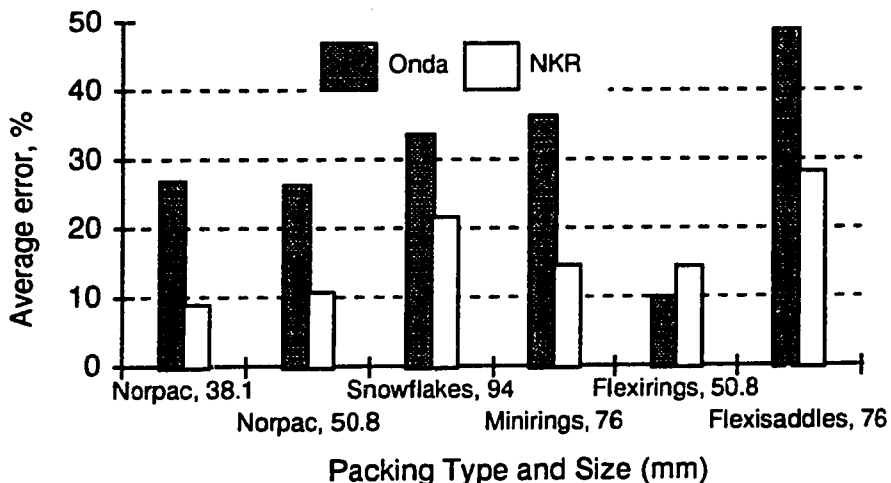
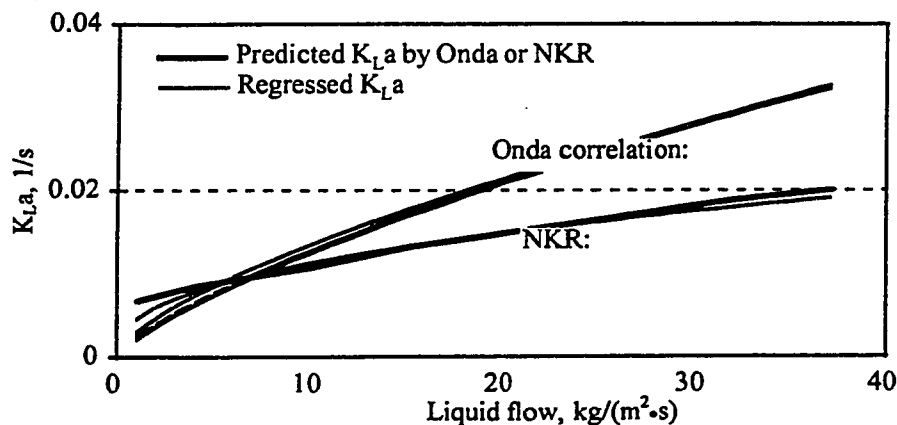


Fig. 10. Regression equations of the Onda and NKR predicted $K_L a$ as a function of the liquid flow rate.



on $K_L a$ for conventional VOC stripping operations.

As indicated earlier, the NKR approach does not result in a simple equation similar to parametric models, and the solution procedure of NKR methods consists of complicated calculations that only a computer program can carry out efficiently. A copy of the program is available from the authors. This program is written in FORTRAN, and it includes the values of the smoothing parameters obtained in the development stage. These values are presented in Table 4.

A hypothetical set of conditions, shown in Table 5, was used to investigate the predictive abilities of the Onda correlation and of the NKR solution, and to compare the predictions to mass transfer theory for air stripping towers. The analysis consisted of assessing the impact on the predictions of varying liquid loading, and results are shown in Fig. 10. The points associated with the predicted lines were regressed using the expression $K_L a = \alpha L_f^\beta$, where L_f is the liquid loading and α and β are the regressed parameters. The value of β for the Onda simulation equals 2/3. Davidson's (1959) comparison of theory with experimental data indicates, however, that the liquid flow rate exponent, β , should be appreciably less than 2/3. Streamline theory (laminar flow conditions) in conjunction with the penetration model showed that the liquid phase $K_L a$ should be proportional to the liquid flow rate to the 1/3 power (Vivian and Peaceman 1956). However, experimental data obtained by Vivian and King (1964) and Vivian and Peaceman (1956) suggested that $K_L a$ should be proportional to the Reynolds number (and thus to L_f) to the power of approximately 0.4. The NKR solution yielded a β of 0.5, which is in closer agreement with the theory.

Conclusions

The NKR was used in order to improve the accuracy of mass transfer coefficient predictions in air stripping towers. As a first step, parameter optimization of the nonparametric model was performed using the least squares cross validation technique with a large set of new experimental data. Four key variables were used in the model development. They are packing surface area, Henry's constant, and liquid and gas

Table 4. Values of the smoothing factors developed based on the Narbaitz et al. (1990) data base.

$K_L a$	Packing surface area	Gas flow	Liquid flow	Henry's law constant
1.444	7.0816	0.0463	0.0493	0.0163

Table 5. Hypothetical conditions for the $K_L a$ determination using Onda and NKR methods in Fig. 10.

Packing surface area (m^2/m^3)	Packing diameter (cm (in.))	Gas flow ($kg/(m^2 \cdot s)$)	Liquid flow ($kg/(m^2 \cdot s)$)	Compound ($T = 20^\circ C$)
115	5.08 (2)	0.6	1-40	C_2Cl_4

flow rates. In the validation step, the NKR model had an average error of 14.9%, which represents 50% improvement over the Onda model predictions. An evaluation for a set of hypothetical conditions showed that the NKR predictions yielded a relationship between $K_L a$ and liquid loading that was in closer agreement with the theory.

Acknowledgment

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List of symbols

AAE	absolute average error
AGE	average algebraic error
a_t	total specific surface area of packing (L^2/L^3)
a_w	wetted specific surface area of the packing (L^2/L^3)
c_0	liquid effluent VOC concentration at depth Z (Fig. 2) (M/L^3)
c_1, c_2	VOC concentrations in the liquid at the depths z_1 and z_2 (M/L^3)
D_G	gas diffusion coefficient (L^2/T)
D_L	liquid diffusion coefficient (L^2/T)
d_p	nominal packing diameter (L)
$E(y X = x)$	optimal estimate from regressing y on x
$f_x(x)$	marginal density function of x
$f(x, y)$	joint density function of x and y
Fr_L	liquid phase Froude number ($= L_f^2 a_t / \rho_L^2 g$) (dimensionless)
g	gravitational constant (L/T^2)
G	gas mass flux (M/L^2T)
h	smoothing parameter
k	number of neighboring observations
k_G	chemical-specific gas phase mass transfer coefficient (L/T)
k_L	chemical-specific liquid phase mass transfer coefficient (L/T)
K_L	overall (liquid phase based) mass transfer coefficient (L/T)
$(K_L a)_{exp}$	experimental mass transfer coefficient
$(K_L a)_{pre}$	predicted mass transfer coefficient
$K(f)$	kernel function
L_f	liquid mass flux (M/L^2T)
MISE	mean integrated squares error
$m(x)$	expected value of the dependent variable y at x
n	number of data points
p	number of variables
P_t	total operating pressure

R	stripping factor (dimensionless)	z	$= z_2 - z_1$ (Fig. 2)
Re_L	liquid phase Reynolds number ($= L_t/a_t\mu_L$) (dimensionless)	α, β, γ	regression parameters
w_i	weight	ρ_L	density of the liquid (M/L ³)
We_L	liquid phase Weber number ($= L_t^2/a_t\rho_L\sigma_t$) (dimensionless)	ρ_G	density of the gas (M/L ³)
x, X, x_i	independent variables	σ_c	surface tension of packing material (M/L ²)
y	dependent variable	σ_L	surface tension of liquid (M/L ²)
		μ_L	liquid viscosity (M/LT)
		μ_G	gas viscosity (M/LT)

ENCYCLOPEDIA OF

ENVIRONMENTAL

ANALYSIS

— AND —

REMEDICATION

Robert A. Meyers

Editor

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Most VOCs are not removed by conventional water treatment operations. In the amendment to the SDWA in 1986, the U.S. EPA recognized air stripping as a best available technology for VOC removal. Aeration exploits the natural tendency of VOCs to volatilize from water into air by allowing intimate contact between these two phases. This contact can be accomplished in a variety of physical arrangements, including bubbling air through a pool of water, spraying water into a stream of air, whirling air and water together in a mechanical device, or in a tower filled with packing material. The key features for improved mass transfer in aeration systems are a high interfacial surface area between the two phases and a reasonable amount of turbulence to bring VOCs to the interface where the transfer occurs. The impact of these factors is maximized in an air stripping packed tower setting. In countercurrent towers (Fig. 1), the most common type of flow arrangement, water is distributed across the top of the packing material and allowed to trickle down the packing while clean air is blown from the bottom of the column. The VOCs are transferred to the air stream as the water flows down the column. Thus, the cleanest air contacts the cleanest water which allows VOC concentrations in the water to be reduced to very low levels. Compared to other aeration processes, countercurrent packed tower aeration has generally proven to be the best suited for treatment of drinking water due to its ability to achieve high removal efficiencies at a low cost (1,2). Furthermore, compared to other groundwater treatment technologies, air stripping is very attractive because of its low cost, ease of operation, and high efficiency especially for VOCs with low affinity for adsorption.

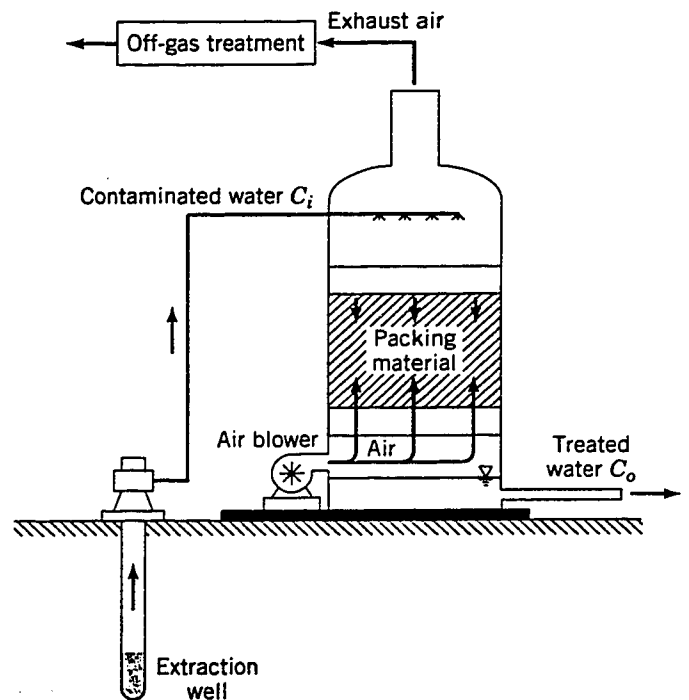


Figure 1. Countercurrent packed tower.

VOLATILE ORGANIC COMPOUNDS, AIR STRIPPING FROM CONTAMINATED GROUNDWATER

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MASS-TRANSFER CORRELATIONS

Groundwater contamination by trace levels of volatile organic compounds (VOCs) has emerged as a major water quality issue.

The most important parameter in the design of an air stripping tower is the volumetric-based overall liquid-phase mass-transfer coefficient $K_L a$. Engineers often calculate $K_L a$ using a mass-transfer correlation because they are easy to use and avoid costly pilot-scale tests. However, predictions via classical mass-transfer correlations have shown 30–50% deviations for full-scale air stripping towers (2–4). Thus more accurate methods for predicting $K_L a$ are necessary.

This article will review current methods used to predict the mass-transfer coefficient for countercurrent air stripping packed towers. It includes a short review of air stripping theory, a discussion of theoretical and empirical approaches for predicting $K_L a$, an assessment of accepted parametric correlations, and a description of novel nonparametric techniques (see AIR STRIPPING OF VOCS).

DESIGN OF AIR STRIPPING PACKED TOWERS

Theory and practice of air stripping in packed columns have been extensively researched in the past 50 years (5–9). The changes in concentration that occur as the liquid percolates down the column are controlled by (1) the resistances to mass transfer in both liquid and gas phases and (2) VOCs equilibrium partitioning coefficient between the two phases. At the low concentrations encountered in air stripping applications the partitioning coefficient is Henry's law constant, which is a function of the compound in question and of temperature. The importance or dominance of one mass-transfer resistance over the other is dependent on the volatility of the compound involved. The higher the Henry's law constant, the greater the magnitude of the liquid-phase resistance. For many VOCs, such as TCE and PCE, the mass-transfer resistance arises almost exclusively from the liquid-phase resistance. For lower volatility organics, such as bromoform, the gas-phase resistance is important, and for even less volatile compounds, the gas-phase resistance will be controlling. Regardless of the relative magnitude of the resistance by the individual phases, the concept of overall resistance is frequently used because it only requires concentration measurements in a single phase.

In designing a packed column for fixed operating conditions, the designer calculates the necessary packing depth, Z , that yields a prespecified removal. The most critical variable in this calculation is the overall liquid (or gas) phase mass-transfer coefficient, K_L (or K_G). The overall mass-transfer coefficient takes into account the resistance to mass transfer in both phases, which permits design calculations to be based just on the change in concentration in a single phase. As it is nearly impossible to measure the interfacial area, a , $K_L a$ (the product of K_L and a) is generally used instead of K_L . $K_L a$ is sometimes called the volumetrically based overall liquid-phase mass-transfer coefficient and its unit is 1/time. Air stripping packed towers are generally designed based on the change in liquid-phase concentrations and $K_L a$.

Using the Kavanaugh and Trussell (5) approach, the packing depth element z , ie, from depth z_1 to z_2 (Fig. 2), is given by:

$$z = \int_{z_1}^{z_2} dz = \frac{L_M}{K_L a \rho_L} \int_{c_1}^{c_2} \frac{dc}{c - c^*} \quad (1)$$

where K_L = overall liquid-phase mass-transfer coefficient (m/s); a = effective interfacial surface area (m^2/m^3); ρ_L = the liquid density (kg/m^3); c^* = VOC concentration in liquid phase that is in equilibrium with the VOC concentration in the gas

phase (kg/m^3); c_1 and c_2 = VOC concentrations in the liquid at depths z_1 and z_2 , respectively (kg/m^3); and L_M = the liquid mass flow rate per unit cross-sectional area ($\text{kg}/\text{m}^2\text{s}$).

Air stripping applications are generally analyzed using the transfer unit model (5,6). It assumes that (1) the mass-transfer coefficient is constant throughout the tower, (2) plug flow conditions prevail, (3) the volumetric air to water ratio, G/L , is constant, ie, the volume of the VOCs removed from the water is too small to affect the volume of the air or water flows, (4) Henry's law applies, and (5) the operation is isothermal. These assumptions are generally considered to be met in current air stripping applications. Using these assumptions, equation 1 can be solved analytically to yield:

$$z = \left[\frac{L_M}{K_L a \rho_L} \right] * \left[\frac{R}{R-1} \left\{ \frac{c_1(1-1/R) + c_0/R}{c_2(1+1/R) + c_0/R} \right\} \right] \\ = [\text{HTU}] * [\text{NTU}] \quad (2)$$

where $R = HG_M/P_i L_M$ = the stripping factor (dimensionless); HTU = the height of a transfer unit (m); NTU = the number of transfer units (dimensionless); c_0 = the liquid effluent VOCs concentration which corresponds to depth Z , the bottom of the packing media in Figure 2 (kg/m^3); H = the Henry's law coefficient on a volume to volume basis (1/atm); P_i = the total operating pressure (atm); and G_M = the gas mass flow rate per unit cross-sectional area ($\text{kg}/\text{m}^2\text{s}$). The value of NTU indicates the difficulty in removing the solute from the liquid phase, while HTU characterizes the mass-transfer efficiency from the liquid to the gas phase.

For the total packing height, Z , equation 2 becomes:

$$Z = \left[\frac{L_M}{K_L a \rho_L} \right] * \left[\frac{R}{R-1} \left\{ \frac{c_1/c_0(R-1) + 1}{R} \right\} \right] \\ = [\text{HTU}] * [\text{NTU}] \quad (3)$$

where c_1 is the liquid influent concentrations at $z = 0$ (kg/m^3). This is the most frequently used equation. The mass-transfer coefficient $K_L a$ can be obtained from either equations 2 or 3, as

$$K_L a = \frac{L_f}{z \rho_L} \text{NTU} \quad (4)$$

In a column with multiple sampling ports, when the section of the column being analyzed does not include the bottom of the column, the gas-phase concentration entering this section

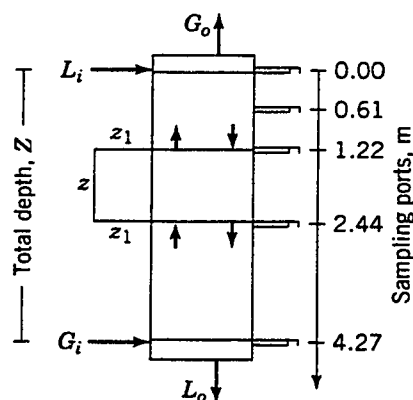


Figure 2. Definition of tower parameters used in analysis.

is not zero, and equation 2 must be used to calculate $K_L a$. Equation 3 is only valid for an inflow gas concentration equal to zero. Rearranging equation 4 gives:

$$NTU = K_L a \left\{ \frac{z \rho_L}{L_M} \right\} \quad (5)$$

During experimental studies including pilot-scale tests, the liquid-phase VOC concentrations are measured at several packing depths. Based on these concentrations, one NTU versus $\left\{ \frac{z \rho_L}{L_M} \right\}$, can be plotted and if mass transfer is described by equation 5, it should yield a straight line with a slope equal to $K_L a$.

The above model assumes that the mass-transfer coefficient is constant within the entire packing depth. However, this has been proven to be invalid, at least at the entrance of the column up to a certain depth. It has been shown that a natural frequency of distribution will develop in packed beds of sufficient height (4,10). This height is referred to as the bed depth required to reach the packing's natural distribution frequency. It has been shown that $K_L a$ is not constant within the column using a packing depth of 4.3 m (Fig. 3) (4). However, it is not yet clear if the observed variations (Fig. 3b) are related to the depth or to the concentration gradient change or to both. This contradicts the assumption of constant mass-transfer co-

efficient $K_L a$ when varying the packing depth. After the packing natural distribution frequency is reached, the flow pattern should be constant; therefore, the interfacial area should also be constant. Thus, the changes in $K_L a$ with depth must be related to the mass-transfer coefficient K_L , rather than to the effective surface area a .

It should also be noted that generally only an influent sample and an effluent sample are collected, so $K_L a$ is calculated based on only two points. As the influent and effluent samples are frequently used instead of samples from the top and the bottom of the packing, the resulting $K_L a$ also includes the additional removal that occurs between the distribution system and the top of the packing, and that occurring between the bottom of the packing and the reservoir below. These end effects normally result in an additional 10–20% VOC removal.

The stripping factor, R , is also important in sizing air stripping towers. A stripping factor of 1.0 is the minimum stripping factor that could, in theory, achieve complete removal of a specific VOC. However, a packed tower would need to be infinitely tall to achieve complete removal. Further, for a stripping factor of less than unity, the system is limited by equilibrium, and the fractional removal is asymptotic to the value of the stripping factor. Therefore, the values of the liquid and gas flow rates are generally selected to give stripping factor greater than three.

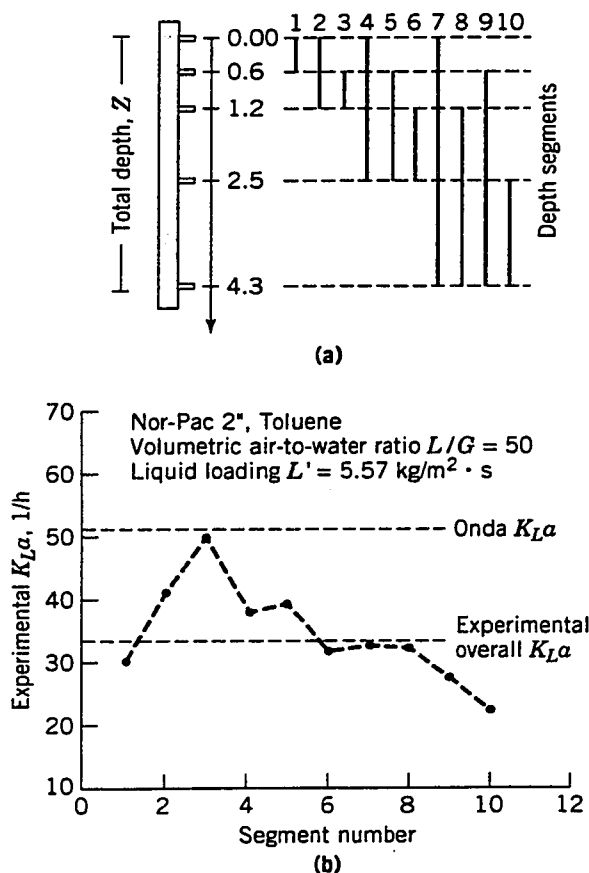


Figure 3. (a) Depth segments with decreasing mean concentration gradient (4); (b) $K_L a$ vs segment depth (initial liquid distribution has distribution capacity lower than natural distribution frequency of packing).

PREDICTION OF THE TRANSFER COEFFICIENT

There are two main types of approaches to predict the mass-transfer coefficient: theoretical and empirical. Theoretical and empirical approaches fall in the category of parametric approaches and are discussed in this section. Alternative approaches based on nonparametric methods, which have been developed recently, are discussed in a later section.

Theoretical Approach

Strict theoretical solutions of the transfer process in packed towers based on first principles are obtained for simple, particular cases of little practical value. This includes the theoretical solution for a laminar liquid film falling over a plate surface (6) and the three well-known models of Davidson (9). There are many theories which attempted to interpret or explain the operation of interface mass-transfer between liquid and gas phases. These are (1) film model (11), (2) penetration model (12), (3) surface renewal model (13), and (4) film-surface renewal model (14). A detailed description of these models is available (14). Based on simplifying assumptions, these models produced simple expressions for the mass-transfer coefficient. In commenting on these models, the following has been stated (6):

"They are all (ie, mass transfer models) speculations, and are continually being revised. It is helpful to keep in mind that transfer coefficients for mass transfer are expediently used to deal with situations which are not well understood.... The ultimate interpretation or explanation of the transfer coefficient will come only when the problems of fluid mechanics are solved, at which time, it will be possible to abandon the concept of transfer coefficient."

Existing mass-transfer correlations provide for individual calculation of mass-transfer coefficient in gas phase and in liquid phase separately. The two-film theory assumes that the overall resistance to mass transfer is equal to the sum of the

resistance in the gas film and the resistance in the liquid film. Therefore,

$$\frac{1}{K_L} = \frac{1}{k_L} + \frac{1}{Hk_G} \quad (6)$$

where K_L = the overall liquid-phase mass-transfer coefficient (m/h), k_L = the individual liquid mass-transfer phase coefficient (m/h), H = Henry's law constant (dimensionless), and k_G = the individual gas mass-transfer phase coefficient (m/h).

Equation 6 will hold true if the following conditions are satisfied (15):

- The interface is in equilibrium and H must be constant. If H is not constant, the value of the equilibrium line slope at the relevant concentration must be employed.
- There must be no significant resistance other than those represented by $1/k_L$ and $1/k_G$. The individual phase coefficients, k_L and k_G , are those measured in the absence or suppression of resistance to mass transfer in the other phase.
- The hydrodynamic conditions (interfacial area, etc) must be the same as those prevailing during the measurements of the individual phase resistances.
- The mass-transfer resistances of the two phases must not interact, ie, k_L and k_G are independent and the ratio k_L/k_G must be constant at all points of the interface.

The above-mentioned conditions are rarely met in common mass-transfer equipment, especially those which provide a wide distribution of liquid surface lifetimes such as randomly packed towers (15). In such equipment a wide variation in local values of k_L (and in k_G) exists. Continuous change in effective surface area is expected even at fixed flow rates. In another study, it was concluded that the average overall mass-transfer coefficient for an individual countercurrent surface exposure will be higher than the prediction of equation 6 (16). However, the net observed overall mass-transfer coefficients for packed towers appear to be less than the predictions generated by equation 6 (15). These conflicting results have been linked to the possibility that the gas-liquid interface may not be in equilibrium as assumed by equation 6 (17). In such a case, the transfer of mass encounters higher interfacial resistance than the prediction of equation 6. In conclusion, theory falls short of producing a satisfying prediction of mass-transfer coefficients in air stripping towers.

Empirical Approach

Most successful works in the area of air stripping mass-transfer coefficient predictions are based on empirically derived parametric correlations. There are three stages in developing a parametric correlation, including data collection, model development, and model evaluation. Each of these involves some difficulties. In data collection there are problems in measuring the components of the transfer process such as the interfacial surface area. Model evaluation has been limited by the scarcity of full-scale data with acceptable quality, and model development has been hampered by the absence of a proven theoretical relationship. This has resulted in a large number of different correlations obtained by regressing experimental data with assumed relationships.

Dimensional analysis simplifies modeling and experimental work by combining variables into a smaller number of dimensionless groups. Also, it guarantees the dimensional con-

sistency of the resulting relationship(s). The main feature of dimensional analysis is the assumption of certain aspects of similarity between model and prototype. There are many possible sets of independent dimensionless groups that can be used. It appears desirable to have groups which depend on kinetic viscosity ν , gravity g , surface tension σ , and mass-transfer coefficient k , ie, four dimensionless groups (18). The groups are usually chosen so that each of the variables μ , g , k , and σ would appear in one group only, ie,

$$N_1^k = f_1(N_2^g, N_3^\mu, N_4^\sigma) \quad (7)$$

where f_1 is the functional relationship that relates the four dimensionless numbers N_1^k , N_2^g , N_3^μ , N_4^σ , each of which depends on the specified variable. It has been indicated (6) that the transfer process in packed towers can be better described using a relationship that involves the three dimensionless numbers, ie,

$$Sh = f_2(Re, Sc) \quad (8)$$

where f_2 is the functional relationship that relates Sh to Re and Sc ; Sh = Sherwood number (k/Da); Re = Reynolds number = L (or G)/ $a\mu$; and Sc = Schmidt number = $\mu/\rho D$, where k = mass-transfer coefficient (m/s), D = molecular diffusivity of the contaminant (m^2/s), μ = dynamic viscosity ($kg/m\cdot s$), and ρ = density (kg/m^3) (6). The variables k , μ , ρ , and D pertain to either the liquid- (L) or gas- (G) phases. However, the form of the functional relationships, f_s in equations 7 and 8, are not provided because they are not known.

Most investigators regressed equations formed of dimensionless numbers. They developed empirical correlations based on the theory by raising some dimensionless numbers to specific exponents in accordance with simple theoretical models. For example, the penetration theory, which assumes laminar flow between surface renewals, predicts $k_L a$ to be proportional to the 1/3 power of the liquid flow rate, L , and the 1/2 power of the diffusion coefficient D (7,9). These findings lead one to assume that $k_L a$ correlations for packed tower absorption data should include Reynolds number to the 1/3 power and the Schmidt number to the 1/2 power. The validity of these results is directly dependent on the validity of the assumptions used in the development of these theories, namely the penetration model.

A functionality was established and accepted to be representative of the relationship between the variables that affect the transport process (19). This functionality has the following form for both liquid and gas phases,

$$Sh = c Re^\alpha Sc^\beta \quad (9)$$

where c , α , and β are parameters to be estimated. The relationship form presented by equation 9 has been widely utilized to obtain regression equations (20). Equation 9 is of the form of the Cobb-Douglas model (21):

$$Y = b_0 \prod X_i^{b_i} \quad (10)$$

where Φ represents the multiplication of all X_i terms, b_i = parameters to be estimated statistically to reflect reality, X_i = independent variables that affect the regressed quantity Y . The Cobb-Douglas model dominated the literature and practice until the early 1970s, when its deficiencies became obvious and practical alternatives became available through the development of high speed computers. The Cobb-Douglas model has several attractive features (21):

- It can, by a suitable choice of the values of the parameters b_i , represent a broad range of the important characteristics of the relationship sought.
- These parameters can be immediately interpreted in terms of the characteristics of the regressed quantity Y , which is a great pedagogical and practical advantage.
- The parameters b_i are easy to estimate statistically. This is because the multiplicative equation can be transformed into a linear function by expressing the variables in terms of their logarithms.

However, the model inherently implies that certain features of the relationship remain the same regardless of the values of the variables. This general remark is in disagreement with conclusions which showed that the nature (and exponents) of the mass-transfer correlations should change with the values of the variables (22). Furthermore, the parameters of the model (eg, c , α , and β of eq. 9) are generally obtained using least squares regression, which has certain limitations and requires large sets of accurate data to yield satisfactory results.

The lack of an accepted form of the functional relationship resulted in the almost exclusive use of the empirical approach as compared to a purely theoretical approach. In the empirical approach a form of the functional relationship f is assumed and its parameters are determined via a parametric regression method. Many different mathematical forms have been proposed in the literature (4,20,23).

A review of the literature showed that five main approaches are used to obtain experimental data and to develop a model.

1. The first approach uses packing with simple geometry where the interfacial surface area is supposed to be known such as for plates, cylinders and spheres (8,18,24,25). In this case, the mass-transfer coefficient k_L and/or k_G is determined by dividing the observed $k_L a$ or $k_G a$ value by the "known" interfacial area. The experimental data are then regressed.
2. The second approach assumes k_G to be substantially the same for the same operating conditions in vaporization and absorption (26–28). First $k_G a_v$ and $k_G a$ are determined for vaporization and absorption, respectively, for the same operating conditions. Data for the effective area for absorption, a , are then determined using the following equation:

$$\frac{\text{System specific during absorption}}{\text{System specific during vaporisation}} = \frac{k_G a}{k_G a_v} = \frac{a}{a_v}$$

where a_v = the dry surface area (m^2/m^3) and a = the effective surface area during absorption. The experimental data are then regressed

3. The third approach conducts experiments in which the resistance to mass transfer is located in one phase only. To obtain k_G or k_L the transfer is carried out using a pure solution in the liquid phase or gas phase, respectively; k_L has been determined by absorbing pure CO_2 into water (29). This offers zero resistance in the gaseous phase. Ammonia absorption experiments or measurements of the rate of evaporation of naphthalene packing into air have given $k_G a$ (26). In these

experiments the liquid phase presented no resistance to the transfer of mass. The obtained data are then regressed.

4. The fourth approach goes through the following steps (8,30):
 - k_G is obtained from the evaporation of naphthalene Raschig rings and Berl saddles.
 - The effective surface area is obtained by comparing the k_G values from the previous step with the $k_G a$ values on ammonia absorption where the resistance to mass transfer in the liquid phase is assumed to be negligible (31).
 - The values of k_L are calculated by dividing the measured $k_L a$ values by the effective area determined in the second step. The experimental data are then regressed.
5. A fifth approach uses a well-accepted correlation to determine one of the transfer components, ie, a , k_L , or k_G . For example, research has proceeded as follows (32):
 - The interfacial areas are assumed to follow the Onda correlation for the wetted surface area a_w (33).
 - k_L data are obtained by dividing measured $k_L a$ by the wetted areas, a_w , from the previous step.
 - k_G data are obtained by dividing the measured $k_G a$ by the wetted areas a_w from the first step. The experimental data are then regressed.

Tens of correlations have been developed during the last fifty years. Excellent reviews of some of these correlations are available (20,34). The most widely accepted models for VOC packed tower air stripping are described in detail below (26,30,35–39).

Sherwood and Holloway Model. Sherwood and Holloway (35) studied the desorption of O_2 , H_2 , and CO_2 from water into a countercurrent flow of air, in columns filled with a variety of packing materials, over ranges of water flow rates ranging from 0.27 to 43 $kg/m^2/s$ and gas flow rates ranging from 0.04 to 1.8 $kg/m^2/s$. The solutes were all gases, with Henry's law constants sufficiently large such that the liquid-phase resistance controlled; this was indeed confirmed by the absence of an effect of gas flow rate on the mass-transfer rate constant. The transfer rate constant was correlated as follow:

$$\frac{K_L a}{D_L} = 10.764 m \left(\frac{0.3048 L_M}{\mu_L} \right)^{1-n} \left(\frac{\mu_L}{\rho_L D_L} \right)^{0.5} \quad (11)$$

$K_L a$ = overall liquid-phase mass-transfer coefficient (1/h); L_M = liquid loading rate ($kg/m^2/h$); μ_L = viscosity of liquid ($kg/h/m$); ρ_L = density of liquid (kg/m^3); m, n = coefficients dependent on the packing material; D_L = solute liquid-phase molecular diffusion coefficient (m^2/h). Values of the empirically determined coefficients n and m are available for some of packings (Table 1) (6,7,35).

Shulman Model. This model estimates k_L , k_G , and a , separately (26,30,36). The following equations are used to calculate k_L and k_G :

$$\frac{k_L d_s}{D_L} = 25.1 (L_M d_s / \mu_L)^{0.45} (\mu_L / \rho_L / \rho_L D_L)^{0.5} \quad (12)$$

$$\frac{k_G d_s}{D_G} = 1.195 (1 - \epsilon)^{0.36} (G_M d_s / \mu_G)^{0.64} (\mu_G / \rho_G D_G)^{0.33} \quad (13)$$

where k_L = liquid-phase mass-transfer coefficients (m/h);

Table 1. Operated Empirical Constants for the Sherwood and Holloway Correlation

Packing Type	Size, in. (mm)	Empirical Constants		Compound Tested	Reference
		<i>m</i>	<i>n</i>		
Raschig rings (ceramic)	2.0 (50)	80	0.22	O ₂ , H ₂ , CO ₂	35
	1.5 (38)	90	0.22		
	1.0 (25)	100	0.22		
	0.5 (12.5)	280	0.35		
Berl saddles (ceramic)	1.5 (38)	160	0.28		
	1.0 (25)	170	0.28		
	0.5 (12.5)	150	0.28		
	1.0 (25)	12	0.25		
Saddles (plastic)	1.0 (25)	63	0.28	Chloroform	3
	1.0 (25)	27	0.22	THMs	6
	1.0 (25)	696	0.55	Chloroform	3
	1.0 (25)	972	0.68	Carbon tetrachloride, PCE, TCE, chloroform	3
Tri-Packs (plastic)	1.0 (25)	41	0.14	Bromoform	3
	2.0 (50)	43	0.16	1,1,1-Trichloroethane	3
	2.0 (50)	66	0.28	1,1-Dichloroethane Trichloroethylene	3 3

k_G = gas-phase mass-transfer coefficients (m/h); G_M = gas mass flux (kg/m²/h); μ_G = viscosity of gas (kg/h/m); ρ_G = density of gas (kg/m³); D_G = solute gas-phase molecular diffusion coefficient (m²/h); d_s = diameter of a sphere having the same surface area as a unit of packing (m); and ϵ = void fraction of the packing. The interfacial area is given by the following equation:

$$a_w = mG^m L'^p \quad (14)$$

where G' and L' are the liquid and gas loading rates in lb/h/ft². Values of m , n , and p for some packings (Table 2). The ranges of L_m and G_m used in the development of the Shulman correlation were 3.5–32 kg/m²/s and from 0.14–1.4 kg/m²/s, respectively.

Onda Model. The Onda correlation consists of three separate equations (37). They provide for independent calculation of the individual liquid- and gas-phase mass-transfer coefficients, k_L and k_G , as well as the wetted specific interfacial surface area for mass transfer, a_w :

$$k_L = 0.0051(L_M/a_w \mu_L)^{2/3} (\mu_L/\rho_L D_L)^{-1/2} (a_i d_p)^{0.4} (\rho_L/\mu_L g)^{-1/3} \quad (15)$$

$$k_G = c a_i D_G (G_M/a_w \mu_G)^{0.7} (\mu_G/\rho_G D_G)^{1/3} (a_i d_p)^{-2} \quad (16)$$

$$a_w = a_i \left\{ 1 - \exp \left[-1.45 (\sigma_c/\sigma_L)^{0.75} (Re_L)^{-0.1} \times (Fr_L)^{-0.05} (We_L)^{0.2} \right] \right\} \quad (17)$$

in which a_w = wetted surface area of the packing (m²/m³); a_i = total surface area of packing (m²/m³); d_p = nominal packing diameter (m); g = gravitational constant (m/h²); c = constant = 2 if $d_p < 15$ mm, otherwise $c = 5.23$; σ_c = surface tension of packing material (kg/m²); σ_L = surface tension of liquid (kg/m²); $Re_L = L_M/a_i \mu_L$ = liquid-phase Reynolds number (dimensionless); $Fr_L = L_M^2 a_i / \rho_L g$ = liquid-phase Froude number (dimensionless); $We_L = L_M^2 / a_i \rho_L \sigma_L$ = liquid-phase Weber number (dimensionless).

The original Onda work was based on 400 data points from engineered stripping absorption and evaporation systems

using liquid mass flow rates of $0.8 < L_M < 43$ kg/m²/s and gas mass flow rates of $0.014 < G_M < 1.7$ kg/m²/s. It consists mostly of data from laboratory experiments with primarily small packings. The largest packing were 2.54 cm (1 in.) in size, but the majority of the data points were for much smaller packing materials. A nice feature of this model is that it can be used directly, ie, it does not contain parameters that are dependent on the packing geometry. The value of such parameters for the Sherwood and Holloway and the Shulman models for a particular packing, especially for the newer types of packing, may not be available in the literature. In which case pilot-scale tests are required to calibrate these models. The Onda model avoids this need.

Evaluation of Existing Correlations

The literature shows that existing models generally yield satisfactory results for lab data. These data are primarily comprised of small size packings of traditional shapes (38,39). However, 30–50% deviations from predictions are often reported in full-scale applications (2–4). Current applications utilize modern packings that have different shapes and different hydraulic responses from those used to develop the above mass-transfer correlations. Also the modern packing in full-scale stripping applications are 2.54–15.24 cm (1–6 in.) in size and made of propylene, whereas the correlations were primarily based on much smaller ceramic packing materials. In addition, the above correlations were developed for solute concentrations encountered in chemical engineering applications, whereas groundwater air stripping involves solute concentrations that are generally several orders of magnitude smaller. Evaluations using large modern packings in full-scale air strippers have been rather limited and some are of questionable quality.

The lack of good predictive ability of existing correlations for full-scale applications is due to (1) the extrapolative nature of the predictions; (2) the limited operating conditions in the databases used to develop the correlations; (3) the

Table 2. Interfacial Areas for Shulman Correlation for $L' > 7500^a$

Packing	Size, in. (mm)	Range of L'	α	γ	γ
Raschig rings	0.5 (12.5)	500-1500	8200	$3.15(10^{-4})L' - 0.3$	-1.04
		1500-4500	9.32	$0.151(10^{-4})L' + 0.148$	-0.111
	1 (25)	500-1500	0.274	0	0.552
		1500-4500	463	$0.528(10^{-4})L' - 0.0793$	-0.47
	1.5 (38)	500-1500	1.32	$0.675(10^{-4})L' - 0.1013$	0.274
		1500-4500	4.85	$0.148(10^{-4})L' - 0.022$	0.140
	2 (50)	500-1500	0.401	0	0.481
		1500-4500	0.95	0	0.362
Berl saddles	0.5 (12.5)	500-1500	0.0336	0.0529	0.761
		1500-4500	2.54	0.0529	0.170
	1 (25)	500-1500	15.89	$0.686(10^{-4})L' - 0.1029$	0
		1500-4500	238	$0.420(10^{-4})L' - 0.0630$	-0.359
	1.5 (38) ^b	500-1500	0.613	-0.0508	0.455
		1500-4500	46.5	$0.325(10^{-4})L' - 0.0996$	0.1355

^a L' and G' are in lb/h/ft² (26,30,36).

^b For $G' < 800$ only.

limitations of parametric regression techniques used to generate these models; and (4) the changing nature of mass-transfer relationships from one set of operating conditions to another, that are not well understood and are poorly mimicked by current models (4,40). As correlations, the Onda, Schulman, and Sherwood and Holloway models are limited to the packing and ranges of the operating conditions within which they were either developed or verified. They are not necessarily reliable outside these ranges.

The potential applicability of the Shulman and the Sherwood and Holloway models is limited. For the Shulman correlation, values for the crucial effective interfacial area for mass transfer are available only for limited number of packing types. Various models have been evaluated with data for 0.0125 m ceramic Berl saddles. It has been noted that the Shulman model underpredicts low K_La values and overpredicts high values (38). For the Sherwood and Holloway correlation, parameter values for new packings are lacking. Its developmental database included ceramic Raschig rings and Berl saddles only. This model was developed based on the assumption that only the liquid-phase resistance controls the mass-transfer operation. It has been indicated that this correlation appears applicable only as a data-fitting relation for a given set of experimental test results (3). In an attempt to determine the value of m and n for other conditions of packings and compounds. A fairly wide variation in the constants has been found as a function of raw water source, packing type, and compound (41). The Sherwood and Holloway relationship would anticipate m and n to be a function of packing but not of compound or water source. It has been indicated that the Sherwood and Holloway correlation may give K_La estimates suitable for design purposes for highly volatile compounds under specific conditions with a stripping factor R of 10-15 (38).

The Onda model should not be used for stripping factors (R) below 1.0 because it produces unpredictable results (38). The Onda correlation systematically overestimates the mass-transfer coefficient K_La for packings having a diameter larger than 2.54 cm, which are typically used in full-scale applications. Most studies that used full-scale data with modern, large-size packings of more than 2.54 cm (2-4) concluded that the Onda correlation overestimates the overall volumetric

mass-transfer coefficient. The average error was found to be 40% and safety factors of 1.47 and 1.68 would be required to account for 68 and 90% of their evaluation data, respectively (4). For 81 of 85 full-scale systems reviewed, the Onda predictions overestimate the K_La with an average error of 35% (2). This error should be even larger because the experimental K_La values included end effects and the calculation of the error was based on the deviation relative to the Onda predictions rather than to the experimental values. In practice, these inaccuracies have been temporarily overcome by reducing the correlation predictions by a safety factor of 1.3 to 1.5. However, the correlations do not always overestimate K_La , and sometimes they overestimate K_La by a factor greater than 1.5.

Improvements to the Onda Model

Attempts have been made to improve the Onda correlation using large-scale data. Two of the main attempts are presented below.

Gossett Method. It has been asserted that gas-phase resistance was underestimated by the Onda correlation (38). In an effort to build on this hypothesis, a link of transfer rate prediction to relative gas-phase resistance values was sought using the following equation (42):

$$\%E = 100[(1 - a') - 1] + \%R_G[(1/b') - (1/a')] \quad (18)$$

in which $\%E$ = percentage difference between Onda-predicted K_La and measured K_La , a' and b' = modification factors for the Onda individual liquid-phase and gas-phase mass-transfer coefficients, respectively, and R_G = percent gas-phase control as predicted by the Onda correlations = $k_La/(H^*k_ga)$ (3). a' and b' are packing-dependent; they can be arrived at using equation 18 given supporting data (42). The adjustment values computed produced no improvement in the predictive capabilities of the Onda correlation for related data (3).

Djebbar and Narbaitz Method. The Onda correlation was found to overestimate K_La for larger packing diameters (2-4).

An equation was proposed to correct for the Onda prediction as a function of the packing diameter (4).

$$K_L\alpha' = \frac{K_L\alpha}{0.834 + 0.293 \ln(d)} \quad (19)$$

where d = the packing nominal diameter in cm; and $K_L\alpha$ and $K_L\alpha'$ = the Onda and the corrected Onda mass-transfer coefficient, respectively. This correction is applicable to packings larger than 2.54 cm in diameter. It is based on the Narbaitz (43) database, which has been developed in a large pilot-scale study using several modern large-diameter packings and numerous full-scale operating conditions. The minimum stripping factor in this database was 3, well above the critical value of 1. More details about this database are available (43). The experimental $K_L\alpha$ values were based on concentrations strictly within the packing media, so they are free of end effects. The result of applying this correction to experimental data from three different databases reduced the prediction errors from 35 to 17% (4).

NONPARAMETRIC METHODS

In the parametric approach, the performance of a process (the dependent variables) is predicted using a mathematical function of a set of design and operational variables (the independent variables) and a set of constants (parameters), for example,

$$y = g(x_i) = \alpha x_1^\beta x_2^\gamma \quad (20)$$

where y is the dependent variable being predicted; x_1 and x_2 are the independent variables; and α , β , and γ are the parameters. The parameters are usually determined by parameter estimation methods such as least squares regression.

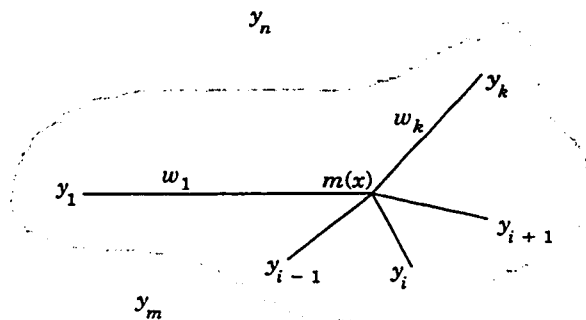
Nonparametric models are alternative methods that overcome some of the shortcomings of the parametric regression approach. The nonparametric approach frees the discriminate analysis from rigid distributional assumptions, like those of the least squares method. The main advantage of these techniques is the avoidance of model form selection. Indeed, in nonparametric estimation, there is no need to assume a relationship of prespecified form, since a relationship, which is possibly complicated or of unorthodox shape, is generated by the data points themselves. In recent years nonparametric methods have shown exceptional performance as regression tools, especially if used for pattern recognition and function estimation. They have been successfully applied in other domains such as geology, hydrology, process control, and in market forecasting (44-47).

Two nonparametric methods have recently been applied (48,49). These methods are the nonparametric kernel regression (NKR) and neural networks (NNS).

Nonparametric Kernel Regression

In nonparametric kernel regression, the value of a dependent variable y at a given value of the independent variable x can be estimated through a weighted average around x , that is:

$$E(K_L\alpha x) = m(x) = \frac{1}{k} \sum_{i=1}^k w_i(x)y_i \quad (21)$$



where $m(x)$ = the expected value of the independent variable y at x ; k = the number of neighboring observations; y_i = the observation at x_i ; and w_i = weight. The basic idea of the local average $m(x)$ is equivalent to the procedure of finding a local weighted least squares estimate (46). As such, this estimate $m(x)$ takes advantage of the fact that more information about $m(x)$ is contained in the surrounding of x rather than in points far away from x . Therefore more weight is given to the information contained in the neighborhood of x and less weight is given to the information contained in points far from x . In parametric estimation equal weight is given to the information in all points, even though the process behavior within the neighborhood of x is likely to be different from the process behavior in points far from x especially in nonlinear processes such as air stripping. The NKR method has been applied and the prediction improved by more than 50% compared to the Onda model using the Narbaitz database (Fig. 4) (4,43,49).

Neural Network Method

Neural networks have emerged as a powerful prediction tool. The neural network approach has been used to simulate $K_L\alpha$ (48). In recent years neural networks (NNs) have shown exceptional performance as regression tools, especially if used for pattern recognition and function estimation. The most important characteristic of NNs is that no assumption has to be made about the form of the functional relationship. Other important characteristics of NNs are their high nonlinearity, their ability to infer subtle, unknown relationships from data, and their capability to generalize, meaning they can respond correctly to patterns that are only broadly similar to the original train-

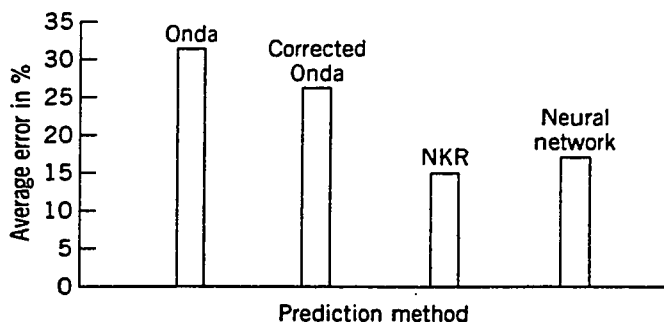
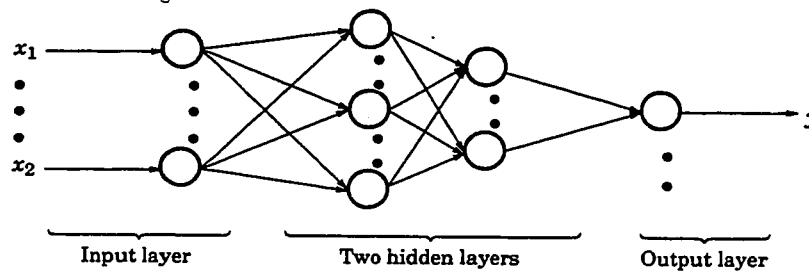


Figure 4. Comparison between the Onda correlation, corrected Onda, NKR, and NN (4).

ing patterns. NNs are inspired by the functioning mode of the animal brain in which a great number of neurons are interconnected by their synapses as shown below. By analogy the

neuron is defined as the basic unit of the network. This neuron can receive one or more inputs, calculate the weighted sum, and produce a unique output through the transfer function (4).



The K_La predictions by neural networks improved by more than 50% compared to the Onda correlation using the Narbaitz database (see Fig. 4). The neural network predictions were based on four variables only. They are liquid and gas flow rates, packing surface area, and Henry's law constant. Also note that the error for the modified Onda was larger than the 17% reported earlier because a somewhat different database was used in the evaluations in Figure 4. The NN predictions were comparable to those obtained by NKR, and research on the use of these techniques for the prediction of K_La is continuing.

CONCLUSIONS

Mass-transfer theory in countercurrent air stripping towers is complex and not well understood. Air stripping tower designers using existing correlation should be aware of the limitations the model being used. Traditional correlations greatly overestimate K_La for modern large-size packings used in current full-scale air stripping applications. The Onda model is still the best correlation for the prediction of K_La . However, a safety factor in the vicinity of 1.5 should be used. The corrected Onda correlation proposed by Djebbar and Narbaitz (4) is recommended when designing modern stripping towers, yet a safety factor of 1.3 is still necessary to ensure adequate designs.

New prediction tools based on nonparametric techniques are under development. They have shown promising results and may constitute an alternative to the shortcomings of the Onda correlation and parametric approach in general.

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IMPROVED ONDA CORRELATIONS FOR MASS TRANSFER IN PACKED TOWERS

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ABSTRACT

A comprehensive database for VOC stripping in packed towers was gathered from 15 field and pilot-scale studies. This database is used to develop a new correlation based on the Onda model. The development of this new correlation addressed the shortcomings of the Onda correlation which were identified in previous studies. The average error in the new correlation was less than 26 % for both the development and the validation data.

KEYWORDS

Volatile organic compounds, packed tower, air stripping, Onda correlation, random structured and packing.

INTRODUCTION

An estimate of the mass transfer coefficient, $K_L a$, is necessary for the designer to determine the dimensions of a packed tower to strip volatile organic compounds (VOCs) from contaminated ground water. This estimate can be obtained using a pilot scale study which is expensive. A common alternative approach is to use mass transfer correlations. Tens of correlations have been developed during the past fifty years (Au-Yeung and Ponter, 1982), however, only few of them have been tested for conditions that are of environmental concern.

Among existing models, there is agreement in the recent literature (Staudinger et al., 1990; Roberts et al., 1985 and Lamarche and Droste, 1989, Djebbar and Narbaitz, 1995) that the Onda model (1968) is the best $K_L a$ correlation for air stripping applications. The literature shows that this model yields satisfactory results for lab data, i.e., conditions that are similar to those under which this model has been developed. However, 30 to 50 percent deviations from predictions are often reported in full-scale applications (Lenzo et al., 1990, Staudinger et al., 1990 and Djebbar and Narbaitz, 1995). The lack of good predictive ability is due to: a) the extrapolative nature of the predictions; b) the limited operating conditions in the databases used to develop the correlations; c) the limitations of the parametric regression techniques used to generate these models; and d) the changing nature of mass transfer relationships from one set of operating conditions to another, that are not well understood and are poorly mimicked by current parametric models (Djebbar and Narbaitz, 1995; Bravo et al., 1992).

The objective of this paper is to address some of the above concerns and propose new correlations based on the Onda et al. work. Point (a) and (b) are addressed through the new database gathered for this study. Point (c) is under investigation by the authors (Narbaitz and Djebbar, 1996). Point (d) is addressed through the improvement introduced to the Onda correlations.

NEED FOR AN IMPROVED MODEL

The Onda model consists of three separate equations for the calculation of the individual liquid and gas phase mass transfer coefficients, k_L and k_G , as well as the wetted specific interfacial surface area for mass transfer, a_w . These equations are (Onda et al., 1968):

$$k_L = 0.0051(L_f / a_w \mu_L)^{2/3} (\mu_L / \rho_L D_L)^{-1/2} (a_t d_p)^{0.4} (\rho_L / \mu_L g)^{-1/3} \quad (1)$$

$$k_G = c a_t D_G (G / a_w \mu_G)^{0.7} (\mu_G / \rho_G D_G)^{1/3} (a_t d_p)^{-2} \quad (2)$$

$$a_w = a_t \left\{ 1 - \exp \left[-1.45 (\sigma_c / \sigma_L)^{0.75} (Re_L)^{0.1} (Fr_L)^{-0.05} (We_L)^{0.2} \right] \right\} \quad (3)$$

in which k_L = chemical-specific liquid phase mass transfer coefficient (L/T); k_G = chemical-specific gas phase mass transfer coefficient (L/T); a_w = wetted specific surface area of the packing (L²/L³); a_t = total specific surface area of packing (L²/L³); L_f = liquid mass flux (M/L²T); G = gas mass flux (M/L²T); ρ_L = density of the liquid (M/L³); ρ_G = density of the gas (M/L³); D_L = liquid diffusion coefficient (L²/T); D_G = gas diffusion coefficient (L²/T); d_p = nominal packing diameter (L); g = gravitational constant (L/T²); c = constant = 2 if $d_p < 15$ mm, otherwise $c = 5.23$; σ_c = surface tension of packing material (M/T²); σ_L = surface tension of liquid (M/T²); $Sc_L = \mu_L / \rho_L D_L$; $Er = a_t d_p$; $Mc = \sigma_c / \sigma_L$; $Re_L = L_f / a_t \mu_L$ = liquid phase Reynolds number (dimensionless); $Fr_L = L_f^2 a_t / \rho_L^2 g$ = liquid phase Froude number (dimensionless); $We_L = L_f^2 / a_t \rho_L \sigma_L$ = liquid phase Weber number (dimensionless); μ_L = liquid viscosity (M/LT); and, μ_G = gas viscosity (M/LT). M, L, and T refer to mass, length, and time units, respectively.

The two phase resistance theory postulates that the total resistance to interfacial mass transfer is equal to the sum of the individual liquid phase and gas phase resistances, therefore:

$$\frac{1}{K_L a} = \frac{1}{k_L a} + \frac{1}{H k_G a} \quad (4)$$

where $K_L a$ = the overall (liquid phase based) mass transfer coefficient, H is the Henry's constant expressed as the ratio of the mass concentration in the gas phase to that of the liquid phase (m³ liquid/m³ air). The original Onda work was based on 400 data points from engineered stripping systems. It consists mostly of data from laboratory experiments and it uses traditional packings of less than 25 mm in size. Onda and his coworkers claimed that their model gives results within $\pm 20\%$. In Roberts et al., (1985) and Lamarche and Droste (1989) studies the Onda correlations yielded an average standard deviation in the 20% ranges for packing with diameter smaller than 15 mm. These test conditions are typical of laboratory test conditions.

Beside the general limitations enumerated in the introduction, which also apply to the Onda correlations, the later was found to overestimate mass transfer coefficient in full scale columns that use modern packings. Some attempts have been made to improve the predictive ability of the Onda model (Djebbar and Narbaitz, 1995, and Gossett et al., 1985). However, these attempts did not address the basic limitations of the Onda model, and Staudinger et al. (1991) found that the Gossett et al. (1985) modification did not improve the predictions when applied to his database.

In subsequent study, Dvorak et al. (1996) found that the Onda correlations overestimate the gas phase mass transfer coefficient especially at low gas flow rates, which result in underestimation of the overall mass transfer coefficient. Dvorak et al. (1996) concluded that the Onda correlations appear to result in significant prediction errors for large random packing materials, and they recommended further improvement to the Onda correlations. Dvorak et al. (1996) indicated that the form of the Onda correlations is appropriate and that the parameters of the correlations only should be changed to reflect modern operating conditions. They also indicated that the source of the error appears to in the wetted surface area and/or the liquid-film resistance equations.

In their study, Djebbar and Narbaitz (1995) found that $K_L a$ is not constant along the depth of the tower as assumed by the theory. This phenomena is not accounted for by present correlations. This finding is confirmed by the work of Gross and Termaath (1985), who conducted experiments in which the only variable that changed was the packing depth. Gross and Termaath found that $K_L a$ decreases with the

increase in the depth of the packing. Observed increases or decreases in $K_L a$ in the upper part of the column are related to the adjustment of the wetted packing surface area associated with the shift from the liquid distribution pattern of the distributor to the natural flow distribution pattern of the packing (Djebbar and Narbaitz, 1995). The Onda correlations systematically overestimate mass transfer coefficient $K_L a$ for larger diameter packings that are typically used in full-scale applications. The average error is found to be 40 % and a safety factor of 1.47 would be required to account for 68 % of Djebbar and Narbaitz database (Djebbar and Narbaitz, 1995).

At the 68% confidence level, typical errors in the variables produce an error in the Onda predictions in the range of 5 to 15%. Large part of the observed deviation is therefore attributed to the lack of fit of the Onda model, which points to the possibility of improving the Onda correlations.

From previous studies it appears that: (i) the functional relationship of the Onda correlations seems to be correct, (ii) the depth of the tower should be included in the correlations, (iii) the source of error appears to be in the surface area and/or the liquid-film resistance equations. The objective of this paper is to address these concerns and propose new correlations based on the Onda model. To undertake such task a database that is comprehensive and representative of real world application is required.

DATABASE

Experimental data in the public domain were surveyed, and evaluated against strict criteria. When necessary, supporting information was obtained directly from the appropriate researchers. The studies chosen from the literature encompass a wide variety of operating conditions. These studies were conducted with modern full scale operating conditions in mind. They include new packing media, optimum striping factors in the range of 2 to 7, typical liquid loading rates of 0.4 to 2 m/s. This database is the most comprehensive database gathered up to date. The total number of data points is 1450 data points, which is about three times the Onda et al. database and took, in total, 12 literature studies to generate. Table 1 contains the packing used in this database with their main characteristics, and Table 2 contains the VOCs used in this database with their main characteristics. As Table 1 shows, this database contains performance data of structured packing.

Table 1 Names and main characteristics of packings in the database.		
Packing	Diameter (mm)	Surface area (m²/m³)
Random packing		
Rashig Rings	13	400
Ceramic Saddles	13, 25	466, 259
Pall Rings;	16, 25, and 50	341, 220, 108
Tellerettes	25 and 50	180, 125
Norpac	38 and 50	145, 100
Hi-Flow Rings	50	97
Flexiring	50	115
Tripac	50	157
Cascade Minirings	50 and 76	210, 141
Flexisaddles	76	88.6
LANPACTM	89	137
Snowflakes	94	91.8
Structured packing		
Munters	16	420
Flexipac	50	131

To interpret results accurately, certain physical property data such as liquid density, diffusion coefficient, and Henry's Law constant. Great care had to be taken in determining these physical properties because they considerably effect the resulting mass transfer coefficient.

Compound name	Chemical formula	Henry's cst. at 20°C
Dichloromethane	CH ₂ Cl ₂	0.0725
Bromoform	CHBr ₃	0.028
Chloroform	CHCl ₃	0.11677
Bromodichloroethane	CHCl ₂ Br	0.095
Dibromochloroethane	CHClBr ₂	0.036
Carbon Tetrachloride	CCl ₄	0.985
Chloroethane	C ₂ H ₅ Cl	0.3968
1,1-Dichloroethane	C ₂ H ₄ Cl ₂	0.182
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	0.059
1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	0.561
1,1,2,2-Tetrachloroethane	C ₂ H ₂ Cl ₄	0.016
Vinylchloride	C ₂ H ₃ Cl	0.923
cis-1,2-Dichloroethylene	C ₂ H ₂ Cl ₂	0.125
Trichloroethylene	C ₂ HCl ₃	0.302
Tetrachloroethylene	C ₂ Cl ₄	0.557
1,2-Dichloropropane	C ₃ H ₆ Cl ₂	0.096
Benzene	C ₆ H ₆	0.23
Toluene	C ₆ H ₅ CH ₃	0.19
Xylene	CH ₃ C ₆ H ₄ CH ₃	0.45
Ethylbenzene	C ₈ H ₁₀	0.27

Henry's constant values were obtained from experimental studies such as those reported in Haarhoff and Cleasby (1990), Gossett (1987), and Lamarche and Droste (1989). The liquid phase diffusion was determined using Wilke and Chang correlation (Wilke and Chang, 1955), and the gas phase diffusion was determined using the semi-empirical Fuller equation derived from kinetic theory principles (Staudinger, 1986).

DEVELOPMENT OF AN IMPROVED MASS TRANSFER CORRELATION

The evaluation process was conducted using basic statistical tools. The absolute average error, AAE, is given by:

$$AAE = \frac{1}{n} \sum_{i=1}^n \frac{|(K_L a)_{exp} - (K_L a)_{pre}|}{(K_L a)_{exp}} \quad (5)$$

and the average algebraic error, AGE, is given by:

$$AGE = \frac{1}{n} \sum_{i=1}^n \frac{(K_L a)_{exp} - (K_L a)_{pre}}{(K_L a)_{exp}} \quad (6)$$

where n = the number of data points; and, $(K_L a)_{exp}$ and $(K_L a)_{pre}$ = the experimental and the predicted mass transfer coefficients, respectively. AAE is a measure of average absolute deviation. AGE measures the overall over-or under-estimation. As suggested by Roberts et al. (1985) the standard error of $K_L a$ should be based on its logarithm transform, SEE;

$$SEE = \left\{ \frac{1}{n} \sum_{i=1}^n (\text{Log } (K_L a)_{exp} - \text{Log } (K_L a)_{pre})^2 \right\}^{0.5} \quad (7)$$

Finally, the interval limited by one standard deviation defines the expected 68% confidence level and it is given by:

By using a nonlinear, multiple regression program based upon the algorithm of Marquardt, the experimental results were fitted to a modified Onda correlations as will be explained in the following. The modifications of the Onda correlations took into account the concerns noted in previous sections. In each of the following, the data is randomly divided into two groups: one for development and the second for validation.

Modern applications of packed tower rarely use packing with small diameter. Furthermore, previous studies concluded that the Onda correlations is reasonably accurate for small packing diameters (Roberts et al., 1985; Lamarche and Droste, 1989). Roberts et al. (1985) found that 68% of the predicted values lie within a factor of 1.21 from the observed value of the database they developed. This accuracy agrees closely with Onda's own assessment (Onda et al. (1968)). Therefore, the Onda correlations are adopted for packing diameter that are smaller than 15 mm. The database used in this study contains packing larger than 15 mm, 70% of which have packing diameter equal or superior than 25 mm (1 inch).

Some modifications were introduced to the Onda correlations to account for the shortcomings pointed out in previous sections. First, the liquid phase mass transfer correlation, equation 1, was rendered dimensionless through the use of the Sherwood number, $Sh = \frac{k_L}{D_L a_i}$. Second, the gas phase Reynolds number was added to the surface area correlation. Finally, the dimensionless number Zd , which is equal to the ratio of packing height to packing diameter, is added to the liquid phase correlation, equation 1.

The result of the first series of analysis, through regressing the whole database, is shown in Figure 1. This figure shows two distinct regions with two different trends. One corresponds to packing with diameters smaller than 25 mm, the second corresponds to packings with diameters larger than or equal to 25 mm. Plot of the results with other variables didn't show any particular trend. Consequently, the database was divided into two groups: smaller than 25 mm, and larger than or equal to 25 mm.

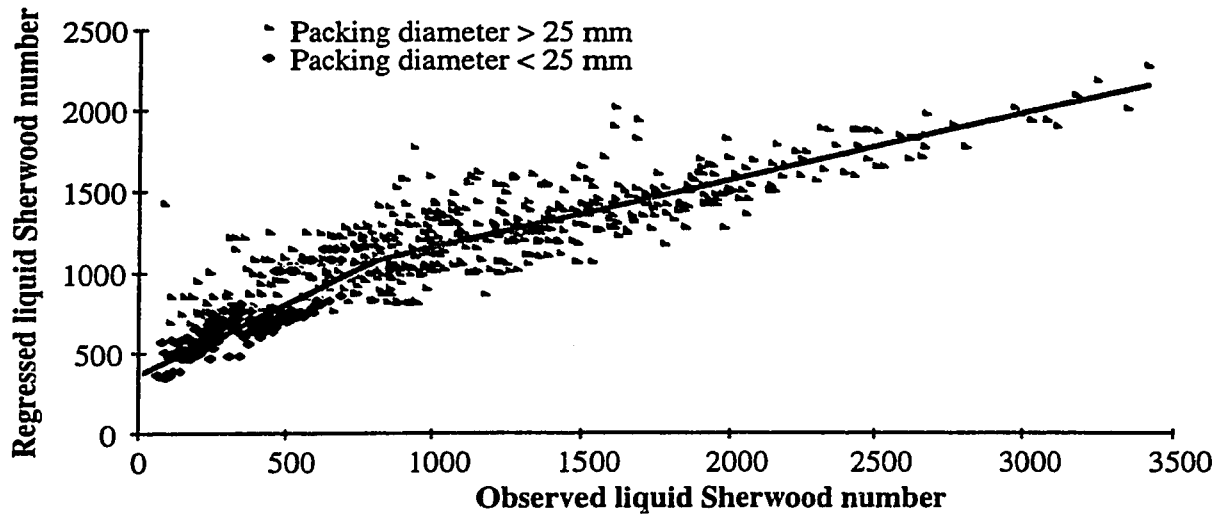


Figure 1. Two region defined by packing diameter equal 25 mm.

The database with packing diameters larger than 25 mm contains 1078 data points. These data were further divided into two groups. The first group contains 500 data points and the second group contains 578 data points. The first data group were regressed using the new correlations forms and the following equations were obtained.

$$a_w = a_i \left\{ 1 - \exp \left[-0.095 (Re_L)^{0.41} (Re_g)^{0.01} (Fr_L)^{-0.48} (We_L)^{0.38} (Er)^{0.56} (M_c)^{0.75} \right] \right\} \quad (9)$$

$$\frac{k_L}{a_i D_L} = (0.15E - 08)(L_f / a_w \mu_L)^{0.65} (Sc_L)^{1.15} (\rho_L / \mu_L g)^{1.8} (Er)^{1.4} (Zd)^{-0.6} \quad (10)$$

$$\frac{k_G}{a_i D_G} = 0.97(G_f / a_i \mu_G)^{0.6} (Sc_G)^{1.5} (Er)^{0.43} \quad (11)$$

Figure 4 shows the results of goodness of fit tests for the 500 data points that constitute the developmental data set. The improved correlations produced an average error of 23.5%, with 68% of the data is within a band limited by a factor of 1.29 from the best fit line. The developmental data set as a whole is slightly overestimated with an average algebraic error of 13%.

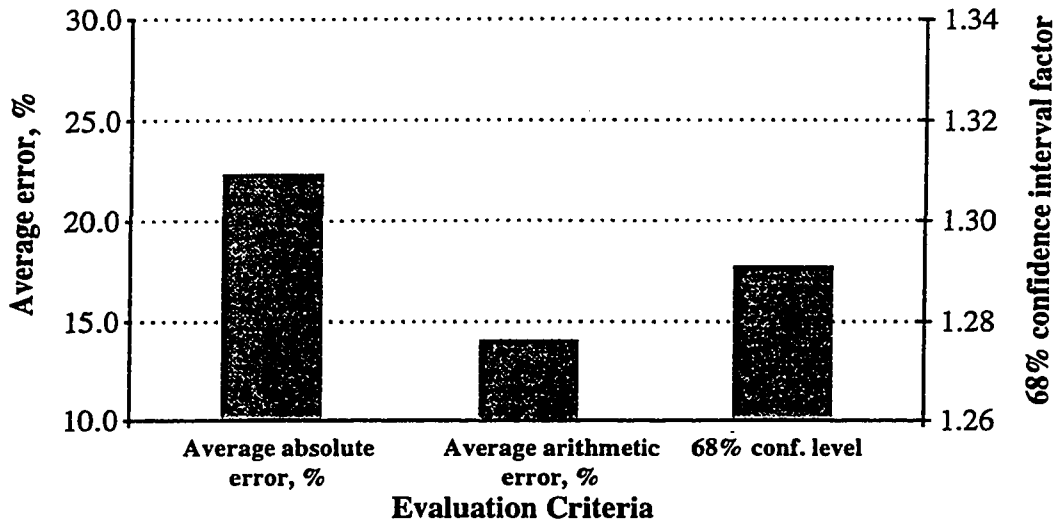


Figure 2. Results of the improved correlations using the developmental data set.

Figure 3 presents a comparison between the Onda and the improved models. The average absolute error is 22% for the improved correlations while it is 29% for the Onda model. As expected, the Onda correlations overestimated the mass transfer coefficient, and the average overestimation was 24%. The improved correlations barely overestimated the results (AGE = 0.7%).

Figure 4 shows the variation of the error with the packing depth. The Onda correlations are independent of the packing depth and, hence, produce a constant value, while the improved model's predictions vary with the packing depth. The improved correlations tend to overestimate $K_L a$ at low packing depth. This may be due to residues of end effects in the data which are more important in short columns. Also, It may be due to the effect of liquid distribution system. Djebbar and Narbaitz (1995) found that the liquid distribution system highly affects the transfer characteristics in the upper parts of the tower, and therefore it has a higher impact in short columns.

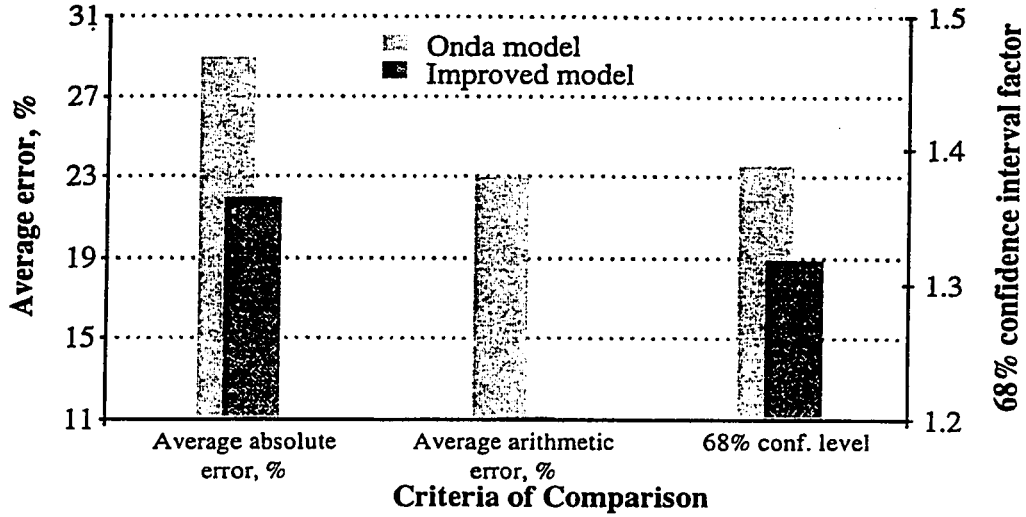


Figure 3. Average errors and F factor for the validation data set.

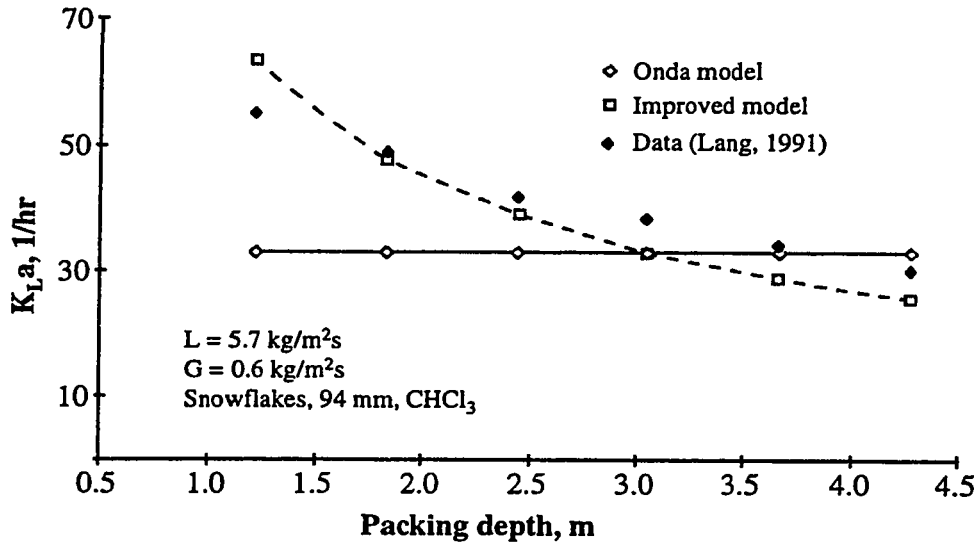


Figure 4. Effect of packing depth on simulated $K_L a$.

CONCLUSION

Improved correlations which are based on the Onda model are presented. A comprehensive database formed of full-scale experiments from different sources was used in the development as well as in the validation of the improved correlations. This database is by far the most comprehensive and representative of real world applications of VOC stripping in packed towers. The improved correlations addressed several of the previously identified shortcomings of the Onda correlations. The average error for the validation as well as for the development data was found to be less than 26%.

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APPENDIX A4.1

“NEURAL NETWORK ESTIMATION OF AIR STRIPPING MASS TRANSFER COEFFICIENTS”

Presented at the 1995 WEFTEC, Miami Beach.

NEURAL NETWORK ESTIMATION OF AIR STRIPPING MASS TRANSFER COEFFICIENTS

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ABSTRACT

Existing parametric correlations have difficulties predicting the mass transfer coefficient for volatile organic chemicals (VOCs) in modern air stripping packed towers. Neural networks have emerged as a powerful prediction tool. They do not require model form selection which is a must for parametric regressions. In this study a neural network approach was used to predict the mass transfer coefficient of air stripping towers. Although based on only four variables, the predictions improved by more than 50% as compared to the Onda correlation, the best existing parametric correlation.

KEYWORDS: air stripping, mass transfer coefficients, neural networks, parametric regression, nonparametric regression, volatile organic compounds.

INTRODUCTION

Many environmental problems fall short of complete theoretical solutions because of their complexity and our limited knowledge of the processes involved. Often, parametric regression techniques are used to model such processes. These techniques require that the form of the functional relationship, that relates the dependent variables to the independent variables, be known or be assumed. The overall mass transfer coefficient in air stripping packed towers, $K_L a$, is an example of such a problem. There are tens of parametrically regressed correlations for the estimation of $K_L a$ in the chemical engineering literature. The superiority of the parametric approach is evident when the real form of the functional relationship is known; however, this is often not the case. The functional relationship for the mass transfer coefficient in packed towers is usually assumed to have the following form (Welty et al., 1976):

$$K_L a = \alpha(X)^\beta(Y)^\gamma \dots = g(X, Y, \dots, \alpha, \beta, \gamma, \dots) \quad (1)$$

where X and Y = dimensionless numbers such as Reynolds and Schmidt numbers which are functions of the operating variables; and α , β and γ = parameters. The parametric regression approach reduces to the determination of the values of the parameters using a parametric estimation method such as least squares regression.

Among all the existing parametric models, there is agreement in the recent literature (Roberts et al., 1985, Staudinger et al., 1990) that the Onda model (1968) is the best mass transfer correlation. The literature shows that this model yields satisfactory results for lab data. However, 30 to 50 percent deviations have been reported in full-scale applications (Lenzo et al., 1990, Staudinger et al., 1990 and Djebbar and Narbaitz, 1995). The lack of good predictive ability is due to: a) the extrapolative nature of the predictions; b) the limited operating conditions in the databases used to develop the correlations; c) the parametric regression techniques used to generate these models; and d) the changing nature of mass transfer relationships from one set of operating conditions to another, which are not well understood and are poorly mimicked by current parametric models (Djebbar and Narbaitz, 1995; Bravo et al., 1992).

Over recent years neural networks (NN) have shown exceptional performance as regression tools, especially if used for pattern recognition and classification. The most important characteristic of NN is that no assumption has to be made about the form of the functional relationship. Other important characteristics of NN are their high nonlinearity, their ability to infer subtle, unknown relationships from data, and their capability to generalize, meaning they can respond correctly to patterns that are only broadly similar to the original training patterns. These characteristics make the NN well-suited for predicting the mass transfer coefficient in packed towers. The objective of this study is to use NN to predict $K_L a$. It is expected that NN will overcome the shortcomings of existing approaches. To achieve this, a large new pilot-scale air stripping database is used. The results of this new approach will be compared to the Onda model predictions.

PARAMETRIC VERSUS NEURAL NETWORK APPROACHES

Parametric models are the most common technique used to describe processes. They predict performance variables (i.e., $K_L a$) as a mathematical function of a set of design variables (independent variables, X and Y in Equation 1) and a set of constants (parameters α , β and γ in Equation 1). The values of the parameters are usually determined by a parameter estimation method, such as the least squares regression, which have certain limitations and require large sets of accurate data to yield satisfactory results. For the optimal properties of the least square estimates to be valid in parametric approach, it is essential that the following assumptions hold: (i) the values of the operating variables are exactly known; (ii) the model form is known; (iii) the errors and the observed responses at each set of operating conditions have the same variance; (iv) the errors (and the observed values of the responses) are not correlated and thus are statistically independent; (v) the errors are identically and normally distributed with zero mean and variance σ^2 . It is obvious that the above assumptions are almost never satisfied. A key assumption of parametric modeling is that the model form, i.e. a mathematical expression to describe g in Equation (1), is known. However, this form is often unknown and always to some extent subjectively assumed (Adamowski and Feluch, 1991). Once regressed, these models can be readily applied using a simple calculator. It is also important to add that the smoothing process in parametric regression considers the entire data set, which makes it vulnerable to deviations due to outliers.

A fundamental concern in parametric regression modeling is the number of degrees of freedom. While it is statistically valid to obtain an equation with as little as a single degree of freedom, the resulting equation is of very limited value as insufficient data was used to develop it. Thus, the larger the data set used to develop parametric regression relationships, the greater the confidence in that relationship. Good quality data (assumption (i)) that are a must for parametric regression are rare and expensive to access. Insufficient good quality data is always a major limiting factor in the application of parametric regression methods.

NN, however, are very successful in estimating any type of function because they are highly nonlinear, in that they can capture complex interactions among the input variables in a system without any prior knowledge about the nature of these interactions. They can generalize, in that they can correctly process data that only broadly resembles the data they were trained on, i.e. developed, originally. They tolerate imprecise or incomplete data, approximate results, and the presence of complex nonlinear behavior (Hammerstrom, 1993a & b; Hayken et al., 1994; Zaabab et al., 1995). They are highly parallel, i.e., their numerous independent operations can be executed simultaneously. Parallel hardware can execute parallel calculations hundreds or thousands of times faster than conventional hardware.

But, NN are slow and expensive to train. However, once trained, the results are obtained quickly. They may fail to find a satisfactory solution, however, this is much less of a problem than in parametric regression. Perhaps there is no learnable function or perhaps the data is insufficient. It can be hard to account for NN results as these results depend on thousands of calculations involving the input pattern and the connection weights. In addition, the NN approach does not result in an explicit relationship between the independent and dependent variables. Showing how the weights "cause" a result may be more complex than showing how a computer program works. This is because the values of the weights are themselves the result of a complex machine learning procedure. The above concerns are rather theoretical and NN have been successfully applied in many fields (De Veaux et al., 1993; French et al., 1992; Hammerstrom, 1993a & b; Haykin, 1994). The main advantage of NN over parametric approach is the avoidance of model form selection. Indeed, in NN there is no need to assume a relationship of pre-specified form, as a relationship of possibly complicated or unorthodox shape is generated by the data points themselves.

PARAMETRIC APPROACH

All existing mass transfer prediction models are parametric. These models have been discussed in Djebbar and Narbaitz (1995), Au-Yeung and Pontar (1983), etc. As indicated earlier, the Onda model is considered the best correlation. The Onda model consists of three separate equations for the calculation of the individual liquid and gas phase mass transfer coefficients, k_L and k_G , as well as the wetted specific interfacial surface area for mass transfer, a_w . These equations are:

$$k_L = 0.051 (L_r / a_w \mu_L)^{2/3} (\mu_L / \rho_L D_L)^{-1/2} (a_i d_p)^{0.4} (\rho_L / \mu_L g)^{-1/3} \quad (2)$$

$$k_G = ca_i D_G (G / a_w \mu_G)^{0.7} (\mu_G / \rho_G D_G)^{1/3} (a_i d_p)^{-2} \quad (3)$$

$$a_w = a_i \{1 - \exp[-1.45(\sigma_c / \sigma_L)^{75} (Re_L)^{0.1} (Fr_L)^{-0.05} (We_L)^{0.2}]\} \quad (4)$$

in which k_L = local liquid phase mass transfer coefficient (L/T); k_G = local gas phase mass transfer coefficient (L/T); a_w = wetted specific surface area of the packing (L^2/L^3); a_i = total specific surface area of the packing (L^2/L^3); L_t = liquid mass flux (M/L^2T); G = gas mass flux (M/L^2T); ρ_L = density of the liquid (M/L^3); ρ_G = density of the gas (M/L^3); D_L = liquid diffusion coefficient (L^2/T); D_G = gas diffusion coefficient (L^2/T); d_p = nominal packing diameter (L); g = gravitational constant (L/T^2); c = constant = 2 if $d_p < 15$ mm otherwise $c = 5.23$; σ_c = surface tension of the packing material (M/L^2); σ_L = surface tension of the liquid (M/L^2); $Re_L = L_t / a_i \mu_L$ = liquid phase Reynolds number (dimensionless); $Fr_L = L_t^2 a_i / \rho_L^2 g$ = liquid phase Froude number (dimensionless); $We_L = L_t^2 a_i \rho_L \sigma_L$ = liquid phase Weber number (dimensionless); μ_L = liquid viscosity (M/LT); and, μ_G = gas viscosity (M/LT). M, L and T refers to mass, length and time units, respectively.

The two phase resistance theory postulates that the total resistance to interfacial mass transfer is equal to the sum of the individual liquid phase and gas phase resistances, therefore:

$$\frac{1}{K_L a} = \frac{1}{k_L a} + \frac{1}{H_c k_G a} \quad (5)$$

where $K_L a$ = the overall (liquid phase based) mass transfer coefficient; H_c is the Henry's constant expressed as the ratio of the mass concentration in the gas phase to that in the liquid phase; and $a = a_w$ in equation 4.

NN APPROACH

Research on NN begun in 1943 with the work of McCulloch and Pitts (1943). They demonstrated the capacity of NN to calculate logic functions. But application of NN really started in 1982 with the works of Hopfield (1982). NN can be defined as a highly parallel adaptive system capable of auto-improving by learning. These networks are inspired by the functioning mode of animal brain in which a great number of neurons are interconnected by their synapses. By analogy we define the neuron as the basic unit of the network. This neuron can receive one or more input, calculate the weighted sum and produce a unique output through the transfer function (Figure 1). Many transfer functions are available but the most common one is the standard sigmoid (Figure 1).

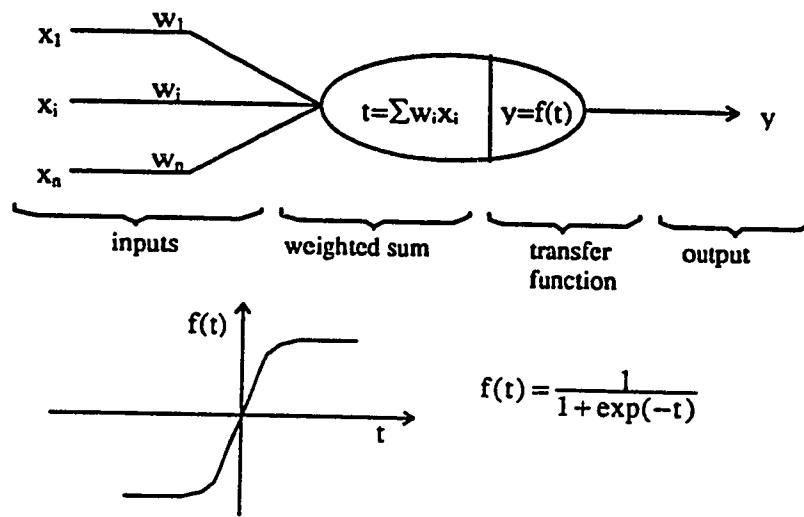


FIGURE 1: Architectural graph of a neuron

NN can be looked at as an association of a number of neurons; therefore, several type of network architectures are possible. However, the best performing are the multilayer networks, which are able to simulate nonlinear problems. The main idea of neural computing is the decomposition of the input-output relationship into a series of linearly separable steps using hidden layers;

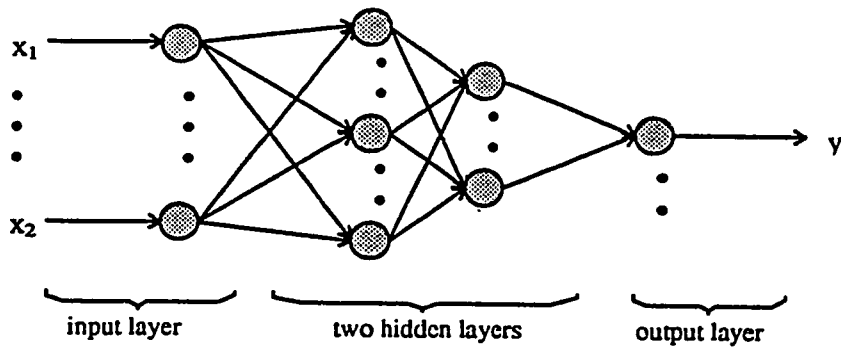


FIGURE 2: Fully connected network with two hidden layers and one output layer

The mechanism of learning of a NN is as follows. First, we define the n input variables, the m output variables and p neurons on the predefined hidden layer. At first the weights at each connection are fixed randomly. Once the network is set, it is clear that for a set of inputs it produces a set of outputs that are different from the observed ones. At this stage, it is necessary to change the weights at each connection so that the outputs will coincide, as close as possible, with the corresponding observed outputs. The known errors on the output layer are propagated back to the hidden layers to determine the appropriate weight changes on the hidden layers. This process of weights calibration is called training, and it may take long time. However, once trained, the network response is instantaneous. The main difficulties with this process is the choice of the network architecture and to a lesser degree the training algorithm. Various NN topologies have been proposed to date such as Hopfield nets, Hamming nets, Carpenter/Grossberg classifiers, perceptrons, multilayer perceptrons, and Kohonen self-organizing feature maps. Recent success in neural network research is mainly attributed to the achievements of multilayer perceptrons with backpropagation training algorithms.

CALCULATION OF WEIGHTS BY BACK PROPAGATION

Back-propagation algorithm has been proposed by Le Cun (1987), which permits the adjustment of the weights of all connections in the network. In back-propagation algorithms the exact number of hidden neurons and the connectivity between layers must be specified before learning can begin. The most common way to choose the number of hidden neurons is by trial and error. In practice, though, one can't guarantee that the back-propagation will find the correct weights for a given number of neurons and a particular training data set.

It is impossible to attribute the deviation between the network output(s) and the observed output(s) to a particular weight(s) of a particular neuron(s). In back-propagation we use neurons with differentiable non linear transfer functions. The algorithm calculates the partial derivative of the error relative to each weight in each neuron of the network. Then, using a gradient descent procedure, an error criteria relative to the error at the output layer (in terms of the weights) is minimized. This can be done as follows:

Define (Figure 3):

x_i^s = output of the neuron j in the layer s

w_{ji}^s = weight of the neuron j of the layer $(s-1)$ to neuron i of layer (s)

t_j^s = weighted sum of the inputs to neuron j of layer (s)

so we have

$$t_j^s = \sum_{i=1}^n w_{ji}^s x_i^{s-1} \quad \text{and} \quad x_j^s = f(t_j^s) \quad (6)$$

The desired output is noted $D=(d_1, \dots, d_i, \dots, d_m)$ and the actual output is noted $x=(x_1, \dots, x_i, \dots, x_m)$. A quadratic form, $E(w)$, to evaluate the error, where w represent the weights is used;

$$E(w) = \frac{1}{2} \sum_k (d_k - x_k)^2 \quad (7)$$

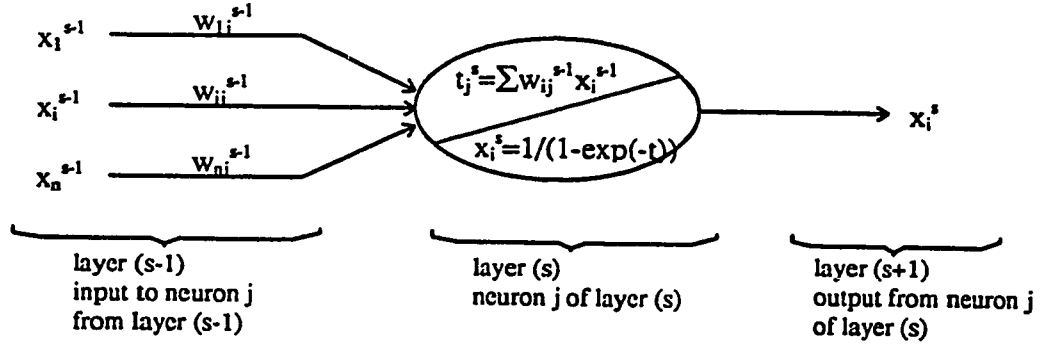


FIGURE 3: Definition of terms used in the backpropagation training algorithm

Weight adjustment is done through a gradient descent procedure, i.e.,

$$\begin{aligned} (w_{ij}^s)_{\text{adjusted}} &= w_{ij}^s + \Delta w_{ij}^s \\ \Delta w_{ij}^s &= -C_1 \frac{\delta E(w)}{\delta w_{ij}^s} \end{aligned} \quad (8)$$

where C_1 is a learning coefficient that determines the speed of learning. The learning process is carried out as follow:

- (i) input is presented to the network
- (ii) an output is obtained
- (iii) determine the relative deviation e_j^s for each weight as follows,

$$e_j^s = - \frac{\delta E(w)}{\delta w_{ij}^s} \quad (9)$$

where

$$\frac{\delta E(w)}{\delta w_x^s} = \frac{\delta E(w)}{\delta t_j^s} \frac{\delta t_j^s}{\delta w_x^s} - e_j^s x_i^{s-1} \quad (10)$$

for the hidden layer

$$e_j^s = f(t_j^s) \sum_k e_k^{s+1} w_{kj}^{s+1} \quad (11)$$

and for the output layer

$$e_k = 2(d_k - x_k) f(t_k) \quad (12)$$

Hence, we can determine all e_j^s starting from the output layer moving backward (back-propagation) and finding all $\frac{\delta E(w)}{\delta w_{ji}^s}$ and then modifying the weights. This process is repeated until a convergence criteria is reached. Back-propagation is essentially a gradient descent method over an error surface.

The network architecture and the learning algorithm (back-propagation) presented here are merely representative. Not all the details apply to all networks. Structural elements such as nodes, connections, layers, and weights are practically universal, but the arrangements between them vary. For example, some networks lack a hidden layer, and some have more than one. Other variations include nodes that feed back to earlier nodes, connections that skip layers, and layers that are partly connected. No effective procedure has yet been published the optimal architecture for NN for backpropagation prior to training of the network. However, an excessive number of hidden nodes will cause bad generalization properties. In such cases, the NN would not be able to interpolate effectively between adjacent training data points. Too few hidden nodes, though, will limit the competence of the network to locate an adequate "relationship"

between response and predictor variables. Various networks with different number of hidden nodes should be trained, and the network which performs best on a test data set is then selected as the most adequate architecture. Also, nodes with very small weights would indicate the relative importance of this particular node compared to the other nodes.

SCALING OF THE DATA

The input node activities of the neural network should be small enough that the sigmoidal hidden nodes are not saturated, i.e., their absolute values should not be too large. It is also imperative that the input values to the net are of the same absolute order. During training each weight is adjusted according to the overall error gradient, which is directly proportional to the magnitude of the input node. A very small input node will thus prevent the weight that connects it to the hidden layer from making a significant contribution to the derivative of the objective function and will slow down the training process. Scaling is often accomplished through linear or logarithmic transformations. The latter is beneficial if the values of a specific variable or function vary over different orders of magnitude. The logarithmically and linearly scaled values are usually zero-mean-centered.

DESCRIPTION OF THE DATA BASE

A critical part of this research is the data to be used. Experimental data in the public domain are abundant, however, acceptable quality data that are representative of real world applications are not. A new data base has been developed by Narbaitz et al. (1995) in a large pilot-scale study using several modern large diameter packings and numerous full scale operating conditions.

A schematic representation of the air stripping tower is shown in Figure 4. It consists of a 30-inch- (0.76 m) diameter tower, with a total height of 29 ft (8.84 m) and filled with 15 ft (4.57 m) of packing. This tower can treat up to 200 gpm. It has five sampling ports within the packing located at 0, 2, 4, 8 and 14 ft (0.0, 0.61, 1.22, 2.44 and 4.27 m) from the top of the packed zone, respectively. To break any wall flow, the column is equipped at 4 ft (1.22 m) intervals with aluminum redistributor rings that extend 3 inches (7.62 cm) inwards from the column wall. The characteristics of the packings tested are summarized in Table 1. The VOCs were studied in three multicomponent mixtures (Table 2) consisting of approximately 100 $\mu\text{g/l}$ of each VOC. Table 2 lists the Henry's law constants and the diffusion coefficients of the VOCs considered, as reported by Gossett (1987) and Haarhoff and Cleasby (1990). The minimum stripping factor was three, well above the critical value of one (Roberts et al., 1985). More details about this data base can be found in Narbaitz et al. (1995). The overall experimental $K_L a$ values were obtained based on the values of the VOC concentrations at five depths. These concentrations are strictly within the packing media, so they are free of end effects. Thus, the Narbaitz et al. data base has a particular advantage, because they are used directly in the analysis without correcting for end effects.

Table 1 Characteristics of the packing material used in the Narbaitz et al. data base

Packing name	Company	diameter cm(in)	surface area (m^2/m^3)
Cascade Miniring #2	Glitsch Inc.	7.62 (3)	150.86
Flexiring #2	Koch	5.08 (2)	114.78
Flexisaddle #3	Koch	7.62 (3)	88.55
Tripack #1	Jeager Inc.	5.08 (2)	157.42
Nor-Pac #3	NSW	3.8 (1.5)	100.03
Nor-Pac #4	NSW	5.08 (2)	145
Snowflakes	Glitsch Inc.	9.4 (3.7)	91.83

Table 2 Characteristics of the chemical compounds in the data base					
Group	Compound Name	Formula	Diffusion (m/s)		H (20 °C) dimensionless
			Gas E-10	Water E-6	
GI	Chloroform	CHCl ₃	9.23	9.18	0.117
	1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	8.13	8.28	0.561
	Carbon Tetrachloride	CCl ₄	8.18	8.22	0.986
	Trichloroethylene	C ₂ HCl ₃	8.45	8.46	0.302
	Tetrachloroethylene	C ₂ Cl ₄	7.61	7.59	0.557
GII	Chloroform	CHCl ₃	9.23	9.18	0.117
	Bromodichloromethane	CHCl ₂ Br	9.09	8.72	0.095
	Chlorodibromomethane	CHBr ₂ Cl	8.96	8.37	0.036
	Bromoform	CHBr ₃	8.83	8.08	0.028
GIII	Toluene	C ₆ H ₅ N	7.98	8.31	0.190
	Chlorobenzene	C ₆ H ₅ Cl	7.48	7.7	0.160
	M-Xylene	C ₈ H ₈	7.21	7.52	0.450
	M-Dichlorobenzene	C ₆ H ₄ Cl ₂	7.29	7.24	0.150

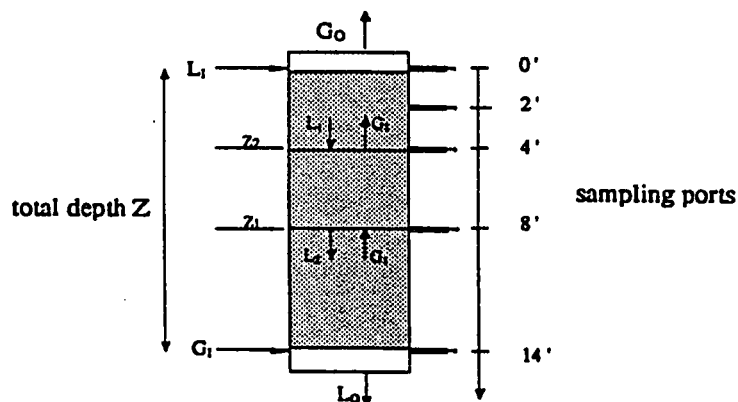


FIGURE 4. Tower used in the Narbaitz et al. data base development

The experimental $K_L a$ is calculated by the following equation (Djebbar and Narbaitz, 1995):

$$K_L a = \left[\frac{L_r}{z \rho_L} \right] * \left[\frac{R}{R-1} \text{Ln} \left\{ \frac{c_1 (1-1/R) + c_o / R}{c_2 (1-1/R) + c_o / R} \right\} \right] \quad (13)$$

where $R = \frac{HG}{P_i L_r}$ = the stripping factor (dimensionless); c_o = the liquid effluent VOC concentration at depth Z , the bottom of the packing media (Figure 4) (M/L^3); c_1 and c_2 = the VOC concentrations in the liquid at the depths z_1 and z_2 , respectively (M/L^3) and $z = z_2 - z_1$ (Figure 4); H = the Henry's law coefficient on a volume to volume basis ($1/\text{atm}$); P_i = the total operating pressure (atm).

METHOD OF ANALYSIS

A FORTRAN program was developed to conduct the NN analysis based on the algorithm presented earlier. Two thirds of the 538 data points were used to determine the optimum values of the weighting factors and the best network architecture. The remaining one third of the data were used to validate the proposed prediction tool and to compare it with the Onda model predictions.

The evaluation of the Onda correlations was conducted using basic statistical tools. The absolute average error, AAE, is given by:

$$AAE = \frac{1}{n} \sum_{i=1}^n \frac{|(K_L a)_{exp} - (K_L a)_{pre}|}{(K_L a)_{exp}} \quad (14)$$

and the average algebraic error, AGE, is given by:

$$AGE = \frac{1}{n} \sum_{i=1}^n \frac{(K_L a)_{exp} - (K_L a)_{pre}}{(K_L a)_{exp}} \quad (15)$$

where n = the number of data points; and, $(K_L a)_{exp}$, and $(K_L a)_{pre}$ = the experimental and the predicted overall mass transfer coefficients, respectively. AAE is a measure of average absolute deviation, while the AGE is a measure of the overall over- or under- estimation.

RESULTS

Four variables, believed to have the greatest impact in the transfer operation, liquid and gas flow rates, packing surface area, and the Henry's law constant were used in the input layer and $K_L a$ used in the output layer. After a series of simulations a scheme of one hidden layer with five neurons was selected (as shown below),

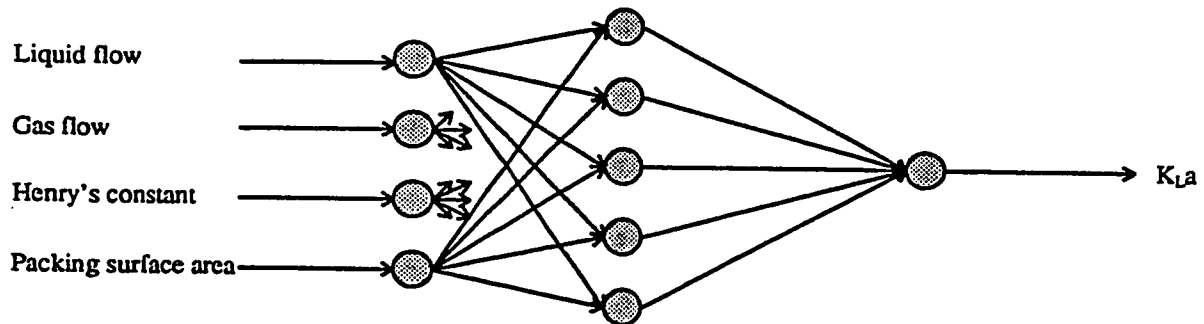


FIGURE 5: Architecture of the selected network; one hidden layer with five neurons.

The results of the training stage in Figure 6 show a very high correlation between the simulated and the experimental data. The average error, 12.5%, is far superior to any of the previous parametric correlations at the developmental stage. For example, the Onda model had an average error of 20% for its developmental data set even though it involves 10 variables.

The results of the validation phase were also impressive. The NN predictions are superior to those of the Onda model as shown in Figure 7 and 8. The Onda model predictions had twice the average error of the NN predictions: 30% and 15%, respectively (Figure 9). The large error of the Onda model is caused by the overestimation of $K_L a$ in 83% of the cases (Figure 9). This is consistent with the findings of other reports in the literature. An overestimation of $K_L a$ is extremely undesirable as it results in an undersized tower. Fortunately the NN predictions only overestimated the $K_L a$ in 20% of the cases. Figure 10 shows that the NN approach was superior to the Onda model for all the packings. This superiority is also evident from the average error versus packing diameter in Figure 11 and versus liquid flow rate in Figure 12. As shown in Figure 11, the magnitude of the Onda model's errors tends to be function of the packing diameter as found by Djebbar and Narbaitz (1995). Lenzo et al. (1990) and Staudinger et al. (1990) also showed that the quality of the Onda predictions deteriorate with increasing packing size. The Onda correlation's predictive quality was unaffected by liquid loading, while the NN predictions improved with increasing liquid loading (Figure 12). Presently, NN modeling is being extended to include other variables, such as packing depth, packing diameter, physico-chemical characteristics of the gas and liquid involved, etc. In addition, the validation is being enlarged to incorporate other data sets.

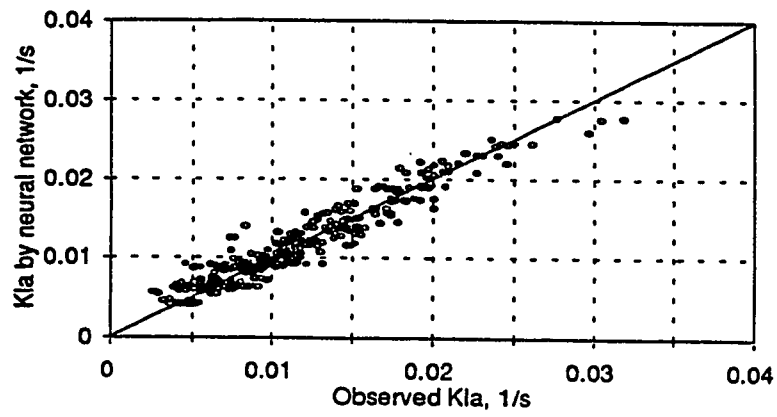


FIGURE 6. Neural network simulations of K_{1a} versus observed K_{1a} for the data used in the training stage

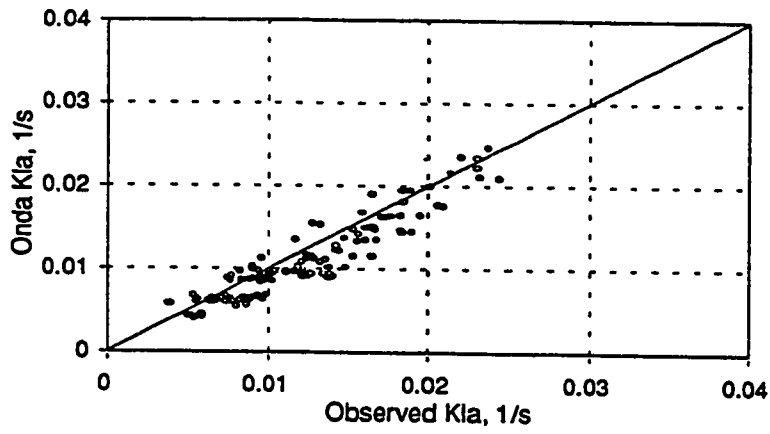


FIGURE 7. Neural network predicted K_{1a} versus observed K_{1a} for the validation data.

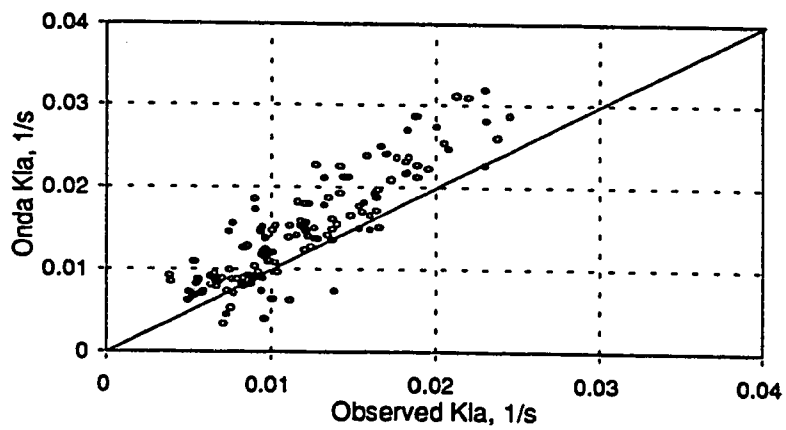


FIGURE 8. Onda predicted K_{1a} versus observed K_{1a} for the validation data

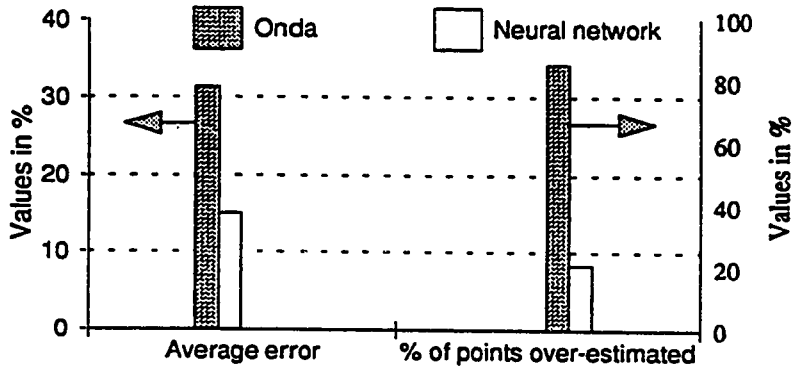


FIGURE 9. Comparison between the Onda correlation and the Neural network method for the validation data.

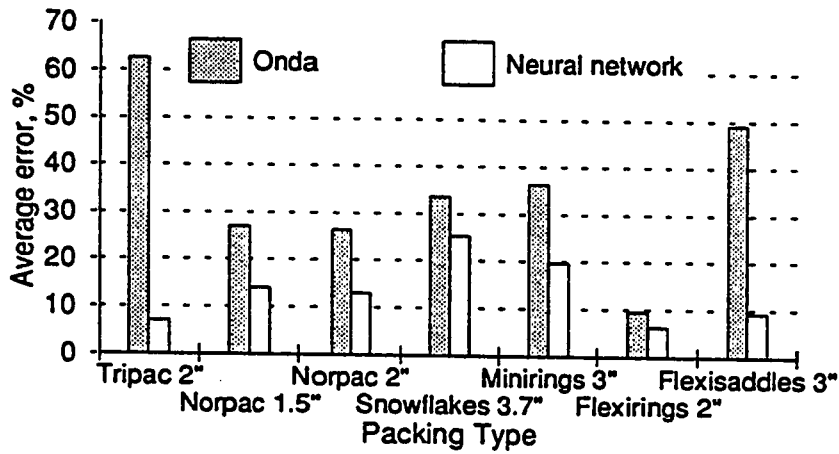


FIGURE 10. Average error in the neural network and the Onda predictions for several packing types for the validation data.

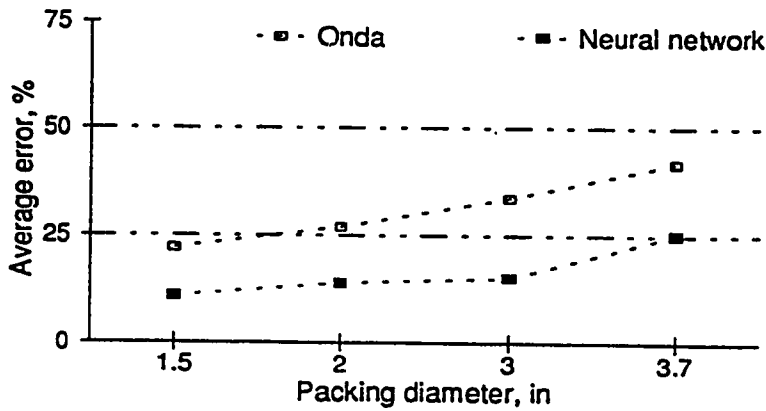


FIGURE 11. Average error in the neural network and the Onda predictions versus packing diameter for the validation data.

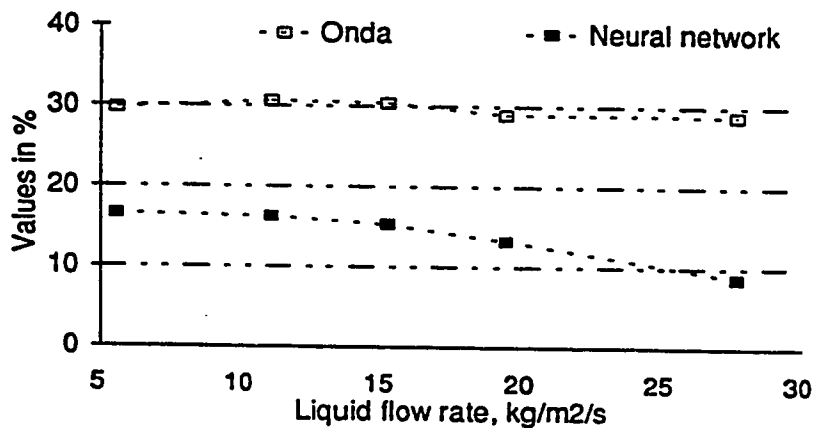


FIGURE 12. Average error in the neural network and Onda predictions versus liquid flow rate for the validation data.

CONCLUSION

This paper presents a nontraditional approach to the analysis of mass transfer coefficient in air stripping towers using a neural network model. As a first step, weights optimization and architecture selection of the NN model was performed using a large new set of experimental data. Four key variables were used in the model development. They are packing surface area, Henry's constant, and liquid and gas flow rates. In the validation step, the NN model had an error of 15% which represents 50% improvement over the Onda model predictions.

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APPENDIX A4.2

NETWORK SELECTION APPROACH AND TRAINING

Architecture Selection

The exact number of hidden neurons and the connectivity between layers must be specified prior to the network training. There is no effective procedure that identifies the optimal architecture of the network prior to training. The number of hidden layers and number of neurons in each hidden layer is determined via a trial and error procedure. There some general guidelines for the selection of the architecture and training, these are:

- An excessive number of hidden nodes may cause the network to memorize the training data. In such cases, the NN would not be able to interpolate effectively between adjacent training data points.
- Too few hidden nodes, on the other hand, will limit the network's ability to locate an adequate "relationship" between response and predictor variables.
- The network with the most compact architecture is preferable, therefore the architecture selection starts with the smallest number of hidden layer and neurons and increases in size as necessary.
- The initial step in the analysis investigates the required input to the network. Experience learned in previous work using the parametric and nonparametric approaches (Djebbar and Narbaitz, 1995b, 1998, Narbaitz and Djebbar, 1996) was used to select the input variables. The selection of the input variables was done via atrial and error procedure and by incrementing the number of inputs from one up. Several training runs were conducted using different numbers and combinations of variables. The best input representation consists of eight dimensionless numbers. These are liquid and gas phases Reynolds numbers, liquid and gas phases Schmidt numbers, Froude number, Weber number, packing efficiency number, and the geometry number, Ge .
- The first hidden layer should not contain more neurons than the number of input variables, i.e., eight, to avoid memorization of the network.
- If the data is noisy, which is in our case, it is helpful to have less neurons in the first hidden layer than in the following one, i.e., the second hidden layer.
- Nodes with very small relative weights usually indicate the small importance of the particular node compared to the other nodes, and its elimination should be investigated.

Training and Validation Data.

Various networks with different numbers of hidden nodes should be trained, and the network with the best performance on a test data set should be selected as the most adequate solution. It

is important to have training and validation data, which must be separate. The following considerations defined the subdivision:

- The subdivision was completely random. Some of the validation data were not used in the training. For example Michael et al., 1991 Rukovena (1987), Raczko et al. (1985), Hess et al. (1983), and Cline et al. (1985). However, some other validation data.
- The data transformation was done via a trial and error procedure. Linear, logarithmic and normal transformation were used using the following equations, respectively:

$$x_t = ax + b \quad (4a-1)$$

$$x_t = \text{Log}\left(\frac{x}{\bar{x}}\right) \quad (4a-1)$$

$$x_t = \frac{x - \bar{x}}{s_d} \quad (4a-1)$$

where x_t = the transform of x ; \bar{x} = sample mean value; and s_d = sample standard deviation, a and b coefficients that transforms x to values between -1 and 1. However, the normal transformation produced better results.

- Training will end if one of the following conditions is met: (i) the number of iteration equals 25,000, or (ii) the error between successive iteration is smaller than 0.001%. All the training sessions ended at the maximum number of iterations. An example of a training session produced the following results:

Table 4A.1. Errors resulting from a typical training session.

Number of iterations	100	1000	10000	15,000	20,000	25,000
Elapsed time, hrs	0.096	0.95	9.1	14.2	18.9	23.2
Error, %	70	44	35	33	31	30

- A typical training session lasts about 24 hrs in a Pentium Pro, 300 MHz IBM compatible PC.

APPENDIX A5

DATA BASE

Table A5-1 Studies author as presented in Table A5-3.

ID	Author	Number of data points
1	Narbaitz et al. (1998)	698
2	Cummins (1988)	105
3	Cummins and Westrick (1983)	104
4	Lamarche And Droste	150
5	Roberts et al. (1985)	300
6	Gossett et al. (1985)	280
7	Lang (1991)	67
8	Gross and Termaath (1983)	54
9	Michael et al. (1991)	6
10	Rukovena (1987)	54
11	Byers and Morton, 1985	24
12	Hess et al. (1983), Cline et al. (1985), Raczko et al. (1985)	90
13	Umphress et al. (1982)	12

Table A5-2. Surface critical tension of several material (N/m²)

Packing Material	Water	Ceramic	PVC	Polyethylene	Glass	Carbon	Paraffin	Metallic
ID #	1	2	3	4	5	6	7	8
Surface Critical tension	0.073	0.061	0.04	0.033	0.073	0.056	0.02	0.071

Table A5-3. Summary of the data

Audio ID	Packed depth, m	Liquid flow, kg/m ² /s	Gas flow, kg/m ² /s	Liquid Temperature, °C	Liquid viscosity, mPa·s	Gas viscosity, mPa·s	Liquid Density, kg/m ³	Gas Density, kg/m ³	Henry's Constant, atm	Liquid Critical Surface Tension, N/m ²	Dry Surface Area, m ² /m ³	Packing Diameter, mm	Tower Diameter, m	Observed Height, m	Compound ID	Packing ID
1	4.27	5.55	0.17	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	35.2	26	115
1	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	31.8	27	115
1	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	62.6	26	115
1	4.27	11.03	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	59.1	26	115
1	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	61.6	26	115
1	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	61.7	26	115
1	4.27	15.16	0.45	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	61.2	26	115
1	4.27	19.36	0.58	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	62.4	26	115
1	4.27	19.36	1.15	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	144.4	50.8	1	93.3	26	115
1	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	1.04E-09	9.46E-06	0.1459	0.072	144.4	50.8	1	101.1	26	115
1	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	1.04E-09	9.46E-06	0.1459	0.072	144.4	50.8	1	14.9	7	58
1	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	17.0	7	58
1	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	18.0	7	58
1	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	29.0	7	58
1	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	31.5	7	58
1	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	32.2	7	58
1	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	38.4	7	58
1	4.27	15.16	0.45	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	48.5	7	58
1	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	48.9	7	58
1	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	144.4	50.8	1	55.7	7	58
1	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.18E-10	8.54E-06	0.6834	0.072	144.4	50.8	1	61.8	7	58
1	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	9.18E-10	8.54E-06	0.6834	0.072	144.4	50.8	1	17.5	17	58
1	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	18.1	17	58
1	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	18.8	17	58
1	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	32.9	17	58
1	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	33.7	17	58
1	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	34.0	17	58
1	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	42.8	17	58
1	4.27	15.16	0.45	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	53.9	17	58
1	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	52.2	17	58
1	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	144.4	50.8	1	62.9	17	58
1	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.24E-10	8.47E-06	1.2189	0.072	144.4	50.8	1	70.0	17	58
1	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	9.24E-10	8.47E-06	1.2189	0.072	144.4	50.8	1	20.4	11	58
1	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	20.9	11	58
1	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	21.7	11	58
1	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	37.0	11	58
1	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	37.7	11	58
1	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	38.2	11	58
1	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	48.7	11	58
1	4.27	15.16	0.45	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	62.4	11	58
1	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	59.3	11	58
1	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	144.4	50.8	1	71.3	11	58
1	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.54E-10	8.72E-06	0.3806	0.072	144.4	50.8	1	79.4	11	58
1	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	9.54E-10	8.72E-06	0.3806	0.072	144.4	50.8	1	16.4	26	58
1	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	144.4	50.8	1	17.1	26	58
1	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	144.4	50.8	1	17.6	26	58

1	47	4.27	9.27	0.86	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	144.4	50.8	1	31.0	26	58
1	48	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	144.4	50.8	1	33.7	26	58
1	49	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	144.4	50.8	1	32.2	26	58
1	50	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	144.4	50.8	1	41.3	26	58
1	51	4.27	15.16	0.45	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	144.4	50.8	1	51.9	26	58
1	52	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	144.4	50.8	1	51.1	26	58
1	53	4.27	19.36	1.15	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	144.4	50.8	1	59.4	26	58
1	54	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	8.59E-10	7.82E-06	0.7073	0.072	0.033	144.4	50.8	1	65.5	26	58
1	55	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	8.59E-10	7.82E-06	0.7073	0.072	0.033	144.4	50.8	1	18.2	27	58
1	56	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	18.9	27	58
1	57	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	19.6	27	58
1	58	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	33.4	27	58
1	59	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	34.3	27	58
1	60	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	34.7	27	58
1	61	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	43.8	27	58
1	62	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	9.01E-10	8.57E-06	0.2843	0.072	0.033	144.4	50.8	1	55.2	27	58
1	63	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	53.4	27	58
1	64	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	63.7	27	58
1	65	4.27	23.49	0.70	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	70.0	27	58
1	66	4.27	27.62	0.82	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	144.4	50.8	1	17.1	7	58
1	67	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	17.3	7	58
1	68	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	30.6	7	58
1	69	4.27	5.55	0.66	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	32.4	7	58
1	70	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	17.3	9	58
1	71	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	18.5	9	58
1	72	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	30.5	9	58
1	73	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.45E-10	7.94E-06	0.1975	0.072	0.033	144.4	50.8	1	32.6	9	58
1	74	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	17.1	10	58
1	75	4.27	19.36	1.15	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	17.3	10	58
1	76	4.27	23.49	0.70	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	33.7	10	58
1	77	4.27	27.62	0.82	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	144.4	50.8	1	29.9	10	58
1	78	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	11.8	8	58
1	79	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	13.2	8	58
1	80	4.27	5.55	0.66	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	18.9	8	58
1	81	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	22.2	8	58
1	82	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	13.3	48	58
1	83	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	15.4	48	58
1	84	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.14E-10	7.75E-06	0.5555	0.072	0.033	144.4	50.8	1	17.6	48	58
1	85	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	26.7	48	58
1	86	4.27	19.36	1.15	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	35.0	17	53
1	87	4.27	23.49	0.70	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	39.9	17	53
1	88	4.27	27.62	0.82	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	144.4	50.8	1	39.3	17	53
1	89	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	41.9	17	53
1	90	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	49.4	17	53
1	91	4.27	5.55	0.66	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	69.4	17	53
1	92	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	34.6	11	53
1	93	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	41.4	11	53
1	94	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	39.2	11	53

1	95	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.23E-10	7.46E-06	0.1852	0.072	0.033	144.4	50.8	1	44.1	11	53
1	96	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	49.3	11	53
1	97	4.27	19.36	1.15	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	50.9	11	53
1	98	4.27	23.49	0.70	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	51.2	11	53
1	99	4.27	27.62	0.82	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	144.4	50.8	1	61.3	11	53
1	100	4.27	5.55	0.17	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	88.6	11	53
1	101	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	17.0	26	53
1	102	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	17.6	26	53
1	103	4.27	11.03	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	25.8	26	53
1	104	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	27.9	26	53
1	105	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	30.7	26	53
1	106	4.27	15.16	0.45	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	29.4	26	53
1	107	4.27	19.36	0.58	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	35.1	26	53
1	108	4.27	19.36	1.15	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	40.3	26	53
1	109	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	1.04E-09	9.46E-06	0.1459	0.072	0.033	102	50.8	1	55.3	26	53
1	110	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	1.04E-09	9.46E-06	0.1459	0.072	0.033	102	50.8	1	22.5	27	53
1	111	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	23.6	27	53
1	112	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	22.5	27	53
1	113	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	32.9	27	53
1	114	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	37.0	27	53
1	115	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	37.5	27	53
1	116	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	41.6	27	53
1	117	4.27	15.16	0.45	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	55.2	27	53
1	118	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	68.0	27	53
1	119	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	102	50.8	1	27.8	7	53
1	120	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.18E-10	8.54E-06	0.6834	0.072	0.033	102	50.8	1	31.4	7	53
1	121	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	9.18E-10	8.54E-06	0.6834	0.072	0.033	102	50.8	1	28.7	7	53
1	122	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	29.7	9	53
1	123	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	22.3	9	53
1	124	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	24.1	9	53
1	125	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	27.8	9	53
1	126	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	32.4	9	53
1	127	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	21.9	10	53
1	128	4.27	15.16	0.45	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	23.2	10	53
1	129	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	25.8	10	53
1	130	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	102	50.8	1	30.3	10	53
1	131	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.24E-10	8.47E-06	1.2189	0.072	0.033	102	50.8	1	16.0	8	53
1	132	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	9.24E-10	8.47E-06	1.2189	0.072	0.033	102	50.8	1	17.4	8	53
1	133	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	18.4	8	53
1	134	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	23.4	8	53
1	135	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	27.0	48	53
1	136	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	24.5	48	53
1	137	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	34.1	48	53
1	138	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	40.8	48	53
1	139	4.27	15.16	0.45	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	27.7	42	53
1	140	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	28.0	42	53
1	141	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	102	50.8	1	36.9	42	53
1	142	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.54E-10	8.72E-06	0.3806	0.072	0.033	102	50.8	1	37.5	42	53

1	143	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	9.54E-10	8.72E-06	0.3806	0.072	0.033	102	50.8	1	26.7	51	53
1	144	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	26.9	51	53
1	145	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	36.9	51	53
1	146	4.27	5.55	0.66	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	42.5	51	53
1	147	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	25.4	44	53
1	148	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	28.3	44	53
1	149	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	34.3	44	53
1	150	4.27	15.16	0.45	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	35.0	44	53
1	151	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	76.2	27	53
1	152	4.27	19.36	1.15	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	102	50.8	1	58.1	27	53
1	153	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	8.59E-10	7.82E-06	0.7073	0.072	0.033	102	50.8	1	61.2	27	53
1	154	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	8.59E-10	7.82E-06	0.7073	0.072	0.033	102	50.8	1	60.8	27	53
1	155	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	60.8	27	53
1	156	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	58.5	17	53
1	157	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	59.4	17	53
1	158	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	102	50.8	1	61.7	17	53
1	159	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.04E-09	9.02E-06	0.12	0.072	0.033	102	50.8	1	61.7	17	53
1	160	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.04E-09	9.02E-06	0.12	0.072	0.033	102	50.8	1	62.6	17	53
1	161	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.04E-09	9.02E-06	0.12	0.072	0.033	102	50.8	1	54.0	26	53
1	162	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.04E-09	9.02E-06	0.12	0.072	0.033	102	50.8	1	56.3	26	53
1	163	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.02E-09	8.66E-06	0.0455	0.072	0.033	102	50.8	1	60.3	26	53
1	164	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.02E-09	8.66E-06	0.0455	0.072	0.033	102	50.8	1	61.2	26	53
1	165	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.02E-09	8.66E-06	0.0455	0.072	0.033	102	50.8	1	61.8	26	53
1	166	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.02E-09	8.66E-06	0.0455	0.072	0.033	102	50.8	1	48.2	7	53
1	167	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.01E-09	8.36E-06	0.0354	0.072	0.033	102	50.8	1	51.3	7	53
1	168	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.01E-09	8.36E-06	0.0354	0.072	0.033	102	50.8	1	55.4	7	53
1	169	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.01E-09	8.36E-06	0.0354	0.072	0.033	102	50.8	1	59.0	7	53
1	170	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.01E-09	8.36E-06	0.0354	0.072	0.033	102	50.8	1	57.6	7	53
1	171	4.27	5.55	0.17	24.5	9.04E-04	1.83E-05	9.01E-10	8.57E-06	0.2843	0.072	0.033	102	50.8	1	39.6	6	53
1	172	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	102	50.8	1	43.7	6	53
1	173	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	102	50.8	1	57.2	6	53
1	174	4.27	11.03	0.33	24.5	9.04E-04	1.83E-05	9.01E-10	8.57E-06	0.2843	0.072	0.033	102	50.8	1	61.7	6	53
1	175	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	102	50.8	1	65.7	6	53
1	176	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	102	50.8	1	42.3	27	53
1	177	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	9.01E-10	8.57E-06	0.2843	0.072	0.033	102	50.8	1	50.0	27	53
1	178	4.27	19.36	0.58	24.5	9.04E-04	1.83E-05	9.01E-10	8.57E-06	0.2843	0.072	0.033	102	50.8	1	60.8	27	53
1	179	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.01E-10	8.57E-06	0.2843	0.072	0.033	102	50.8	1	64.8	27	53
1	180	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	9.01E-10	8.57E-06	0.2843	0.072	0.033	102	50.8	1	77.0	27	53
1	181	4.27	5.55	0.17	24.5	9.04E-04	1.83E-05	8.45E-10	7.94E-06	0.1975	0.072	0.033	102	50.8	1	83.7	27	53
1	182	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	102	50.8	1	46.8	17	53
1	183	4.27	5.55	0.66	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	102	50.8	1	53.1	17	53
1	184	4.27	11.03	0.33	24.5	9.04E-04	1.83E-05	8.45E-10	7.94E-06	0.1975	0.072	0.033	102	50.8	1	61.7	17	53
1	185	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	102	50.8	1	68.0	17	53
1	186	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	102	50.8	1	79.7	17	53
1	187	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.45E-10	7.94E-06	0.1975	0.072	0.033	102	50.8	1	85.1	17	53
1	188	4.27	19.36	0.58	24.5	9.04E-04	1.83E-05	8.45E-10	7.94E-06	0.1975	0.072	0.033	102	50.8	1	46.4	26	53
1	189	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	8.45E-10	7.94E-06	0.1975	0.072	0.033	102	50.8	1	52.7	26	53
1	190	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	8.45E-10	7.94E-06	0.1975	0.072	0.033	102	50.8	1	61.2	26	53

1	191	4.27	5.55	0.17	24.5	9.04E-04	1.83E-05	8.14E-10	7.75E-06	0.5555	0.072	0.033	102	50.8	1	66.2	26	53
1	192	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	102	50.8	1	78.3	26	53
1	193	4.27	5.55	0.66	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	102	50.8	1	83.7	26	53
1	194	4.27	11.03	0.33	24.5	9.04E-04	1.83E-05	8.14E-10	7.75E-06	0.5555	0.072	0.033	102	50.8	1	43.7	7	53
1	195	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	102	50.8	1	50.0	7	53
1	196	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	102	50.8	1	59.0	7	53
1	197	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.14E-10	7.75E-06	0.5555	0.072	0.033	102	50.8	1	62.1	7	53
1	198	4.27	19.36	0.58	24.5	9.04E-04	1.83E-05	8.14E-10	7.75E-06	0.5555	0.072	0.033	102	50.8	1	74.3	7	53
1	199	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	8.14E-10	7.75E-06	0.5555	0.072	0.033	102	50.8	1	79.2	7	53
1	200	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	8.14E-10	7.75E-06	0.5555	0.072	0.033	102	50.8	1	48.2	6	53
1	201	4.27	5.55	0.17	24.5	9.04E-04	1.83E-05	8.23E-10	7.46E-06	0.1852	0.072	0.033	102	50.8	1	53.1	6	53
1	202	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	102	50.8	1	61.7	6	53
1	203	4.27	5.55	0.66	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	102	50.8	1	66.2	6	53
1	204	4.27	11.03	0.33	24.5	9.04E-04	1.83E-05	8.23E-10	7.46E-06	0.1852	0.072	0.033	102	50.8	1	79.2	6	53
1	205	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	102	50.8	1	84.2	6	53
1	206	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	102	50.8	1	56.1	17	95
1	207	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.23E-10	7.46E-06	0.1852	0.072	0.033	102	50.8	1	55.2	17	95
1	208	4.27	19.36	0.58	24.5	9.04E-04	1.83E-05	8.23E-10	7.46E-06	0.1852	0.072	0.033	102	50.8	1	30.7	17	95
1	209	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	8.23E-10	7.46E-06	0.1852	0.072	0.033	102	50.8	1	34.7	17	95
1	210	4.27	27.62	0.82	24.5	9.04E-04	1.83E-05	8.23E-10	7.46E-06	0.1852	0.072	0.033	102	50.8	1	29.3	17	95
1	211	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	46.1	17	95
1	212	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	45.7	17	95
1	213	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	31.2	17	95
1	214	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	31.2	17	95
1	215	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	40.8	17	95
1	216	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	43.1	17	95
1	217	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	12.2	48	43
1	218	4.27	19.34	0.57	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	16.4	48	43
1	219	4.27	19.34	1.14	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	15.8	48	43
1	220	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	18.5	48	43
1	221	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	15.7	50	43
1	222	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	15.5	50	43
1	223	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	21.5	7	57
1	224	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	20.3	7	57
1	225	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	23.1	7	57
1	226	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	38.6	7	57
1	227	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	41.5	7	57
1	228	4.27	19.34	0.57	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	40.8	7	57
1	229	4.27	19.34	1.14	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	53.6	7	57
1	230	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	91.8	94	1	60.3	7	57
1	231	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	64.5	7	57
1	232	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	72.4	7	57
1	233	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	82.2	7	57
1	234	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	21.8	17	57
1	235	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	21.1	17	57
1	236	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	21.9	17	57
1	237	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	39.7	17	57
1	238	4.27	19.34	0.57	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	42.2	17	57

1	240	7.47	19.34	1.14	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	39.3	57
1	241	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	91.8	94	1	55.0	57
1	242	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	63.7	57
1	243	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	66.4	57
1	244	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	75.6	57
1	245	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	89.0	57
1	246	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	25.1	57
1	247	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	23.8	57
1	248	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	25.3	57
1	249	4.27	19.34	0.57	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	45.4	57
1	250	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	1	48.3	57
1	251	4.27	5.55	0.16	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	44.8	57
1	252	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	62.9	57
1	253	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	72.5	57
1	254	4.27	11.02	0.32	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	75.7	57
1	255	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	85.5	57
1	256	4.27	11.02	1.30	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	99.6	57
1	257	4.27	15.15	0.45	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	15.0	57
1	258	4.27	19.34	0.57	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	14.1	57
1	259	4.27	23.47	1.14	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	14.5	57
1	260	4.27	23.47	0.69	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	91.8	94	1	28.5	57
1	261	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	27.3	57
1	262	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	39.6	57
1	263	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	29.8	57
1	264	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	91.8	94	1	46.3	57
1	265	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.12E-09	9.20E-06	0.1375	0.071	0.033	91.8	94	1	47.6	57
1	266	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.12E-09	9.20E-06	0.1375	0.071	0.033	91.8	94	1	55.0	57
1	267	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.12E-09	9.20E-06	0.1375	0.071	0.033	91.8	94	1	69.6	57
1	268	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.12E-09	9.20E-06	0.1375	0.071	0.033	91.8	94	1	22.0	57
1	269	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.12E-09	9.20E-06	0.1375	0.071	0.033	91.8	94	1	21.3	57
1	270	4.27	5.55	1.30	28	8.36E-04	1.85E-05	1.11E-09	8.83E-06	0.0521	0.071	0.033	91.8	94	1	22.2	57
1	271	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.11E-09	8.83E-06	0.0521	0.071	0.033	91.8	94	1	40.3	57
1	272	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.11E-09	8.83E-06	0.0521	0.071	0.033	91.8	94	1	42.7	57
1	273	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.11E-09	8.83E-06	0.0521	0.071	0.033	91.8	94	1	40.3	57
1	274	4.27	5.55	1.30	28	8.36E-04	1.85E-05	1.09E-09	8.53E-06	0.0406	0.071	0.033	91.8	94	1	40.3	57
1	275	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.09E-09	8.53E-06	0.0406	0.071	0.033	91.8	94	1	55.0	57
1	276	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.09E-09	8.53E-06	0.0406	0.071	0.033	91.8	94	1	63.8	57
1	277	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.09E-09	8.53E-06	0.0406	0.071	0.033	91.8	94	1	66.0	57
1	278	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	91.8	94	1	74.7	57
1	279	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	91.8	94	1	90.5	57
1	280	4.27	11.02	0.32	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	91.8	94	1	16.7	57
1	281	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	91.8	94	1	18.6	57
1	282	4.27	5.55	1.30	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	91.8	94	1	16.5	57
1	283	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.24E-10	8.13E-06	0.2316	0.071	0.033	91.8	94	1	33.5	57
1	284	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.24E-10	8.13E-06	0.2316	0.071	0.033	91.8	94	1	34.8	57
1	285	4.27	11.02	0.32	28	8.36E-04	1.85E-05	9.24E-10	8.13E-06	0.2316	0.071	0.033	91.8	94	1	33.4	57
1	286	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.24E-10	8.13E-06	0.2316	0.071	0.033	91.8	94	1	37.0	57
1	287	4.27	5.55	1.30	28	8.36E-04	1.85E-05	8.91E-10	7.94E-06	0.6514	0.071	0.033	91.8	94	1	46.5	57
1	288	4.27	5.55	0.33	28	8.36E-04	1.85E-05	8.91E-10	7.94E-06	0.6514	0.071	0.033	91.8	94	1	53.3	57

1	287	4.27	11.02	0.65	28	8.36E-04	1.85E-05	8.91E-10	7.94E-06	0.6514	0.071	0.033	91.8	94	1	64.9	48
1	288	4.27	11.02	1.30	28	8.36E-04	1.85E-05	8.91E-10	7.94E-06	0.6514	0.071	0.033	91.8	94	1	77.1	48
1	289	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.00E-10	7.64E-06	0.2171	0.071	0.033	91.8	94	1	22.8	42
1	290	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.00E-10	7.64E-06	0.2171	0.071	0.033	91.8	94	1	23.7	42
1	291	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.00E-10	7.64E-06	0.2171	0.071	0.033	91.8	94	1	23.8	42
1	292	4.27	11.02	1.30	28	8.36E-04	1.85E-05	9.00E-10	7.64E-06	0.2171	0.071	0.033	91.8	94	1	44.4	42
1	293	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	1.13E-09	9.66E-06	0.1686	0.072	0.033	141.1	76.2	1	43.6	42
1	294	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	141.1	76.2	1	43.4	42
1	295	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	141.1	76.2	1	55.4	42
1	296	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	1.13E-09	9.66E-06	0.1686	0.072	0.033	141.1	76.2	1	66.4	42
1	297	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	141.1	76.2	1	65.9	42
1	298	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	141.1	76.2	1	74.3	42
1	299	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	141.1	76.2	1	88.3	42
1	300	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	1.13E-09	9.66E-06	0.1686	0.072	0.033	141.1	76.2	1	22.8	51
1	301	4.27	19.34	0.96	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	141.1	76.2	1	22.6	51
1	302	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	141.1	76.2	1	23.5	51
1	303	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	9.92E-10	8.71E-06	0.7773	0.072	0.033	141.1	76.2	1	40.2	51
1	304	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	141.1	76.2	1	43.8	51
1	305	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	141.1	76.2	1	42.8	51
1	306	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	9.92E-10	8.71E-06	0.7773	0.072	0.033	141.1	76.2	1	51.3	51
1	307	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	141.1	76.2	1	63.6	51
1	308	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	141.1	76.2	1	61.4	51
1	309	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	141.1	76.2	1	72.3	51
1	310	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	9.92E-10	8.71E-06	0.7773	0.072	0.033	141.1	76.2	1	79.4	51
1	311	4.27	19.34	0.96	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	141.1	76.2	1	23.9	44
1	312	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	141.1	76.2	1	24.5	44
1	313	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	9.98E-10	8.65E-06	1.3993	0.072	0.033	141.1	76.2	1	25.4	44
1	314	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	141.1	76.2	1	49.6	44
1	315	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	141.1	76.2	1	43.8	44
1	316	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	9.98E-10	8.65E-06	1.3993	0.072	0.033	141.1	76.2	1	42.7	44
1	317	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	141.1	76.2	1	59.3	44
1	318	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	141.1	76.2	1	68.5	44
1	319	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	141.1	76.2	1	68.4	44
1	320	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	9.98E-10	8.65E-06	1.3993	0.072	0.033	141.1	76.2	1	75.3	44
1	321	4.27	19.34	0.96	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	141.1	76.2	1	83.4	44
1	322	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	141.1	76.2	1	25.9	7
1	323	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	1.03E-09	8.90E-06	0.4423	0.072	0.033	141.1	76.2	1	28.1	7
1	324	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	141.1	76.2	1	27.8	7
1	325	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	141.1	76.2	1	40.8	7
1	326	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	1.03E-09	8.90E-06	0.4423	0.072	0.033	141.1	76.2	1	40.5	7
1	327	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	141.1	76.2	1	44.0	7
1	328	4.27	11.02	1.30	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	141.1	76.2	1	52.2	7
1	329	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.03E-09	8.90E-06	0.4423	0.072	0.033	141.1	76.2	1	58.9	7
1	330	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	141.1	76.2	1	61.0	7
1	331	4.27	19.34	0.96	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	141.1	76.2	1	69.2	7
1	332	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	141.1	76.2	1	21.5	17
1	333	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	9.28E-10	7.98E-06	0.8258	0.072	0.033	141.1	76.2	1	22.1	17
1	334	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	141.1	76.2	1	22.4	17

1	335	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	141.1	76.2	1	39.2	103
1	336	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	9.28E-10	7.98E-06	0.8258	0.072	0.033	141.1	76.2	1	39.0	103
1	337	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	141.1	76.2	1	38.6	103
1	338	4.27	11.02	1.30	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	141.1	76.2	1	51.2	103
1	339	4.27	15.15	0.45	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	141.1	76.2	1	56.4	103
1	340	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	9.28E-10	7.98E-06	0.8258	0.072	0.033	141.1	76.2	1	58.9	103
1	341	4.27	19.34	0.96	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	141.1	76.2	1	68.3	103
1	342	4.27	23.47	0.69	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	141.1	76.2	1	30.9	103
1	343	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	141.1	76.2	1	47.4	103
1	344	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	141.1	76.2	1	48.9	103
1	345	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	141.1	76.2	1	47.3	103
1	346	4.27	11.02	1.30	28	8.36E-04	1.85E-05	9.86E-10	8.77E-06	0.3856	0.071	0.033	141.1	76.2	1	61.6	103
1	347	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.24E-10	8.13E-06	0.2316	0.071	0.033	141.1	76.2	1	68.1	103
1	348	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.24E-10	8.13E-06	0.2316	0.071	0.033	141.1	76.2	1	73.0	103
1	349	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.24E-10	8.13E-06	0.2316	0.071	0.033	141.1	76.2	1	79.3	103
1	350	4.27	11.02	1.30	28	8.36E-04	1.85E-05	9.24E-10	8.13E-06	0.2316	0.071	0.033	141.1	76.2	1	16.1	103
1	351	4.27	5.55	0.33	28	8.36E-04	1.85E-05	8.91E-10	7.94E-06	0.6514	0.071	0.033	141.1	76.2	1	15.7	103
1	352	4.27	5.55	0.65	28	8.36E-04	1.85E-05	8.91E-10	7.94E-06	0.6514	0.071	0.033	141.1	76.2	1	15.1	103
1	353	4.27	11.02	0.65	28	8.36E-04	1.85E-05	8.91E-10	7.94E-06	0.6514	0.071	0.033	141.1	76.2	1	30.0	103
1	354	4.27	11.02	1.30	28	8.36E-04	1.85E-05	8.91E-10	7.94E-06	0.6514	0.071	0.033	141.1	76.2	1	28.7	103
1	355	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.00E-10	7.64E-06	0.2171	0.071	0.033	141.1	76.2	1	28.2	103
1	356	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.00E-10	7.64E-06	0.2171	0.071	0.033	141.1	76.2	1	39.9	103
1	357	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.00E-10	7.64E-06	0.2171	0.071	0.033	141.1	76.2	1	46.6	103
1	358	4.27	11.02	1.30	28	8.36E-04	1.85E-05	9.00E-10	7.64E-06	0.2171	0.071	0.033	141.1	76.2	1	46.2	103
1	359	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	55.9	103
1	360	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	24.0	103
1	361	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	20.9	103
1	362	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	39.4	103
1	363	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	41.1	103
1	364	4.27	11.02	0.92	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	39.0	103
1	365	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	52.2	103
1	366	4.27	19.34	0.57	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	57.2	103
1	367	4.27	23.47	0.55	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	61.9	103
1	368	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	115	50.8	1	66.5	103
1	369	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	115	50.8	1	27.1	103
1	370	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	115	50.8	1	27.3	103
1	371	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	115	50.8	1	41.0	103
1	372	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	115	50.8	1	43.7	103
1	373	4.27	11.02	0.92	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	115	50.8	1	24.5	103
1	374	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	115	50.8	1	25.7	103
1	375	4.27	19.34	0.57	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	115	50.8	1	40.6	103
1	376	4.27	23.47	0.55	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	44.3	103
1	377	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	25.2	103
1	378	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	27.0	103
1	379	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	41.7	103
1	380	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	44.8	103
1	381	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	17.8	103
1	382	4.27	11.02	0.92	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	22.6	103

384	4.27	13.13	0.49	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	31.7	8	103
385	4.27	19.34	0.57	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	35.6	8	103
386	4.27	23.47	0.55	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	115	50.8	1	17.6	17	37
387	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	115	50.8	1	17.0	17	37
388	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	115	50.8	1	15.9	17	37
389	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	115	50.8	1	17.9	17	37
390	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	115	50.8	1	30.0	48	58
391	4.27	11.02	0.92	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	115	50.8	1	30.9	48	58
392	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	115	50.8	1	34.3	48	58
393	4.27	19.34	0.57	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	115	50.8	1	42.3	48	58
394	4.27	23.47	0.55	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	115	50.8	1	48.0	48	58
395	4.27	5.55	0.16	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	57.4	48	58
396	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	18.1	42	42
397	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	18.9	42	42
398	4.27	11.02	0.32	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	18.0	42	42
399	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	35.9	42	42
400	4.27	11.02	0.92	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	34.2	42	42
401	4.27	15.15	0.45	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	34.4	42	42
402	4.27	19.34	0.57	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	44.8	42	42
403	4.27	23.47	0.55	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	115	50.8	1	56.2	42	42
404	4.27	5.55	0.16	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	70.4	42	42
405	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	19.0	51	58
406	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	115	50.8	1	19.2	51	58
407	4.27	11.02	0.32	28	8.36E-04	1.85E-05	1.12E-09	9.20E-06	0.1375	0.071	0.033	115	50.8	1	21.1	51	58
408	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.12E-09	9.20E-06	0.1375	0.071	0.033	115	50.8	1	35.3	51	58
409	4.27	15.15	0.33	28	8.36E-04	1.85E-05	1.11E-09	8.83E-06	0.0521	0.071	0.033	115	50.8	1	35.2	51	58
410	4.27	19.34	0.55	28	8.36E-04	1.85E-05	1.09E-09	8.53E-06	0.0406	0.071	0.033	115	50.8	1	35.1	51	58
411	4.27	23.47	0.55	28	8.36E-04	1.85E-05	1.09E-09	8.53E-06	0.0406	0.071	0.033	115	50.8	1	45.8	51	58
412	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	1.13E-09	9.66E-06	0.1686	0.072	0.033	88.6	76.2	1	56.6	51	58
413	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	88.6	76.2	1	62.6	51	58
414	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	88.6	76.2	1	66.6	51	58
415	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	1.13E-09	9.66E-06	0.1686	0.072	0.033	88.6	76.2	1	17.7	44	58
416	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	88.6	76.2	1	19.1	44	58
417	4.27	11.02	1.23	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	88.6	76.2	1	20.9	44	58
418	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	88.6	76.2	1	37.0	44	58
419	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	1.13E-09	9.66E-06	0.1686	0.072	0.033	88.6	76.2	1	35.0	44	58
420	4.27	19.34	1.00	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	88.6	76.2	1	36.2	44	58
421	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.14E-09	9.69E-06	0.1727	0.071	0.033	88.6	76.2	1	46.3	44	58
422	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	9.92E-10	8.71E-06	0.7773	0.072	0.033	88.6	76.2	1	57.8	44	58
423	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	88.6	76.2	1	59.1	44	58
424	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	88.6	76.2	1	66.0	44	58
425	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	9.92E-10	8.71E-06	0.7773	0.072	0.033	88.6	76.2	1	23.9	7	96
426	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	88.6	76.2	1	26.2	7	96
427	4.27	11.02	1.23	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	88.6	76.2	1	27.4	7	96
428	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	88.6	76.2	1	36.1	7	96
429	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	9.92E-10	8.71E-06	0.7773	0.072	0.033	88.6	76.2	1	35.8	7	96
430	4.27	19.34	1.00	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	88.6	76.2	1	33.8	7	96

1	431	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.00E-09	8.74E-06	0.7939	0.071	0.033	88.6	76.2	1	47.0	96
1	432	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	9.98E-10	8.65E-06	1.3993	0.072	0.033	88.6	76.2	1	46.0	96
1	433	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	88.6	76.2	1	43.0	96
1	434	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	88.6	76.2	1	41.4	96
1	435	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	9.98E-10	8.65E-06	1.3993	0.072	0.033	88.6	76.2	1	23.5	17
1	436	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	88.6	76.2	1	22.2	17
1	437	4.27	11.02	1.23	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	88.6	76.2	1	22.3	17
1	438	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	88.6	76.2	1	40.6	17
1	439	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	9.98E-10	8.65E-06	1.3993	0.072	0.033	88.6	76.2	1	39.0	17
1	440	4.27	19.34	1.00	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	88.6	76.2	1	35.8	17
1	441	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.01E-09	8.68E-06	1.4314	0.071	0.033	88.6	76.2	1	52.8	17
1	442	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	1.03E-09	8.90E-06	0.4423	0.072	0.033	88.6	76.2	1	53.5	17
1	443	4.27	5.55	0.33	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	88.6	76.2	1	53.8	17
1	444	4.27	5.55	0.65	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	88.6	76.2	1	51.7	17
1	445	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	1.03E-09	8.90E-06	0.4423	0.072	0.033	88.6	76.2	1	31.8	11
1	446	4.27	11.02	0.65	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	88.6	76.2	1	30.2	11
1	447	4.27	11.02	1.23	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	88.6	76.2	1	31.2	11
1	448	4.27	15.15	0.45	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	88.6	76.2	1	56.3	11
1	449	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	1.03E-09	8.90E-06	0.4423	0.072	0.033	88.6	76.2	1	54.6	11
1	450	4.27	19.34	1.00	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	88.6	76.2	1	50.3	11
1	451	4.27	23.47	0.69	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	88.6	76.2	1	72.2	11
1	452	4.27	5.55	0.16	27.5	8.45E-04	1.85E-05	9.28E-10	7.98E-06	0.8258	0.072	0.033	88.6	76.2	1	70.6	11
1	453	4.27	5.55	0.33	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	88.6	76.2	1	74.8	11
1	454	4.27	5.55	0.65	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	88.6	76.2	1	64.9	11
1	455	4.27	11.03	0.33	27.5	8.45E-04	1.85E-05	9.28E-10	7.98E-06	0.8258	0.072	0.033	88.6	76.2	1	10.9	26
1	456	4.27	11.02	0.65	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	88.6	76.2	1	10.3	26
1	457	4.27	11.02	1.23	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	88.6	76.2	1	9.6	26
1	458	4.27	15.15	0.45	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	88.6	76.2	1	20.0	26
1	459	4.27	19.35	0.57	27.5	8.45E-04	1.85E-05	9.28E-10	7.98E-06	0.8258	0.072	0.033	88.6	76.2	1	18.7	26
1	460	4.27	19.34	1.00	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	88.6	76.2	1	16.5	26
1	461	4.27	23.47	0.69	28	8.36E-04	1.85E-05	9.40E-10	8.01E-06	0.8472	0.071	0.033	88.6	76.2	1	26.9	26
1	462	4.27	5.55	0.16	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	27.7	26
1	463	4.27	5.55	0.33	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	26.5	26
1	464	4.27	5.55	0.66	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	30.1	26
1	465	4.27	11.03	0.33	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	22.2	27
1	466	4.27	11.03	0.65	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	20.1	27
1	467	4.27	11.03	1.04	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	22.0	27
1	468	4.27	15.16	0.45	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	41.9	27
1	469	4.27	19.35	0.57	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	40.8	27
1	470	4.27	23.48	0.64	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	36.5	27
1	471	4.27	5.55	0.16	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	54.6	27
1	472	4.27	5.55	0.33	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	52.5	27
1	473	4.27	5.55	0.66	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	55.1	27
1	474	4.27	11.03	0.33	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	50.3	27
1	475	4.27	11.03	0.65	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	27.3	7
1	476	4.27	11.03	1.04	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	28.2	7
1	477	4.27	15.16	0.45	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	44.1	7
1	478	4.27	19.35	0.57	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	39.7	7

1	479	4.27	23.48	0.64	26	8.74E-04	1.84E-05	9.54E-10	8.62E-06	0.7291	0.072	0.033	148	50.8	1	32.9	9	96
1	480	4.27	5.55	0.16	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	27.6	9	96
1	481	4.27	5.55	0.33	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	47.4	9	96
1	482	4.27	5.55	0.66	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	40.1	9	96
1	483	4.27	11.03	0.33	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	34.7	10	96
1	484	4.27	11.03	0.65	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	27.2	10	96
1	485	4.27	11.03	1.04	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	50.0	10	96
1	486	4.27	15.16	0.45	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	37.6	10	96
1	487	4.27	19.35	0.57	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	25.6	8	96
1	488	4.27	23.48	0.64	26	8.74E-04	1.84E-05	9.60E-10	8.56E-06	1.3064	0.072	0.033	148	50.8	1	26.2	8	96
1	489	4.27	5.55	0.33	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	40.2	8	96
1	490	4.27	5.55	0.66	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	29.6	8	96
1	491	4.27	5.55	0.66	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	13.9	48	96
1	492	4.27	11.03	0.33	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	13.5	48	96
1	493	4.27	11.03	0.65	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	26.7	48	96
1	494	4.27	11.03	1.04	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	27.6	48	96
1	495	4.27	15.16	0.45	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	26.4	42	96
1	496	4.27	19.35	0.57	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	31.6	42	96
1	497	4.27	23.48	0.64	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	1	45.1	42	96
1	498	4.27	5.55	0.16	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	48.7	42	96
1	499	4.27	5.55	0.33	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	28.7	51	96
1	500	4.27	5.55	0.66	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	31.1	51	96
1	501	4.27	11.03	0.33	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	49.8	51	96
1	502	4.27	11.03	0.65	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	50.8	51	96
1	503	4.27	11.03	1.04	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	27.9	44	96
1	504	4.27	15.16	0.45	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	29.8	44	96
1	505	4.27	19.35	0.57	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	43.4	44	96
1	506	4.27	23.48	0.64	26	8.74E-04	1.84E-05	8.93E-10	7.90E-06	0.7646	0.072	0.033	148	50.8	1	45.9	44	96
1	507	4.27	5.55	0.33	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	19.7	7	44
1	508	4.27	5.55	0.66	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	21.5	7	44
1	509	4.27	11.03	0.33	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	28.2	7	44
1	510	4.27	11.03	0.65	26	8.74E-04	1.84E-05	1.08E-09	9.56E-06	0.1569	0.072	0.033	148	50.8	1	34.9	7	44
1	511	4.27	5.55	0.33	26	8.74E-04	1.84E-05	1.07E-09	9.08E-06	0.1256	0.072	0.033	148	50.8	1	40.8	7	44
1	512	4.27	5.55	0.66	26	8.74E-04	1.84E-05	1.07E-09	9.08E-06	0.1256	0.072	0.033	148	50.8	1	37.8	7	44
1	513	4.27	11.03	0.65	26	8.74E-04	1.84E-05	1.07E-09	9.08E-06	0.1256	0.072	0.033	148	50.8	1	50.0	7	44
1	514	4.27	11.03	1.04	26	8.74E-04	1.84E-05	1.07E-09	9.08E-06	0.1256	0.072	0.033	148	50.8	1	43.5	7	44
1	515	4.27	5.55	0.33	26	8.74E-04	1.84E-05	1.05E-09	8.72E-06	0.0476	0.072	0.033	148	50.8	1	63.0	7	44
1	516	4.27	5.55	0.66	26	8.74E-04	1.84E-05	1.05E-09	8.72E-06	0.0476	0.072	0.033	148	50.8	1	71.7	7	44
1	517	4.27	11.03	0.33	26	8.74E-04	1.84E-05	1.05E-09	8.72E-06	0.0476	0.072	0.033	148	50.8	1	23.1	17	44
1	518	4.27	11.03	0.65	26	8.74E-04	1.84E-05	1.05E-09	8.72E-06	0.0476	0.072	0.033	148	50.8	1	24.0	17	44
1	519	4.27	5.55	0.33	26	8.74E-04	1.84E-05	1.04E-09	8.41E-06	0.0371	0.072	0.033	148	50.8	1	23.0	17	44
1	520	4.27	5.55	0.66	26	8.74E-04	1.84E-05	1.04E-09	8.41E-06	0.0371	0.072	0.033	148	50.8	1	42.6	17	44
1	521	4.27	11.03	0.65	26	8.74E-04	1.84E-05	1.04E-09	8.41E-06	0.0371	0.072	0.033	148	50.8	1	44.8	17	44
1	522	4.27	11.03	1.04	26	8.74E-04	1.84E-05	1.04E-09	8.41E-06	0.0371	0.072	0.033	148	50.8	1	43.8	17	44
1	523	4.27	5.55	0.33	27	8.54E-04	1.84E-05	9.61E-10	8.71E-06	0.3537	0.072	0.033	148	50.8	1	53.0	17	44
1	524	4.27	5.55	0.66	27	8.54E-04	1.84E-05	9.61E-10	8.71E-06	0.3537	0.072	0.033	148	50.8	1	60.1	17	44
1	525	4.27	11.03	0.65	27	8.54E-04	1.84E-05	9.61E-10	8.71E-06	0.3537	0.072	0.033	148	50.8	1	71.0	17	44
1	526	4.27	11.03	1.04	27	8.54E-04	1.84E-05	9.61E-10	8.71E-06	0.3537	0.072	0.033	148	50.8	1	83.4	17	44

Anchor ID	Data ID	Packed depth, m	Liquid flow, kg/m ² /s	Gas flow, kg/m ² /s	Liquid Temp, °C	Liquid Viscosity, m ² /s	Gas Viscosity, m ² /s	Liquid Density, kg/m ³	Gas Density, kg/m ³	Henry's Coefficient, atm	Liquid Critical Temp, °C	Packing Critical Temp, °C	Dry Surface Area, m ² /m ³	Packing Diameter, mm	Tower Diameter, mm	Observed K _{La} , 1/s	Compound ID
1	527	4.27	5.55	0.33	27	8.54E-04	1.84E-05	9.01E-10	8.07E-06	0.2214	0.072	0.033	148	50.8	1	42.5	11
1	528	4.27	5.55	0.66	27	8.54E-04	1.84E-05	9.01E-10	8.07E-06	0.2214	0.072	0.033	148	50.8	1	39.8	11
1	529	4.27	11.03	0.65	27	8.54E-04	1.84E-05	9.01E-10	8.07E-06	0.2214	0.072	0.033	148	50.8	1	38.4	11
1	530	4.27	11.03	1.04	27	8.54E-04	1.84E-05	9.01E-10	8.07E-06	0.2214	0.072	0.033	148	50.8	1	58.7	11
1	531	4.27	5.55	0.33	27	8.54E-04	1.84E-05	8.68E-10	7.88E-06	0.6227	0.072	0.033	148	50.8	1	59.3	11
1	532	4.27	5.55	0.66	27	8.54E-04	1.84E-05	8.68E-10	7.88E-06	0.6227	0.072	0.033	148	50.8	1	58.8	11
1	533	4.27	11.03	0.65	27	8.54E-04	1.84E-05	8.68E-10	7.88E-06	0.6227	0.072	0.033	148	50.8	1	72.4	11
1	534	4.27	11.03	1.04	27	8.54E-04	1.84E-05	8.68E-10	7.88E-06	0.6227	0.072	0.033	148	50.8	1	86.4	11
1	535	4.27	5.55	0.33	27	8.54E-04	1.84E-05	8.78E-10	7.59E-06	0.2076	0.072	0.033	148	50.8	1	94.4	11
1	536	4.27	5.55	0.66	27	8.54E-04	1.84E-05	8.78E-10	7.59E-06	0.2076	0.072	0.033	148	50.8	1	109.8	11
1	537	4.27	11.03	0.65	27	8.54E-04	1.84E-05	8.78E-10	7.59E-06	0.2076	0.072	0.033	148	50.8	1	30.8	26
1	538	4.27	11.03	1.04	27	8.54E-04	1.84E-05	8.78E-10	7.59E-06	0.2076	0.072	0.033	148	50.8	1	17.4	26
1	539	4.27	5.55	0.17	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	15.8	26
1	540	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	39.1	26
1	541	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	34.1	26
1	542	4.27	11.03	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	31.4	26
1	543	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	37.5	26
1	544	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	54.8	26
1	545	4.27	15.16	0.45	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	53.3	26
1	546	4.27	19.36	0.58	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	66.4	26
1	547	4.27	19.36	1.15	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	35.2	27
1	548	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	1.04E-09	9.46E-06	0.1459	0.072	0.033	227	25.4	1	33.7	27
1	549	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	32.0	27
1	550	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	46.6	27
1	551	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	42.7	27
1	552	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	40.0	27
1	553	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	46.1	27
1	554	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	66.1	27
1	555	4.27	15.16	0.45	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	68.1	27
1	556	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	83.0	27
1	557	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	227	25.4	1	27.0	48
1	558	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.18E-10	8.54E-06	0.6834	0.072	0.033	227	25.4	1	19.1	48
1	559	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	32.6	48
1	560	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	32.4	48
1	561	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	32.4	48
1	562	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	31.0	42
1	563	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	33.4	42
1	564	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	44.0	42
1	565	4.27	15.16	0.45	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	53.7	42
1	566	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	32.4	51
1	567	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.36E-10	8.50E-06	1.2475	0.072	0.033	227	25.4	1	35.5	51
1	568	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.24E-10	8.47E-06	1.2189	0.072	0.033	227	25.4	1	47.8	44
1	569	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	48.8	44
1	570	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	30.3	44
1	571	4.27	5.55	0.66	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	33.6	44
1	572	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	41.9	44
1	573	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	49.8	44
1	574	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	32.4	7
1	574	4.27	11.03	1.31	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	33.2	7

576	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	33.4	7	39
577	4.27	19.36	1.15	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	227	25.4	1	51.6	7	39
578	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	9.54E-10	8.72E-06	0.3806	0.072	0.033	227	25.4	1	52.4	7	39
579	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	57.0	7	39
580	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	63.5	7	39
581	4.27	5.55	0.66	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	70.8	7	39
582	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	74.0	7	39
583	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	32.4	17	39
584	4.27	11.03	1.31	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	32.8	17	39
585	4.27	15.16	0.45	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	33.4	17	39
586	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	46.5	17	39
587	4.27	19.36	1.15	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	227	25.4	1	45.5	17	39
588	4.27	23.49	0.70	24.5	9.04E-04	1.83E-05	8.59E-10	7.82E-06	0.7073	0.072	0.033	227	25.4	1	63.4	17	39
589	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	78.1	17	39
590	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	87.5	17	39
591	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	38.9	11	39
592	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	227	25.4	1	40.5	11	39
593	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.04E-09	9.02E-06	0.12	0.072	0.033	227	25.4	1	40.4	11	39
594	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.04E-09	9.02E-06	0.12	0.072	0.033	227	25.4	1	69.6	11	39
595	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.04E-09	9.02E-06	0.12	0.072	0.033	227	25.4	1	66.8	11	39
596	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.04E-09	9.02E-06	0.12	0.072	0.033	227	25.4	1	71.2	11	39
597	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.02E-09	8.66E-06	0.0455	0.072	0.033	227	25.4	1	86.7	11	39
598	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.02E-09	8.66E-06	0.0455	0.072	0.033	227	25.4	1	106.8	11	39
599	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.02E-09	8.66E-06	0.0455	0.072	0.033	227	25.4	1	115.0	11	39
600	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.02E-09	8.66E-06	0.0455	0.072	0.033	227	25.4	1	31.8	26	39
601	4.27	5.55	0.33	25	8.94E-04	1.83E-05	1.01E-09	8.36E-06	0.0354	0.072	0.033	227	25.4	1	31.2	26	39
602	4.27	5.55	0.66	25	8.94E-04	1.83E-05	1.01E-09	8.36E-06	0.0354	0.072	0.033	227	25.4	1	31.9	26	39
603	4.27	11.03	0.66	25	8.94E-04	1.83E-05	1.01E-09	8.36E-06	0.0354	0.072	0.033	227	25.4	1	55.5	26	39
604	4.27	11.03	1.31	25	8.94E-04	1.83E-05	1.01E-09	8.36E-06	0.0354	0.072	0.033	227	25.4	1	52.5	26	39
605	4.27	5.55	0.17	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	227	25.4	1	54.2	26	39
606	4.27	5.55	0.33	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	227	25.4	1	63.1	26	39
607	4.27	11.03	0.33	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	227	25.4	1	70.0	26	39
608	4.27	11.03	0.66	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	227	25.4	1	82.2	26	39
609	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	9.01E-10	8.57E-06	0.2843	0.072	0.033	227	25.4	1	32.1	27	39
610	4.27	19.36	0.58	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	227	25.4	1	34.1	27	39
611	4.27	23.49	0.70	25	8.94E-04	1.83E-05	9.13E-10	8.60E-06	0.2971	0.072	0.033	227	25.4	1	32.8	27	39
612	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	227	25.4	1	57.9	27	39
613	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	227	25.4	1	55.3	27	39
614	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	227	25.4	1	60.0	27	39
615	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	227	25.4	1	59.3	27	39
616	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.45E-10	7.94E-06	0.1975	0.072	0.033	227	25.4	1	83.3	27	39
617	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	227	25.4	1	85.7	27	39
618	4.27	23.49	0.70	25	8.94E-04	1.83E-05	8.56E-10	7.97E-06	0.2021	0.072	0.033	227	25.4	1	27.4	7	39
619	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	227	25.4	1	31.8	7	39
620	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	227	25.4	1	30.5	9	39
621	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	227	25.4	1	29.9	9	39
622	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	227	25.4	1	36.3	10	39

1	623	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.14E-10	7.75E-06	0.5555	0.072	0.033	227	25.4	1	34.0	10	39
1	624	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	227	25.4	1	29.0	8	39
1	625	4.27	23.49	0.70	25	8.94E-04	1.83E-05	8.25E-10	7.78E-06	0.5684	0.072	0.033	227	25.4	1	26.3	8	39
1	626	4.27	5.55	0.17	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	227	25.4	1	18.7	7	42
1	627	4.27	5.55	0.33	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	227	25.4	1	20.0	7	42
1	628	4.27	11.03	0.33	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	227	25.4	1	20.1	7	42
1	629	4.27	11.03	0.66	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	227	25.4	1	30.6	7	42
1	630	4.27	15.16	0.45	24.5	9.04E-04	1.83E-05	8.23E-10	7.46E-06	0.1852	0.072	0.033	227	25.4	1	33.4	7	42
1	631	4.27	19.36	0.58	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	227	25.4	1	34.1	7	42
1	632	4.27	23.49	0.70	25	8.94E-04	1.83E-05	8.34E-10	7.49E-06	0.1895	0.072	0.033	227	25.4	1	37.8	7	42
1	633	4.27	5.55	0.16	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	47.5	7	42
1	634	4.27	5.55	0.33	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	45.6	7	42
1	635	4.27	5.55	0.66	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	51.8	7	42
1	636	4.27	11.03	0.33	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	20.0	17	42
1	637	4.27	11.03	0.65	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	21.1	17	42
1	638	4.27	11.03	1.30	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	20.7	17	42
1	639	4.27	15.15	0.45	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	35.6	17	42
1	640	4.27	19.35	0.57	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	36.6	17	42
1	641	4.27	19.35	1.14	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	36.8	17	42
1	642	4.27	23.48	0.69	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	44.7	17	42
1	643	4.27	5.55	0.16	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	55.5	17	42
1	644	4.27	5.55	0.33	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	53.3	17	42
1	645	4.27	5.55	0.66	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	63.0	17	42
1	646	4.27	11.03	0.33	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	23.2	11	42
1	647	4.27	11.03	0.65	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	25.2	11	42
1	648	4.27	11.03	1.30	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	24.5	11	42
1	649	4.27	15.15	0.45	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	41.1	11	42
1	650	4.27	19.35	0.57	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	42.3	11	42
1	651	4.27	19.35	1.14	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	42.7	11	42
1	652	4.27	23.48	0.69	27	8.54E-04	1.84E-05	9.79E-10	8.68E-06	0.7609	0.072	0.033	131.2	26.9	1	53.6	11	42
1	655	4.27	5.55	0.66	27	8.54E-04	1.84E-05	9.85E-10	8.62E-06	1.3677	0.072	0.033	131.2	26.9	1	63.9	11	42
1	656	4.27	11.03	0.33	27	8.54E-04	1.84E-05	9.85E-10	8.62E-06	1.3677	0.072	0.033	131.2	26.9	1	64.3	11	42
1	657	4.27	11.03	0.65	27	8.54E-04	1.84E-05	9.85E-10	8.62E-06	1.3677	0.072	0.033	131.2	26.9	1	75.4	11	42
1	658	4.27	11.03	1.30	27	8.54E-04	1.84E-05	9.85E-10	8.62E-06	1.3677	0.072	0.033	131.2	26.9	1	20.0	26	42
1	659	4.27	15.15	0.45	27	8.54E-04	1.84E-05	9.85E-10	8.62E-06	1.3677	0.072	0.033	131.2	26.9	1	22.9	26	42
1	660	4.27	19.35	0.57	27	8.54E-04	1.84E-05	9.85E-10	8.62E-06	1.3677	0.072	0.033	131.2	26.9	1	23.5	26	42
1	661	4.27	19.35	1.14	27	8.54E-04	1.84E-05	9.85E-10	8.62E-06	1.3677	0.072	0.033	131.2	26.9	1	34.9	26	42
1	662	4.27	23.48	0.69	27	8.54E-04	1.84E-05	9.85E-10	8.62E-06	1.3677	0.072	0.033	131.2	26.9	1	36.5	26	42
1	663	4.27	5.55	0.16	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	36.9	26	42
1	664	4.27	5.55	0.33	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	43.5	26	42
1	665	4.27	5.55	0.66	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	52.1	26	42
1	666	4.27	11.03	0.33	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	51.3	26	42
1	667	4.27	11.03	0.65	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	60.4	26	42
1	668	4.27	11.03	1.30	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	19.6	27	42
1	669	4.27	15.15	0.45	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	20.1	27	42
1	670	4.27	19.35	0.57	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	19.9	27	42
1	671	4.27	19.35	1.14	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	35.0	27	42
1	672	4.27	23.48	0.69	27	8.54E-04	1.84E-05	1.02E-09	8.87E-06	0.4315	0.072	0.033	131.2	26.9	1	33.9	27	42

1	673	4.27	5.55	0.16	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	33.7	27	42
1	674	4.27	5.55	0.33	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	44.8	27	42
1	676	4.27	11.03	0.33	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	53.4	27	42
1	677	4.27	11.03	0.65	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	51.3	27	42
1	678	4.27	11.03	1.30	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	62.4	27	42
1	679	4.27	15.15	0.45	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	20.1	7	53
1	680	4.27	19.35	0.57	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	29.7	7	53
1	681	4.27	19.35	1.14	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	27.2	7	53
1	682	4.27	23.48	0.69	27	8.54E-04	1.84E-05	9.16E-10	7.96E-06	0.805	0.072	0.033	131.2	26.9	1	29.0	7	53
1	683	4.27	5.55	0.33	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	34.1	7	53
1	684	4.27	5.55	0.66	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	29.6	7	53
1	685	4.27	11.03	0.65	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	34.0	7	53
1	686	4.27	11.03	1.30	27	8.54E-04	1.84E-05	1.11E-09	9.62E-06	0.1647	0.072	0.033	131.2	26.9	1	39.7	7	53
1	687	4.27	5.55	0.33	27	8.54E-04	1.84E-05	1.09E-09	9.14E-06	0.1315	0.072	0.033	131.2	26.9	1	52.1	7	53
1	688	4.27	5.55	0.66	27	8.54E-04	1.84E-05	1.09E-09	9.14E-06	0.1315	0.072	0.033	131.2	26.9	1	29.0	17	53
1	689	4.27	11.03	0.65	27	8.54E-04	1.84E-05	1.09E-09	9.14E-06	0.1315	0.072	0.033	131.2	26.9	1	34.7	17	53
1	690	4.27	11.03	1.30	27	8.54E-04	1.84E-05	1.09E-09	9.14E-06	0.1315	0.072	0.033	131.2	26.9	1	32.1	17	53
1	691	4.27	5.55	0.33	27	8.54E-04	1.84E-05	1.08E-09	8.77E-06	0.0498	0.072	0.033	131.2	26.9	1	88.4	21	53
1	692	4.27	5.55	0.66	27	8.54E-04	1.84E-05	1.08E-09	8.77E-06	0.0498	0.072	0.033	131.2	26.9	1	88.8	21	53
1	693	4.27	11.03	0.65	27	8.54E-04	1.84E-05	1.08E-09	8.77E-06	0.0498	0.072	0.033	131.2	26.9	1	64.5	50	53
1	694	4.27	11.03	1.30	27	8.54E-04	1.84E-05	1.08E-09	8.77E-06	0.0498	0.072	0.033	131.2	26.9	1	67.8	50	53
1	695	4.27	5.55	0.33	27	8.54E-04	1.84E-05	1.06E-09	8.47E-06	0.0388	0.072	0.033	131.2	26.9	1	65.1	50	53
1	696	4.27	5.55	0.66	27	8.54E-04	1.84E-05	1.06E-09	8.47E-06	0.0388	0.072	0.033	131.2	26.9	1	72.4	50	53
1	697	4.27	11.03	0.65	27	8.54E-04	1.84E-05	1.06E-09	8.47E-06	0.0388	0.072	0.033	131.2	26.9	1	33.9	26	96
1	698	4.27	11.03	1.30	27	8.54E-04	1.84E-05	1.06E-09	8.47E-06	0.0388	0.072	0.033	131.2	26.9	1	28.7	26	96
2	1	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	148	50.8	0.61	41.9	26	96
2	2	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	148	50.8	0.61	46.1	26	96
2	3	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	148	50.8	0.61	43.0	26	96
2	4	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	148	50.8	0.61	52.2	26	96
2	5	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	148	50.8	0.61	48.6	26	96
2	6	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	148	50.8	0.61	55.3	26	96
2	7	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	148	50.8	0.61	55.0	26	96
2	8	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	148	50.8	0.61	65.7	26	96
2	9	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	148	50.8	0.61	65.6	26	96
2	10	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	148	50.8	0.61	98.0	26	96
2	11	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	148	50.8	0.61	36.1	27	96
2	12	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	148	50.8	0.61	36.3	27	96
2	13	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	148	50.8	0.61	43.8	27	96
2	14	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	148	50.8	0.61	50.2	27	96
2	15	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	148	50.8	0.61	44.9	27	96
2	16	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	91.8	94	0.61	51.4	27	96
2	19	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	91.8	94	0.61	56.0	27	96
2	20	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	91.8	94	0.61	60.3	27	96
2	21	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	91.8	94	0.61	61.5	27	96
2	22	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	91.8	94	0.61	57.6	27	96
2	23	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	91.8	94	0.61	62.1	27	96
2	24	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	91.8	94	0.61	88.7	27	96
2	25	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	91.8	94	0.61	34.4	26	96

2	26	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	91.8	94	0.61	47.5	26	96
2	27	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	91.8	94	0.61	59.7	26	96
2	28	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	91.8	94	0.61	36.4	26	96
2	29	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	91.8	94	0.61	45.7	26	96
2	30	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	91.8	94	0.61	53.4	26	96
2	31	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	207	25.4	0.61	32.6	26	96
2	32	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	207	25.4	0.61	44.2	26	96
2	33	5.50	7.47	0.56	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	207	25.4	0.61	61.2	26	96
2	34	5.50	7.47	0.42	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	207	25.4	0.61	24.5	26	96
2	35	5.50	7.47	0.27	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	207	25.4	0.61	24.8	26	96
2	36	5.50	7.47	0.18	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	207	25.4	0.61	28.2	26	96
2	37	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	207	25.4	0.61	28.7	26	96
2	38	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	207	25.4	0.61	30.9	26	96
2	39	5.50	7.47	0.56	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	207	25.4	0.61	40.1	26	96
2	40	5.50	7.47	0.42	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	207	25.4	0.61	41.6	26	96
2	41	5.50	7.47	0.27	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	207	25.4	0.61	77.5	26	96
2	42	5.50	7.47	0.18	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	207	25.4	0.61	47.6	26	96
2	43	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	207	25.4	0.61	47.9	26	96
2	44	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	207	25.4	0.61	54.8	26	96
2	45	5.50	7.47	0.56	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	207	25.4	0.61	66.8	26	96
2	46	5.50	7.47	0.42	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	207	25.4	0.61	61.9	26	96
2	47	5.50	7.47	0.27	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	207	25.4	0.61	63.1	26	96
2	48	5.50	7.47	0.18	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	207	25.4	0.61	71.5	26	96
2	49	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	207	25.4	0.61	78.0	26	96
2	50	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	207	25.4	0.61	87.2	26	96
2	51	5.50	7.47	0.56	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	207	25.4	0.61	102.9	26	96
2	52	5.50	7.47	0.42	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	207	25.4	0.61	60.5	26	96
2	53	5.50	7.47	0.27	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	207	25.4	0.61	73.8	26	96
2	54	5.50	7.47	0.18	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	207	25.4	0.61	104.9	26	96
2	55	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	207	25.4	0.61	64.1	17	115
2	56	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	207	25.4	0.61	53.6	17	115
2	57	5.50	7.47	0.56	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	207	25.4	0.61	57.0	17	115
2	58	5.50	7.47	0.42	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	207	25.4	0.61	45.1	17	115
2	59	5.50	7.47	0.27	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	207	25.4	0.61	50.0	17	115
2	60	5.50	7.47	0.18	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	207	25.4	0.61	47.9	17	115
2	61	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	141.1	76.2	0.61	53.4	17	115
2	62	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	141.1	76.2	0.61	49.5	17	115
2	63	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	141.1	76.2	0.61	41.7	17	115
2	64	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	141.1	76.2	0.61	36.4	17	115
2	65	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	141.1	76.2	0.61	41.4	17	115
2	66	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	141.1	76.2	0.61	34.3	17	115
2	67	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	141.1	76.2	0.61	53.0	17	53
2	68	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	141.1	76.2	0.61	59.1	17	53
2	69	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	141.1	76.2	0.61	35.1	17	53
2	70	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	141.1	76.2	0.61	43.4	17	53
2	71	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	141.1	76.2	0.61	46.2	17	53
2	72	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	141.1	76.2	0.61	32.3	17	53
2	73	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	141.1	76.2	0.61	34.1	17	53

2	74	5.50	7.47	0.85	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	141.1	76.2	0.61	33.0	17	53
2	75	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	141.1	76.2	0.61	31.2	7	100
2	76	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	210	50.8	0.61	36.9	7	100
2	77	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	210	50.8	0.61	34.7	7	100
2	78	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	210	50.8	0.61	50.8	7	100
2	79	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	210	50.8	0.61	58.3	7	100
2	80	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	210	50.8	0.61	59.8	7	100
2	81	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	210	50.8	0.61	61.1	7	100
2	82	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	210	50.8	0.61	84.8	7	100
2	83	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	210	50.8	0.61	85.7	7	100
2	84	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	210	50.8	0.61	79.4	7	100
2	85	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	210	50.8	0.61	33.5	17	100
2	86	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	210	50.8	0.61	38.1	17	100
2	87	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	210	50.8	0.61	35.6	17	100
2	88	5.50	7.47	1.32	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	210	50.8	0.61	54.9	17	100
2	89	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	210	50.8	0.61	58.6	17	100
2	90	5.50	7.47	0.57	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	210	50.8	0.61	60.8	17	100
2	91	5.50	7.47	1.24	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	115	50.8	0.61	67.5	17	100
2	92	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	115	50.8	0.61	68.0	17	100
2	93	5.50	7.47	0.58	26.7	8.60E-04	1.84E-05	8.80E-10	7.66E-06	0.0218	0.072	0.033	115	50.8	0.61	91.1	17	100
2	94	5.50	7.47	1.24	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	115	50.8	0.61	87.6	17	100
2	95	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	115	50.8	0.61	33.1	11	100
2	96	5.50	7.47	0.58	26.7	8.60E-04	1.84E-05	1.15E-09	1.01E-05	0.1685	0.072	0.033	115	50.8	0.61	35.4	11	100
2	97	5.50	7.47	1.24	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	115	50.8	0.61	33.9	11	100
2	98	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	115	50.8	0.61	61.0	11	100
2	99	5.50	7.47	0.58	26.7	8.60E-04	1.84E-05	1.10E-09	9.60E-06	0.1623	0.072	0.033	115	50.8	0.61	61.1	11	100
2	100	5.50	7.47	1.24	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	115	50.8	0.61	64.2	11	100
2	101	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	115	50.8	0.61	79.0	11	100
2	102	5.50	7.47	0.58	26.7	8.60E-04	1.84E-05	1.09E-09	9.12E-06	0.1297	0.072	0.033	115	50.8	0.61	102.3	11	100
2	103	5.50	7.47	1.24	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	115	50.8	0.61	103.2	11	100
2	104	5.50	7.47	0.86	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	115	50.8	0.61	106.2	11	100
2	105	5.50	7.47	0.58	26.7	8.60E-04	1.84E-05	1.07E-09	8.76E-06	0.0491	0.072	0.033	115	50.8	0.61	21.2	26	100
3	1	5.15	6.05	0.64	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	22.1	26	100
3	2	5.15	9.19	0.50	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	20.0	26	100
3	3	5.15	14.40	0.44	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	40.2	26	100
3	4	5.15	19.41	0.38	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	38.7	26	100
3	5	5.15	29.02	0.28	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	38.5	26	100
3	6	5.15	8.77	0.93	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	50.8	26	100
3	7	5.15	13.57	0.75	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	67.0	26	100
3	8	5.15	20.25	0.61	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	68.2	26	100
3	9	5.15	26.09	0.53	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	71.2	26	100
3	10	5.15	35.70	0.34	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	27.3	27	100
3	11	5.15	11.69	1.08	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	26.6	27	100
3	12	5.15	18.37	0.98	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	26.7	27	100
3	13	5.15	25.05	0.76	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	49.9	27	100
3	14	5.15	31.31	0.60	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	49.9	27	100
3	15	5.15	43.42	0.44	20	1.00E-03	1.81E-05	9.02E-10	9.37E-06	0.23	0.073	0.033	207	25.4	0.61	50.5	27	100
3	16	5.15	6.05	0.64	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	64.1	27	100

3	17	5.15	9.19	0.50	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	82.7	27	100
3	18	5.15	14.40	0.44	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	84.0	27	100
3	19	5.15	19.41	0.38	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	85.6	27	100
3	20	5.15	29.02	0.28	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	32.2	7	100
3	21	5.15	8.77	0.93	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	50.0	7	100
3	22	5.15	13.57	0.75	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	33.5	7	100
3	23	5.15	20.25	0.61	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	46.6	7	100
3	24	5.15	26.09	0.53	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	21.2	9	100
3	25	5.15	35.70	0.34	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	37.7	9	100
3	26	5.15	11.69	1.08	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	19.3	9	100
3	27	5.15	18.37	0.98	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	36.4	9	100
3	28	5.15	25.05	0.76	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	35.1	10	100
3	29	5.15	31.31	0.60	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	68.1	10	100
3	30	5.15	43.42	0.44	20	1.00E-03	1.81E-05	7.98E-10	8.31E-06	0.19	0.073	0.033	207	25.4	0.61	35.8	10	100
3	31	5.50	3.49	0.87	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	66.1	10	100
3	32	5.50	4.79	1.14	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	23.6	8	100
3	33	5.50	6.18	1.47	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	61.0	8	100
3	34	5.50	6.18	0.74	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	27.2	8	100
3	35	5.50	8.37	1.00	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	52.4	8	100
3	36	5.50	10.97	1.31	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	15.4	48	100
3	37	5.50	10.97	0.65	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	30.7	48	100
3	38	5.50	13.96	0.80	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	50.2	48	100
3	39	5.50	17.95	1.07	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	57.1	48	100
3	40	5.50	16.95	0.52	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	70.4	48	100
3	41	5.50	19.94	0.66	24.3	9.08E-04	1.83E-05	1.04E-09	9.45E-06	0.1445	0.072	0.033	207	25.4	0.61	79.6	48	100
3	42	5.50	2.00	1.27	21.8	9.62E-04	1.82E-05	7.53E-10	6.95E-06	0.0142	0.072	0.033	207	25.4	0.61	30.0	42	100
3	43	5.50	3.19	1.26	21.8	9.62E-04	1.82E-05	7.53E-10	6.95E-06	0.0142	0.072	0.033	207	25.4	0.61	35.4	42	100
3	44	5.50	4.59	1.21	21.8	9.62E-04	1.82E-05	7.53E-10	6.95E-06	0.0142	0.072	0.033	207	25.4	0.61	48.6	42	100
3	45	5.50	7.78	1.03	21.8	9.62E-04	1.82E-05	7.53E-10	6.95E-06	0.0142	0.072	0.033	207	25.4	0.61	53.9	42	100
3	46	5.50	12.97	0.84	21.8	9.62E-04	1.82E-05	7.53E-10	6.95E-06	0.0142	0.072	0.033	207	25.4	0.61	65.1	42	100
3	47	5.50	1.60	0.94	21.8	9.62E-04	1.82E-05	7.53E-10	6.95E-06	0.0142	0.072	0.033	207	25.4	0.61	82.4	42	100
3	48	5.50	19.94	0.83	24	9.14E-04	1.83E-05	8.48E-10	7.80E-06	0.689	0.072	0.033	207	25.4	0.61	86.0	42	100
3	49	5.50	19.94	0.43	24	9.14E-04	1.83E-05	8.48E-10	7.80E-06	0.689	0.072	0.033	207	25.4	0.61	31.0	51	100
3	50	5.50	19.94	0.24	24	9.14E-04	1.83E-05	8.48E-10	7.80E-06	0.689	0.072	0.033	207	25.4	0.61	35.1	51	100
3	51	5.50	19.94	0.12	24	9.14E-04	1.83E-05	8.48E-10	7.80E-06	0.689	0.072	0.033	207	25.4	0.61	50.8	51	100
3	52	5.50	19.94	0.06	24	9.14E-04	1.83E-05	8.48E-10	7.80E-06	0.689	0.072	0.033	207	25.4	0.61	53.8	51	100
3	53	5.50	19.94	0.04	24	9.14E-04	1.83E-05	8.48E-10	7.80E-06	0.689	0.072	0.033	207	25.4	0.61	61.8	51	100
3	54	5.50	19.94	0.04	24	9.14E-04	1.83E-05	8.48E-10	7.80E-06	0.689	0.072	0.033	207	25.4	0.61	80.7	51	100
3	55	5.50	28.88	0.99	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	88.3	51	100
3	56	5.50	19.26	0.92	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	29.0	44	100
3	57	5.50	28.88	0.99	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	46.4	44	100
3	58	5.50	29.85	0.36	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	46.4	44	100
3	59	5.50	28.88	0.17	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	52.0	44	100
3	60	5.50	28.88	0.99	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	69.1	44	100
3	61	5.50	28.88	0.03	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	85.5	44	100
3	62	5.50	29.85	0.36	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	87.3	44	100
3	63	5.50	28.88	0.17	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61	38.1	26	72
3	64	5.50	28.88	0.17	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61			
3	65	5.50	29.85	0.03	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61			
3	66	5.50	28.88	0.99	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61			
3	67	5.50	28.88	0.36	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61			
3	68	5.50	29.85	0.03	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61			
3	69	5.50	28.88	0.17	14.6	1.15E-03	1.78E-05	7.23E-10	8.15E-06	0.2264	0.074	0.033	207	25.4	0.61			
3	70	5.50	3.49	0.87	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61			

Author ID	Data ID	Packed Depth (m)	Liquid flow (kg/m ² /s)	Gas flow (kg/m ² /s)	Liquid Temperature (C)	Liquid viscosity (m ² /s)	Gas Viscosity (m ² /s)	Liquid Density (kg/m ³)	Gas Density (kg/m ³)	Henry's Constant (km ³ /km ³)	Liquid Critical Turbulence (m ² /s)	Packing Chemical Tension (m ² /s)	Dry Surface Area (m ² /m ³)	Packing Diameter (mm)	Tower Diameter (m)	Observed (Kla) (1/h)	Chamoulin ID	Packing ID
3	73	5.50	4.79	1.14	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	38.8	26	72
3	74	5.50	6.18	1.47	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	41.2	26	72
3	75	5.50	6.18	0.74	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	57.3	26	72
3	76	5.50	6.37	1.00	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	38.8	26	72
3	77	5.50	10.97	1.31	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	49.1	26	72
3	78	5.50	10.97	0.65	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	60.0	26	72
3	79	5.50	13.96	0.80	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	41.0	26	72
3	80	5.50	17.95	1.07	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	50.4	26	72
3	81	5.50	16.95	0.52	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	57.1	26	72
3	82	5.50	19.94	0.66	24.3	9.08E-04	1.83E-05	1.01E-09	8.62E-06	0.044	0.072	0.033	207	25.4	0.61	49.2	27	72
3	83	5.50	3.49	0.87	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	40.1	27	72
3	84	5.50	4.79	1.14	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	42.5	27	72
3	85	5.50	6.18	1.47	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	37.9	27	72
3	86	5.50	6.18	0.74	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	42.1	27	72
3	87	5.50	8.37	1.00	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	50.3	27	72
3	88	5.50	10.97	1.31	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	43.9	27	72
3	89	5.50	10.97	0.65	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	64.3	27	72
3	90	5.50	13.96	0.80	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	49.4	27	72
3	91	5.50	17.95	1.07	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	41.2	27	72
3	92	5.50	16.95	0.52	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	60.4	27	72
3	93	5.50	19.94	0.66	24.3	9.08E-04	1.83E-05	1.02E-09	8.98E-06	0.1162	0.072	0.033	207	25.4	0.61	39.1	17	72
3	94	5.50	3.49	0.87	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	37.3	17	72
3	95	5.50	4.79	1.14	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	42.7	17	72
3	96	5.50	6.18	1.47	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	46.1	17	72
3	97	5.50	6.18	0.74	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	40.5	17	72
3	98	5.50	8.37	1.00	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	55.2	17	72
3	99	5.50	10.97	1.31	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	44.7	17	72
3	100	5.50	10.97	0.65	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	62.8	17	72
3	101	5.50	13.96	0.80	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	50.1	17	72
3	102	5.50	17.95	1.07	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	40.9	17	72
3	103	5.50	16.95	0.52	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	63.6	17	72
3	104	5.50	19.94	0.66	24.3	9.08E-04	1.83E-05	9.92E-10	8.32E-06	0.0343	0.072	0.033	207	25.4	0.61	37.6	26	72
6	1	2.44	15.30	0.09	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	148	50.8	0.444	49.4	26	72
6	2	2.44	15.30	0.14	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	148	50.8	0.444	48.0	26	72
6	3	2.44	15.30	0.29	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	148	50.8	0.444	62.1	26	72
6	4	2.44	15.30	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	148	50.8	0.444	71.0	26	72
6	5	2.44	15.30	1.08	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	148	50.8	0.444	27.8	26	72
6	6	2.44	15.30	0.09	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	148	50.8	0.444	60.9	26	72
6	7	2.44	15.30	0.14	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	148	50.8	0.444	43.6	26	72
6	8	2.44	15.30	0.29	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	148	50.8	0.444	87.8	26	72
6	9	2.44	15.30	0.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	148	50.8	0.444	74.0	26	72
6	10	2.44	15.30	1.08	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	148	50.8	0.444	64.1	26	72
6	11	2.44	15.30	0.09	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	148	50.8	0.444	62.3	26	72
6	12	2.44	15.30	0.14	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	148	50.8	0.444	97.4	26	72
6	13	2.44	15.30	0.29	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	148	50.8	0.444	81.3	26	72
6	14	2.44	15.30	0.65	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	148	50.8	0.444	30.2	26	72
6	15	2.44	15.30	1.08	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	148	50.8	0.444	21.8	26	72
6	16	2.44	15.30	0.09	25	8.94E-04	1.83E-05	1.08E-09	9.50E-06	0.1495	0.072	0.033	148	50.8	0.444	37.6	26	72

Data Base

Author ID	Data ID	Packed Depth (in)	Liquid flow (kgm ² /s)	Gas flow (kgm ² /s)	Liquid Temp (C)	Liquid viscosity (mPa.s)	Liquid Density (kg/m ³)	Gas Viscosity (mPa.s)	Liquid Density (kg/m ³)	Gas Density (kg/m ³)	Henry's Constant (atm)	Liquid Critical Temp (K)	Packing Critical Temp (K)	Dry Surface Area (m ² /m ³)	Packing Diameter (mm)	Tower Diameter (mm)	Observed K _{La} (1/min)	Compound ID
6	17	2.44	15.30	0.14	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	40.2	26
6	18	2.44	15.30	0.29	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	32.6	7
6	19	2.44	15.30	0.65	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	21.8	7
6	20	2.44	15.30	1.08	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	12.9	7
6	21	2.44	15.30	0.09	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	36.1	9
6	22	2.44	15.30	0.14	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	21.0	9
6	23	2.44	15.30	0.29	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	12.7	9
6	24	2.44	15.30	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	37.4	10
6	25	2.44	15.30	1.08	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	18.2	10
6	26	2.44	9.95	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	148	50.8	0.444	11.2	10
6	27	2.44	13.00	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	148	50.8	0.444	28.2	8
6	28	2.44	15.30	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	148	50.8	0.444	12.1	8
6	29	2.44	18.28	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	148	50.8	0.444	7.3	8
6	30	2.44	20.65	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	148	50.8	0.444	45.0	27
6	31	2.44	22.95	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	148	50.8	0.444	50.4	27
6	32	2.44	9.95	0.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	148	50.8	0.444	52.7	27
6	33	2.44	13.00	0.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	148	50.8	0.444	51.8	27
6	34	2.44	15.30	0.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	148	50.8	0.444	54.9	27
6	35	2.44	18.28	0.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	148	50.8	0.444	46.8	17
6	36	2.44	20.65	0.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	148	50.8	0.444	52.2	17
6	37	2.44	22.95	0.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	148	50.8	0.444	54.5	17
6	38	2.44	9.95	0.65	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	0.033	148	50.8	0.444	55.4	17
6	39	2.44	13.00	0.65	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	0.033	148	50.8	0.444	39.6	26
6	40	2.44	15.30	0.65	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	0.033	148	50.8	0.444	47.3	26
6	41	2.44	18.28	0.65	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	0.033	148	50.8	0.444	52.7	26
6	42	2.44	20.65	0.65	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	0.033	148	50.8	0.444	55.4	26
6	43	2.44	22.95	0.65	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	0.033	148	50.8	0.444	73.8	26
6	44	2.44	9.95	0.65	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	93.2	26
6	45	2.44	13.00	0.65	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	40.5	7
6	46	2.44	15.30	0.65	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	50.4	7
6	47	2.44	18.28	0.65	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	57.2	7
6	48	2.44	20.65	0.65	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	60.8	7
6	49	2.44	22.95	0.65	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	0.033	148	50.8	0.444	78.3	7
6	50	2.44	9.95	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	43.2	6
6	51	2.44	13.00	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	55.8	6
6	52	2.44	15.30	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	54.0	6
6	53	2.44	18.28	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	57.6	6
6	54	2.44	20.65	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	61.7	6
6	55	2.44	22.95	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	0.033	148	50.8	0.444	78.8	6
6	56	2.44	15.30	0.14	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	207	25.4	0.444	40.8	26
6	57	2.44	15.30	0.29	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	207	25.4	0.444	60.9	26
6	58	2.44	15.30	0.54	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	207	25.4	0.444	33.7	26
6	59	2.44	15.30	0.51	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	0.033	207	25.4	0.444	35.5	26
6	60	2.44	15.30	0.81	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	207	25.4	0.444	39.1	26
6	61	2.44	15.30	0.14	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	207	25.4	0.444	40.4	26
6	62	2.44	15.30	0.29	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	207	25.4	0.444	37.6	26
6	63	2.44	15.30	0.54	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	207	25.4	0.444	40.4	26
6	64	2.44	15.30	0.51	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	0.033	207	25.4	0.444	37.6	26

6	113	2.44	15.30	0.54	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	108	50.8	0.444	76.8	27	72
6	114	2.44	15.30	0.99	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	108	50.8	0.444	48.6	17	72
6	115	2.44	15.30	0.09	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	61.8	17	72
6	116	2.44	15.30	0.14	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	69.6	17	72
6	117	2.44	15.30	0.29	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	78.6	17	72
6	118	2.44	15.30	0.54	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	77.4	17	72
6	119	2.44	15.30	0.99	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	85.8	17	72
6	120	2.44	15.30	0.09	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	48.6	26	72
6	121	2.44	15.30	0.14	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	61.2	26	72
6	122	2.44	15.30	0.29	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	70.2	26	72
6	123	2.44	15.30	0.54	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	76.8	26	72
6	124	2.44	15.30	0.99	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	75.8	26	72
6	125	2.44	15.30	0.14	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	84.0	26	72
6	126	2.44	15.30	0.29	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	43.8	7	72
6	127	2.44	15.30	0.54	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	56.4	7	72
6	128	2.44	15.30	0.99	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	63.6	7	72
6	129	2.44	15.30	0.29	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	69.6	7	72
6	130	2.44	15.30	0.54	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	76.2	7	72
6	131	2.44	15.30	0.99	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	73.2	7	72
6	132	2.44	9.95	0.99	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	108	50.8	0.444	49.8	6	72
6	133	2.44	13.00	0.99	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	108	50.8	0.444	60.6	6	72
6	134	2.44	15.30	0.99	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	108	50.8	0.444	66.0	6	72
6	135	2.44	18.28	0.99	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	108	50.8	0.444	72.0	6	72
6	136	2.44	20.65	0.99	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	108	50.8	0.444	70.2	6	72
6	137	2.44	22.95	0.99	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	108	50.8	0.444	74.4	6	72
6	138	2.44	9.95	0.99	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	60.0	27	24
6	139	2.44	13.00	0.99	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	67.2	27	24
6	140	2.44	15.30	0.99	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	70.2	27	24
6	141	2.44	18.28	0.99	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	69.0	27	24
6	142	2.44	20.65	0.99	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	73.2	27	24
6	143	2.44	22.95	0.99	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	108	50.8	0.444	62.4	17	24
6	144	2.44	9.95	0.99	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	69.6	17	24
6	145	2.44	13.00	0.99	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	72.6	17	24
6	146	2.44	15.30	0.99	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	69.0	17	24
6	147	2.44	18.28	0.99	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	73.8	17	24
6	148	2.44	20.65	0.99	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	74.4	17	24
6	149	2.44	22.95	0.99	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	108	50.8	0.444	52.8	26	24
6	150	2.44	9.95	0.99	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	63.0	26	24
6	151	2.44	13.00	0.99	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	70.2	26	24
6	152	2.44	15.30	0.99	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	73.8	26	24
6	153	2.44	18.28	0.99	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	76.2	26	24
6	154	2.44	20.65	0.99	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	46.8	7	24
6	155	2.44	22.95	0.99	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	108	50.8	0.444	60.0	7	24
6	156	2.44	9.95	0.99	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	65.4	7	24
6	157	2.44	13.00	0.99	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	69.0	7	24
6	158	2.44	15.30	0.99	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	58.2	6	24
6	159	2.44	18.28	0.99	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	68.4	6	24
6	160	2.44	20.65	0.99	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	75.6	6	24
6	160	2.44	20.65	0.99	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	48.0	27	24

Data Base

Alloy ID	Packed depth, m	Liquid flow, kg/m ² /s	Gas flow, kg/m ² /s	Liquid Temp, C	Liquid Viscosity, mPa.s	Gas Viscosity, mPa.s	Liquid Density, kg/m ³	Gas Density, kg/m ³	Henry's Constant, atm	Liquid Critical Surface Tension, mN/m	Packing Critical Surface Tension, mN/m	Dry Surface Area, m ² /m ³	Packing Diameter, mm	Tower Diameter, mm	Observed K _{La} , 1/min	Compound ID	Packing ID
6	161	2.44	22.95	0.99	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	108	50.8	0.444	62.4	27	24
6	162	2.44	15.30	0.09	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	210	25.4	0.444	73.2	27	24
6	163	2.44	15.30	0.36	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	210	25.4	0.444	78.0	27	24
6	164	2.44	15.30	0.51	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	210	25.4	0.444	85.8	27	24
6	165	2.44	9.95	0.06	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	94.2	27	24
6	166	2.44	13.00	0.31	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	52.8	17	24
6	167	2.44	15.30	0.51	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	67.2	17	24
6	168	2.44	9.95	0.06	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	74.4	17	24
6	169	2.44	13.00	0.31	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	86.4	17	24
6	170	2.44	15.30	0.51	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	90.0	17	24
6	171	2.44	9.95	0.23	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	98.4	17	24
6	172	2.44	13.00	0.43	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	52.8	26	24
6	173	2.44	15.30	0.81	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	67.8	26	24
6	174	2.44	9.95	0.23	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	76.2	26	24
6	175	2.44	13.00	0.43	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	84.6	26	24
6	176	2.44	15.30	0.81	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	90.0	26	24
6	177	2.44	22.67	0.23	1.31E-03	1.76E-05	5.65E-10	7.08E-06	0.3187	0.074	0.033	210	25.4	0.444	98.4	26	24
6	178	2.44	22.64	0.22	1.00E-03	1.81E-05	6.27E-10	7.89E-06	0.5571	0.073	0.033	210	25.4	0.444	50.4	7	24
6	179	2.44	22.58	0.21	8.01E-04	1.86E-05	9.89E-10	8.12E-06	0.9374	0.071	0.033	210	25.4	0.444	62.4	7	24
6	180	2.44	22.67	0.23	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	210	25.4	0.444	69.0	7	24
6	181	2.44	22.64	0.22	1.00E-03	1.81E-05	8.13E-10	8.28E-06	0.5606	0.073	0.033	210	25.4	0.444	81.6	7	24
6	182	2.44	22.58	0.21	8.01E-04	1.86E-05	1.06E-09	8.85E-06	0.8635	0.071	0.033	210	25.4	0.444	84.6	7	24
6	183	2.44	22.67	0.23	1.31E-03	1.76E-05	6.27E-10	7.89E-06	0.1756	0.074	0.033	210	25.4	0.444	91.2	7	24
6	184	2.44	22.64	0.22	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3019	0.073	0.033	210	25.4	0.444	56.4	6	24
6	185	2.44	22.58	0.21	8.01E-04	1.86E-05	1.10E-09	9.05E-06	0.5002	0.071	0.033	210	25.4	0.444	69.6	6	24
6	186	2.44	22.67	0.23	1.31E-03	1.76E-05	6.85E-10	8.56E-06	0.6693	0.074	0.033	210	25.4	0.444	75.6	6	24
6	187	2.44	22.64	0.22	1.00E-03	1.81E-05	9.23E-10	9.18E-06	0.1168	0.073	0.033	210	25.4	0.444	88.8	6	24
6	188	2.44	22.58	0.21	8.01E-04	1.86E-05	1.20E-09	9.82E-06	0.1898	0.071	0.033	210	25.4	0.444	91.2	6	24
6	189	2.44	22.67	0.23	1.31E-03	1.76E-05	7.94E-10	9.89E-06	0.0474	0.074	0.033	210	25.4	0.444	98.4	6	24
6	190	2.44	22.64	0.22	1.00E-03	1.81E-05	1.07E-09	1.06E-05	0.0725	0.073	0.033	210	25.4	0.444	64.8	27	22
6	191	2.44	22.58	0.21	8.01E-04	1.86E-05	1.39E-09	1.13E-05	0.1078	0.071	0.033	210	25.4	0.444	75.0	27	22
6	192	2.44	9.95	0.51	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	210	25.4	0.444	72.6	27	22
6	193	2.44	13.00	0.51	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	210	25.4	0.444	68.4	17	22
6	194	2.44	15.30	0.51	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	210	25.4	0.444	82.8	17	22
6	195	2.44	18.28	0.51	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	210	25.4	0.444	82.2	17	22
6	196	2.44	20.65	0.51	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	210	25.4	0.444	50.4	26	22
6	197	2.44	22.95	0.50	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	77.4	26	22
6	198	2.44	9.95	0.51	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	79.2	26	22
6	199	2.44	13.00	0.51	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	72.6	7	22
6	200	2.44	15.30	0.51	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	74.4	7	22
6	201	2.44	18.28	0.51	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	76.8	7	22
6	202	2.44	20.65	0.51	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	73.8	6	22
6	203	2.44	22.95	0.50	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	210	25.4	0.444	76.8	6	22
6	204	2.44	9.95	0.51	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	79.8	6	22
6	205	2.44	13.00	0.51	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	54.0	27	22
6	206	2.44	15.30	0.51	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	75.0	27	22
6	207	2.44	18.28	0.51	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	102.0	27	22
6	208	2.44	20.65	0.51	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	61.2	17	22

6	210	2.44	22.95	0.50	25	8.94E-04	1.83E-05	9.87E-10	8.75E-06	0.3903	0.072	0.033	210	25.4	0.444	84.0	22
6	211	2.44	9.95	0.51	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	108.6	22
6	212	2.44	13.00	0.51	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	45.0	22
6	213	2.44	15.30	0.51	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	69.0	22
6	214	2.44	18.28	0.51	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	93.6	22
6	215	2.44	20.65	0.51	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	23.4	7
6	216	2.44	22.95	0.50	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	210	25.4	0.444	42.6	7
6	217	2.44	9.95	0.51	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	66.0	7
6	218	2.44	13.00	0.51	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	16.8	6
6	219	2.44	15.30	0.51	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	28.8	6
6	220	2.44	18.28	0.51	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	47.4	6
6	221	2.44	20.65	0.51	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	52.2	27
6	222	2.44	22.95	0.50	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	210	25.4	0.444	64.2	27
6	223	2.44	15.30	0.09	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	72.6	27
6	224	2.44	15.30	0.14	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	82.8	27
6	225	2.44	15.30	0.22	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	93.6	27
6	226	2.44	15.30	0.33	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	118.2	27
6	227	2.44	15.30	0.51	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	57.0	17
6	228	2.44	15.30	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	75.0	17
6	229	2.44	15.30	0.09	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	81.6	17
6	230	2.44	15.30	0.14	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	95.4	17
6	231	2.44	15.30	0.22	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	106.2	17
6	232	2.44	15.30	0.33	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	129.6	17
6	233	2.44	15.30	0.51	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	57.0	22
6	234	2.44	15.30	0.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	72.6	22
6	235	2.44	15.30	0.09	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	341	16	0.444	78.6	26
6	236	2.44	15.30	0.22	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	341	16	0.444	89.4	26
6	237	2.44	15.30	0.33	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	341	16	0.444	41.9	17
6	238	2.44	15.30	0.51	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	341	16	0.444	43.2	17
6	239	2.44	15.30	0.65	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	341	16	0.444	44.5	17
6	240	2.44	15.30	0.14	25	8.94E-04	1.83E-05	9.67E-10	8.75E-06	0.3903	0.072	0.033	341	16	0.444	46.6	17
6	241	2.44	15.30	0.22	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	341	16	0.444	36.6	17
6	242	2.44	15.30	0.33	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	341	16	0.444	37.1	17
6	243	2.44	15.30	0.51	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	341	16	0.444	35.2	17
6	244	2.44	15.30	0.65	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	341	16	0.444	43.4	17
6	245	2.44	15.30	0.72	25	8.94E-04	1.83E-05	1.06E-09	9.50E-06	0.1495	0.072	0.033	341	16	0.444	41.6	17
6	246	2.44	15.30	0.22	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	341	16	0.444	41.3	17
6	247	2.44	15.30	0.33	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	341	16	0.444	30.6	17
6	248	2.44	15.30	0.51	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	341	16	0.444	28.4	17
6	249	2.44	15.30	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	341	16	0.444	30.6	17
6	250	2.44	15.30	0.72	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	341	16	0.444	30.6	17
6	251	2.44	9.95	0.65	25	8.94E-04	1.83E-05	1.22E-09	1.10E-05	0.0887	0.072	0.033	341	16	0.444	31.2	17
6	252	2.44	13.00	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	27.4	17
6	253	2.44	15.30	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	79.8	27
6	254	2.44	18.28	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	85.8	27
6	255	2.44	20.65	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	85.8	27
6	256	2.44	22.95	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	89.4	27
6	256	2.44	22.95	0.65	25	8.94E-04	1.83E-05	8.71E-10	7.85E-06	0.7259	0.072	0.033	341	16	0.444	97.2	27

Data Base

Alcohol ID	Packed depth, m	Liquid flow, kg/m ² /h	Gas flow, kg/m ² /h	Liquid Temp, °C	Liquid Viscosity, mPa	Gas Viscosity, mPa	Liquid Density, kg/m ³	Gas Density, kg/m ³	Henry's Constant, atm	Liquid Critical Surface Vm ² /s	Packing Critical Vm ² /s	Dry Surface Area, m ² /m ³	Packing Diameter, mm	Tower Diameter, m	Observed KLa, 1/h	Compound ID	Packing ID
6	257	2.44	9.95	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	93.6	27	21
6	258	2.44	13.00	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	85.8	17	21
6	259	2.44	15.30	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	88.2	17	21
6	260	2.44	18.28	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	89.4	17	21
6	261	2.44	20.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	97.2	17	21
6	262	2.44	22.95	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	93.6	17	21
6	263	2.44	9.95	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	93.6	17	21
6	264	2.44	13.00	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	93.6	17	21
6	265	2.44	15.30	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	76.8	17	21
6	266	2.44	18.28	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	81.0	17	21
6	267	2.44	20.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	81.6	17	21
6	268	2.44	22.95	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	94.8	17	21
6	269	2.44	9.95	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	89.4	17	21
6	270	2.44	13.00	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	91.8	17	21
6	271	2.44	15.30	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	65.4	7	21
6	272	2.44	18.28	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	76.2	7	21
6	273	2.44	20.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	86.4	7	21
6	274	2.44	22.95	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	81.6	7	21
6	275	2.44	9.95	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	82.8	7	21
6	276	2.44	13.00	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	90.6	7	21
6	277	2.44	15.30	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	77.4	6	21
6	278	2.44	18.28	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	85.8	6	21
6	279	2.44	20.65	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	91.8	6	21
6	280	2.44	22.95	25	8.94E-04	1.83E-05	9.30E-10	8.57E-06	0.6984	0.072	0.033	341	16	0.444	97.2	6	21
7	1	3.03	20.36	15.2	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	103.8	6	21
7	2	3.03	20.36	10.2	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	57.6	27	21
7	3	3.03	20.36	1.02	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	78.0	27	21
7	4	3.03	16.97	0.85	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	84.0	27	21
7	5	3.03	16.97	0.85	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	103.2	27	21
7	6	3.03	16.97	1.27	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	108.0	27	21
7	7	3.03	16.97	1.06	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	127.2	27	21
7	8	3.03	16.97	1.06	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	65.4	17	21
7	9	3.03	13.58	0.68	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	84.0	17	21
7	10	3.03	13.58	0.68	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	93.6	17	21
7	11	3.03	13.58	1.02	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	108.0	17	21
7	12	3.03	13.58	1.35	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	117.0	17	21
7	13	3.03	20.36	1.02	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	147.6	88.9	0.582	127.2	17	21
7	14	3.03	20.36	1.52	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	148	50.8	0.582	63.0	26	21
7	15	3.03	16.97	0.85	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	148	50.8	0.582	81.0	26	21
7	16	3.03	16.97	1.06	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	148	50.8	0.582	91.8	26	21
7	17	3.03	16.97	1.27	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	148	50.8	0.582	109.8	26	21
7	18	3.03	13.58	0.68	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	148	50.8	0.582	116.4	26	21
7	19	3.03	13.58	1.02	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	148	50.8	0.582	126.0	26	21
7	20	3.03	13.58	1.35	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	148	50.8	0.582	63.0	7	21
7	21	3.03	20.35	1.50	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	78.6	7	21
7	22	3.03	20.35	1.50	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	82.8	7	21
7	23	3.03	20.35	1.00	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	101.4	7	21
7	24	3.03	16.96	0.83	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	109.2	7	21
7	24	3.03	16.96	0.83	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	115.8	7	21

7	25	3.03	16.96	0.83	14	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	75.0	6	21
7	26	3.03	16.96	1.25	14	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	90.0	6	21
7	27	3.03	16.96	1.25	14	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	97.2	6	21
7	28	3.03	13.57	0.67	14	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	112.8	6	21
7	29	3.03	13.57	0.67	14	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	119.4	6	21
7	30	3.03	13.57	1.00	14	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	120.6	6	21
7	31	3.03	13.57	1.34	14	1.17E-03	1.78E-05	6.84E-10	7.94E-06	0.4261	0.074	0.033	110	50.8	0.582	67.7	26	60
7	32	3.03	2.03	0.73	24	9.14E-04	1.83E-05	9.06E-10	8.51E-06	0.6687	0.072	0.033	213	25.4	0.582	75.5	26	60
7	33	3.03	2.03	0.73	24	9.14E-04	1.83E-05	9.06E-10	8.51E-06	0.6687	0.072	0.033	213	25.4	0.582	67.7	23	60
7	34	3.03	2.03	0.73	24	9.14E-04	1.83E-05	9.06E-10	8.51E-06	0.6687	0.072	0.033	213	25.4	0.582	71.8	23	60
7	35	3.03	2.03	0.73	24	9.14E-04	1.83E-05	9.06E-10	8.51E-06	0.6687	0.072	0.033	213	25.4	0.582	23.1	27	60
7	36	3.03	2.03	0.73	24	9.14E-04	1.83E-05	8.89E-10	8.54E-06	0.272	0.072	0.033	210	50.8	0.582	29.6	27	60
7	37	3.03	2.03	0.73	24	9.14E-04	1.83E-05	8.89E-10	8.54E-06	0.272	0.072	0.033	210	50.8	0.582	35.4	27	60
7	38	3.03	2.03	0.73	24	9.14E-04	1.83E-05	8.89E-10	8.54E-06	0.272	0.072	0.033	210	50.8	0.582	45.7	27	60
7	39	3.03	2.03	0.73	24	9.14E-04	1.83E-05	8.89E-10	8.54E-06	0.272	0.072	0.033	210	50.8	0.582	47.6	27	60
7	40	3.03	2.03	0.73	24	9.14E-04	1.83E-05	8.03E-10	7.71E-06	0.3981	0.072	0.033	210	50.8	0.582	57.4	27	60
7	41	3.03	2.03	0.73	24	9.14E-04	1.83E-05	8.03E-10	7.71E-06	0.3981	0.072	0.033	210	50.8	0.582	22.3	26	60
7	42	8.18	12.00	4.53	7.2	1.42E-03	1.75E-05	5.72E-10	7.74E-06	0.1498	0.075	0.033	147.6	88.9	0.582	28.4	26	60
7	43	8.18	12.00	4.53	7.2	1.42E-03	1.75E-05	5.15E-10	6.94E-06	0.2706	0.075	0.033	147.6	88.9	0.582	16.9	26	60
7	44	3.03	12.90	1.17	10.5	1.29E-03	1.76E-05	6.37E-10	7.92E-06	0.1806	0.074	0.033	147.6	88.9	0.582	47.7	26	60
7	45	3.03	12.90	1.17	10.5	1.29E-03	1.76E-05	6.37E-10	7.92E-06	0.1806	0.074	0.033	147.6	88.9	0.582	56.2	26	60
7	46	3.03	12.90	1.17	10.5	1.29E-03	1.76E-05	6.37E-10	7.92E-06	0.1806	0.074	0.033	147.6	88.9	0.582	24.6	23	60
7	47	3.03	12.90	1.17	10.5	1.29E-03	1.76E-05	6.37E-10	7.92E-06	0.1806	0.074	0.033	147.6	88.9	0.582	30.0	23	60
7	48	3.03	12.90	1.17	10.5	1.29E-03	1.76E-05	6.37E-10	7.92E-06	0.1806	0.074	0.033	147.6	88.9	0.582	18.7	23	60
7	49	3.03	12.90	1.17	10.5	1.29E-03	1.76E-05	6.37E-10	7.92E-06	0.1806	0.074	0.033	147.6	88.9	0.582	51.6	23	60
7	50	3.03	21.04	1.28	10.5	1.29E-03	1.76E-05	6.37E-10	7.92E-06	0.1806	0.074	0.033	147.6	88.9	0.582	61.1	23	60
7	51	3.03	23.76	1.18	10.5	1.29E-03	1.76E-05	6.37E-10	7.92E-06	0.1806	0.074	0.033	147.6	88.9	0.582	64.2	27	60
7	52	3.03	20.36	1.02	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	71.8	27	60
7	53	3.03	20.36	1.02	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	84.2	27	60
7	54	3.03	20.36	1.52	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	59.8	26	60
7	55	3.03	20.36	1.52	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	67.7	26	60
7	56	3.03	16.97	0.85	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	75.5	26	60
7	57	3.03	16.97	0.85	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	67.7	23	60
7	58	3.03	16.97	1.06	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	71.8	23	60
7	59	3.03	16.97	1.06	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	23.1	27	60
7	60	3.03	16.97	1.27	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	29.6	27	60
7	61	3.03	16.97	1.27	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	35.4	27	60
7	62	3.03	13.58	0.68	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	45.7	27	60
7	63	3.03	13.58	0.68	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	57.4	27	60
7	64	3.03	13.58	1.02	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	47.6	27	60
7	65	3.03	13.58	1.02	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	22.3	26	60
7	66	3.03	13.58	1.35	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	28.4	26	60
7	67	3.03	13.58	1.35	10	1.31E-03	1.76E-05	6.03E-10	7.72E-06	0.3526	0.074	0.033	246	22.2	0.582	16.9	26	60
8	1	5.13	9.90	1.12	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	47.7	26	60
8	2	5.13	9.90	0.99	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	56.2	26	60
8	3	5.13	9.90	0.90	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	24.6	23	60
8	4	5.13	14.78	1.12	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	30.0	23	60
8	5	5.13	14.78	0.99	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	18.7	23	60

Unit ID	Packed depth	Liquid flow	Gas flow	Liquid Temp	Liquid Viscosity	Gas Viscosity	Liquid Density	Gas Density	Henry's Constant	Liquid Critical Temp	Packing Critical Temp	Dry Surface Area	Packing Diameter	Tower Diameter	Observed Na	Compound ID
8	5.13	14.78	0.90	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	51.6	23
8	5.13	15.32	1.21	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	61.1	23
8	5.13	18.17	1.43	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	69.0	26
8	5.13	18.44	1.12	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	75.9	26
8	5.13	18.44	0.99	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	83.9	26
8	5.13	18.44	0.90	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	90.1	26
8	5.13	28.61	1.91	18	1.06E-03	1.80E-05	7.99E-10	8.34E-06	0.2718	0.073	0.033	91.8	94	0.902	83.9	26
8	5.13	9.90	1.12	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	136.1	26
8	5.13	9.90	0.99	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	75.9	26
8	5.13	9.90	0.90	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	115.7	26
8	5.13	14.78	1.12	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	73.5	26
8	5.13	14.78	0.99	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	90.1	26
8	5.13	14.78	0.90	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	93.6	26
8	5.13	15.32	1.21	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	90.1	26
8	5.13	18.17	1.43	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	86.9	26
8	5.13	18.17	0.99	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	83.9	26
8	5.13	18.44	1.12	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	83.9	26
8	5.13	18.44	0.99	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	93.6	26
8	5.13	28.61	1.91	18	1.06E-03	1.80E-05	7.19E-10	7.49E-06	0.4998	0.073	0.033	91.8	94	0.902	128.3	26
8	5.13	9.90	1.12	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	88.3	26
8	5.13	9.90	1.12	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	97.3	26
8	5.13	14.78	1.12	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	84.5	26
8	5.13	18.44	1.12	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	97.3	26
8	5.13	9.90	0.98	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	84.5	26
8	5.13	14.78	0.98	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	108.9	26
8	5.13	18.44	0.98	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	84.5	26
8	5.13	9.90	0.89	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	84.5	26
8	5.13	14.78	0.89	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	84.5	26
8	5.13	18.44	0.89	18.3	1.05E-03	1.80E-05	8.06E-10	8.36E-06	0.2761	0.073	0.033	91.8	94	0.902	67.5	26
8	3.05	4.29	0.28	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	81.1	26
8	3.05	4.29	1.13	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	60.1	26
8	3.05	4.29	0.23	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	77.1	26
8	3.05	4.29	3.40	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	96.9	26
8	3.05	4.29	4.29	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	90.7	26
8	3.05	4.29	4.53	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	67.5	26
8	3.05	4.29	5.66	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	73.6	26
8	3.05	8.58	0.28	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	96.9	26
8	3.05	8.58	1.13	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	81.1	26
8	3.05	8.58	2.27	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	83.0	26
8	3.05	8.58	3.40	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	83.0	26
8	3.05	8.58	4.53	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	83.0	26
8	3.05	8.58	5.66	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	83.0	26
8	3.05	17.16	0.28	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	129.7	26
8	3.05	17.16	1.13	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	77.8	26
8	3.05	17.16	2.27	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	109.6	26
8	3.05	17.16	3.40	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	83.0	26
8	3.05	17.16	4.53	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	83.0	26
8	3.05	17.16	5.29	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	129.7	26
8	3.05	22.36	0.28	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	97.8	26
8	3.05	22.36	2.27	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	129.7	26
8	3.05	22.36	2.27	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	113.5	26
8	3.05	22.36	2.27	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	68.1	26

Author ID	Data ID	Packed depth, m	Liquid flow, kg/m ² /s	Gas flow, kg/m ² /s	Liquid Temperature, C	Liquid Viscosity, m ² /s	Gas Viscosity, m ² /s	Liquid Density, kg/m ³	Gas Density, kg/m ³	Henry's Constant, atm	Liquid Critical Turbulence, N/m ² /s	Packing Critical Turbulence, N/m ² /s	Dry Surface Area, m ² /m ³	Packing Diameter, mm	Tower Diameter, m	Observed Compound, kg/m ³	Peak ID
8	54	3.05	22.36	4.15	28	8.36E-04	1.85E-05	1.04E-09	8.93E-06	0.4534	0.071	0.033	91.8	94	0.902	72.7	26
9	39	1.21	6.48	0.60	14	1.17E-03	1.78E-05	9.50E-10	1.14E-05	0.7455	0.074	0.033	148	50.8	0.61	57.8	26
9	40	1.21	6.48	0.80	14	1.17E-03	1.78E-05	9.50E-10	1.14E-05	0.7455	0.074	0.033	148	50.8	0.61	95.9	26
9	41	1.21	7.35	0.27	14	1.17E-03	1.78E-05	6.06E-10	7.20E-06	0.2466	0.074	0.033	148	50.8	0.61	85.6	26
9	42	1.21	6.48	0.40	14	1.17E-03	1.78E-05	6.06E-10	7.20E-06	0.2466	0.074	0.033	148	50.8	0.61	95.9	26
9	43	1.21	6.48	0.60	14	1.17E-03	1.78E-05	6.06E-10	7.20E-06	0.2466	0.074	0.033	148	50.8	0.61	113.5	26
9	44	1.21	6.48	0.80	14	1.17E-03	1.78E-05	6.06E-10	7.20E-06	0.2466	0.074	0.033	148	50.8	0.61	113.5	26
10	1	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	113.5	26
10	2	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	64.2	27
10	3	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	71.8	27
10	4	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	84.2	27
10	5	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	59.8	26
10	6	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	12.8	20
10	7	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	24.6	24
10	8	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	24.4	24
10	9	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	22.0	24
10	10	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	15.3	7
10	11	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	15.5	7
10	12	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	15.5	7
10	13	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	25.0	9
10	14	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	21.4	9
10	15	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	19.3	9
10	16	1.21	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	21.1	10
10	17	1.51	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	18.8	10
10	18	1.51	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	16.5	10
10	19	1.51	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	10.3	20
10	20	1.51	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	11.2	20
10	21	1.51	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	9.6	20
10	22	1.51	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	30.2	53
10	23	1.51	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	30.6	53
10	24	1.51	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	27.9	53
10	25	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	15.5	7
10	26	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	16.8	7
10	27	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	17.4	7
10	28	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	25.4	53
10	29	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	25.1	53
10	30	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	24.3	53
10	31	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	21.2	10
10	32	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	21.4	10
10	33	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	18.9	10
10	34	1.82	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	16.8	20
10	35	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	16.8	20
10	36	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	10.5	20
10	37	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	14.1	20
10	38	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	6.2	20
10	39	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	9.0	20
10	40	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	39.0	24
10	41	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	34.9	24

10	42	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	34.2	72
10	43	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	35.6	72
10	44	2.12	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	33.7	72
10	45	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	31.0	72
10	46	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	14.2	72
10	47	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	15.8	72
10	48	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	16.5	72
10	49	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	16.8	72
10	50	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	19.0	72
10	51	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	19.9	72
10	52	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	30.6	72
10	53	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	30.3	72
10	54	2.42	14.67	0.39	21	9.81E-04	1.81E-05	8.69E-10	8.52E-06	0.3181	0.073	0.033	341	16	0.203	29.4	72
11	1	2.42	13.98	0.29	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5571	0.073	0.061	466	12.7	0.102	29.2	72
11	2	2.42	14.52	0.43	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5571	0.073	0.061	466	12.7	0.102	23.4	72
11	3	2.42	15.14	0.51	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5571	0.073	0.061	466	12.7	0.102	58.4	72
11	4	2.42	13.98	0.29	20	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3019	0.073	0.061	466	12.7	0.102	53.6	72
11	5	2.42	14.52	0.43	20	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3019	0.073	0.061	466	12.7	0.102	45.8	72
11	6	2.42	15.14	0.51	20	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3019	0.073	0.061	466	12.7	0.102	37.1	72
11	7	2.42	13.98	0.29	20	1.00E-03	1.81E-05	8.61E-10	8.71E-06	0.32	0.073	0.061	466	12.7	0.102	23.4	72
11	8	2.42	14.52	0.43	20	1.00E-03	1.81E-05	8.61E-10	8.71E-06	0.32	0.073	0.061	466	12.7	0.102	59.5	72
11	9	2.42	4.66	0.26	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5574	0.073	0.061	466	12.7	0.102	65.9	72
11	10	2.42	5.34	0.40	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5574	0.073	0.061	466	12.7	0.102	57.1	72
11	11	2.42	5.41	0.66	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5574	0.073	0.061	466	12.7	0.102	76.5	72
11	12	2.42	14.05	0.26	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5574	0.073	0.061	466	12.7	0.102	59.7	72
11	13	2.42	13.53	0.40	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5574	0.073	0.061	466	12.7	0.102	49.7	72
11	14	2.42	13.53	0.46	20	1.00E-03	1.81E-05	7.61E-10	7.59E-06	0.5574	0.073	0.061	466	12.7	0.102	5.1	72
11	15	2.42	4.66	0.26	20	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3021	0.073	0.061	466	12.7	0.102	77.4	72
11	16	2.42	5.34	0.40	20	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3021	0.073	0.061	466	12.7	0.102	64.7	72
11	17	2.42	5.41	0.10	20	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3021	0.073	0.061	466	12.7	0.102	54.4	72
11	18	2.42	13.53	0.40	20	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3021	0.073	0.061	466	12.7	0.102	10.4	72
11	19	2.42	13.53	0.46	20	1.00E-03	1.81E-05	8.45E-10	8.46E-06	0.3021	0.073	0.061	466	12.7	0.102	10.2	72
11	20	2.42	4.66	0.26	20	1.00E-03	1.81E-05	8.61E-10	8.71E-06	0.3202	0.073	0.061	466	12.7	0.102	13.8	72
11	21	2.42	5.34	0.40	20	1.00E-03	1.81E-05	8.61E-10	8.71E-06	0.3202	0.073	0.061	466	12.7	0.102	17.3	72
11	22	2.42	5.41	0.10	20	1.00E-03	1.81E-05	8.61E-10	8.71E-06	0.3202	0.073	0.061	466	12.7	0.102	21.5	72
11	23	2.42	13.53	0.40	20	1.00E-03	1.81E-05	8.61E-10	8.71E-06	0.3202	0.073	0.061	466	12.7	0.102	30.1	72
11	24	2.42	13.53	0.46	20	1.00E-03	1.81E-05	8.61E-10	8.71E-06	0.3202	0.073	0.061	466	12.7	0.102	27.2	72
12	1	3.03	17.28	0.24	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.218	0.074	0.033	207	25.4	0.305	19.3	72
12	2	3.03	17.28	0.40	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	51.7	72
12	3	3.03	17.28	0.43	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	17.4	72
12	4	3.03	17.28	0.53	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	36.4	72
12	5	3.03	17.28	0.56	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	32.2	72
12	6	3.03	21.59	0.19	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	27.7	72
12	7	3.03	21.59	0.38	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	26.7	72
12	8	3.03	21.59	0.50	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	24.0	72
12	9	3.03	21.59	0.60	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	18.6	72
12	10	3.03	25.91	0.45	13.9	1.17E-03	1.78E-05	7.08E-10	8.11E-06	0.2179	0.074	0.033	207	25.4	0.305	9.5	72
12	11	3.03	17.28	0.24	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3982	0.074	0.033	207	25.4	0.305	5.2	44

12	12	3.03	17.28	0.40	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	5.1	20	44
12	13	3.03	17.28	0.43	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	29.6	24	44
12	14	3.03	17.28	0.53	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	29.8	24	44
12	15	3.03	17.28	0.56	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	26.8	24	44
12	16	3.03	21.59	0.19	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	27.1	7	44
12	17	3.03	21.59	0.26	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	22.9	7	44
12	18	3.03	21.59	0.38	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	21.4	7	44
12	19	3.03	21.59	0.50	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	27.3	9	44
12	20	3.03	21.59	0.60	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	25.1	9	44
12	21	3.03	25.91	0.45	13.9	1.17E-03	1.78E-05	6.38E-10	7.28E-06	0.3981	0.074	0.033	207	25.4	0.305	22.7	9	44
12	22	3.03	17.28	0.24	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	20.0	10	44
12	23	3.03	17.28	0.40	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	20.8	10	44
12	24	3.03	17.28	0.43	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	18.4	10	44
12	25	3.03	17.28	0.53	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	9.7	20	43
12	26	3.03	17.28	0.56	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	6.2	20	43
12	27	3.03	21.59	0.19	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	3.2	20	43
12	28	3.03	21.59	0.26	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	28.0	24	43
12	29	3.03	21.59	0.38	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	20.7	24	43
12	30	3.03	21.59	0.50	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	15.5	24	43
12	31	3.03	21.59	0.60	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	17.2	24	43
12	32	3.03	25.91	0.45	13.9	1.17E-03	1.78E-05	6.81E-10	7.94E-06	0.4241	0.074	0.033	207	25.4	0.305	13.8	7	43
12	33	3.03	12.96	0.30	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	11.5	7	43
12	34	3.03	17.28	0.30	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	23.8	9	43
12	35	3.03	19.01	0.31	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	17.6	9	43
12	36	3.03	21.60	0.35	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	12.9	9	43
12	37	3.03	25.92	0.42	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	22.4	10	43
12	38	3.03	6.64	0.84	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	9.6	10	43
12	39	3.03	17.28	0.38	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	11.5	20	39
12	40	3.03	17.28	0.83	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	11.2	20	39
12	41	3.03	25.92	0.23	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	6.7	20	39
12	42	3.03	25.92	0.48	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	29.9	24	39
12	43	3.03	25.92	0.87	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	29.4	24	39
12	44	3.03	29.37	0.80	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	30.9	24	39
12	45	3.03	34.56	0.77	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	16.0	7	39
12	46	3.03	43.20	0.69	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	16.8	7	39
12	47	3.03	6.91	0.46	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	17.2	7	39
12	48	3.03	6.05	0.77	12.5	1.22E-03	1.77E-05	6.79E-10	8.03E-06	0.2019	0.074	0.033	207	25.4	0.305	26.5	9	39
12	49	3.03	13.82	0.34	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	207	25.4	0.305	26.0	9	39
12	50	3.03	13.82	0.51	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	207	25.4	0.305	25.6	9	39
12	51	3.03	11.23	0.69	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	207	25.4	0.305	25.5	10	39
12	52	3.03	20.73	0.51	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	207	25.4	0.305	26.6	10	39
12	53	3.03	13.82	0.26	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	207	25.4	0.305	21.7	10	39
12	54	3.03	13.82	0.43	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	207	25.4	0.305	31.9	40	72
12	55	3.03	13.82	0.26	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	207	25.4	0.305	46.2	40	72
12	56	3.03	13.82	0.43	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	207	25.4	0.305	52.2	40	72
12	57	3.03	13.82	0.34	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	60.5	40	72
12	58	3.03	13.82	0.51	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	70.0	40	72
12	59	3.03	11.23	0.69	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305		40	72

12	60	3.03	10.37	0.64	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	44.5	72
12	61	3.03	10.37	0.32	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	57.5	72
12	62	3.03	13.82	0.43	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	63.5	72
12	63	3.03	13.82	0.26	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	53.9	72
12	64	3.03	13.82	0.43	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	38.0	72
12	65	3.03	13.82	0.26	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	55.2	72
12	66	3.03	13.82	0.43	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	74.5	72
12	67	3.03	20.73	0.64	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	70.9	72
12	68	3.03	17.28	0.11	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	77.4	72
12	69	3.03	8.64	0.64	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	180	25.4	0.305	89.7	72
12	70	3.03	17.28	0.11	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	125	50.8	0.305	31.2	72
12	71	3.03	17.28	0.32	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	125	50.8	0.305	36.4	72
12	72	3.03	17.28	0.53	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	125	50.8	0.305	50.4	72
12	73	3.03	24.19	0.15	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	125	50.8	0.305	60.1	72
12	74	3.03	24.19	0.45	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	125	50.8	0.305	65.6	72
12	75	3.03	21.60	0.67	13	1.20E-03	1.78E-05	6.89E-10	8.06E-06	0.2075	0.074	0.033	125	50.8	0.305	44.9	72
12	76	2.88	11.20	0.61	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	47.3	72
12	77	2.88	12.06	0.50	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	67.2	72
12	78	2.88	13.78	0.76	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	57.7	72
12	79	2.88	14.65	0.52	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	51.2	72
12	80	2.88	17.23	0.51	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	40.2	72
12	81	2.88	18.95	0.45	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	69.6	72
12	82	2.88	20.68	0.61	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	65.8	72
12	83	2.88	21.54	0.61	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	83.7	72
12	84	2.88	22.40	0.69	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	62.2	72
12	85	2.88	23.26	0.55	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	10.0	72
12	86	2.88	26.71	0.46	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	13.4	72
12	87	2.88	27.57	0.76	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	15.7	72
12	88	2.88	27.57	1.15	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	17.1	72
12	89	2.88	28.43	0.34	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	21.1	72
12	90	2.88	31.01	1.07	26	8.74E-04	1.84E-05	9.92E-10	8.81E-06	0.4105	0.072	0.033	148	50.8	0.305	27.3	72
13	1	2.32	10.89	1.35	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	26.3	72
13	2	2.32	5.44	0.67	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	36.1	72
13	3	2.32	2.68	0.33	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	44.7	72
13	4	2.32	10.89	1.35	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	44.6	72
13	5	2.32	5.44	0.67	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	47.9	72
13	6	2.32	2.68	0.33	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	4.8	72
13	7	2.32	10.53	1.30	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	5.7	72
13	8	2.32	5.27	0.65	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	3.2	72
13	9	2.32	2.59	0.32	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	3.3	72
13	10	2.32	10.53	1.30	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	13.9	72
13	11	2.32	5.27	0.65	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	3.9	72
13	12	2.32	2.59	0.32	12.5	1.22E-03	1.77E-05	7.41E-10	8.72E-06	0.0793	0.074	0.033	207	25.4	0.305	68.7	72

APPENDIX A6

NEURAL NETWORK FORTRAN PROGRAM

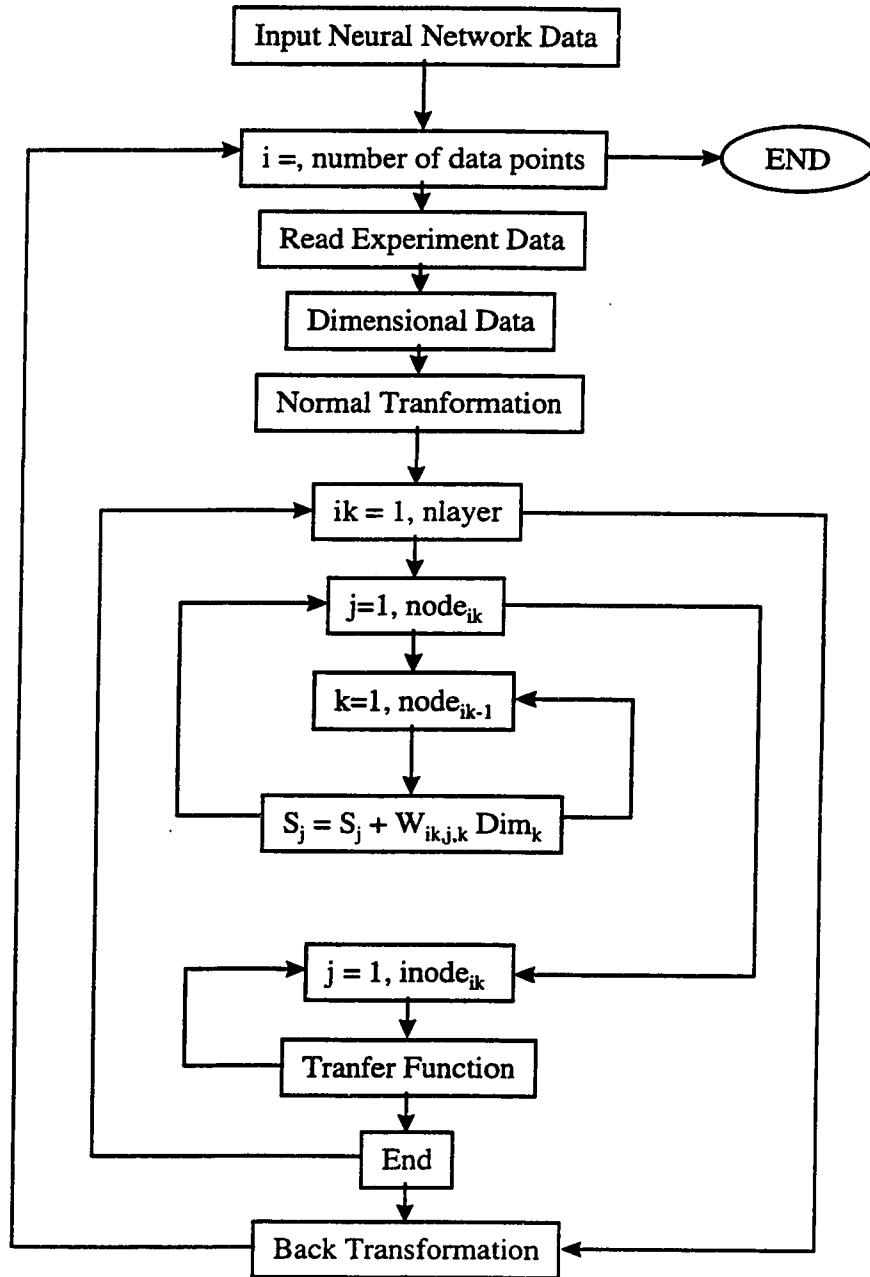


Figure A6-1. Organigram of the Neural Network Solution

THE NEURAL NETWORK FORTRAN PROGRAM

C LAST CHANGE: YD 17 OCT 98 8:09 PM
PROGRAM MASS TRANSFER COEFFICIENT USING NEURAL NETWORK

C LAST UPDATED: YASSINE DJEBBAR 19 JUNE 97 0:28 AM

```
REAL MEAN(20), DEV(20), W(6,10,20), A(20), B(20), SUMM(20)
REAL Y(20), D(6)
INTEGER INODE(20)
CHARACTER*12 INPUT0, INPUT1, INPUT2, OUTPUT
```

```
WRITE(*,*)'THIS PROGRAM ESTIMATES THE MASS TRANSFER COEFFICIENT'
WRITE(*,*)'      FOR AIR STRIPPING TOWERS'
WRITE(*,*)'      BY YASSINE DJEBBAR'
WRITE(*,*)'INPUT_NET, INPUT-DIM, INPUT-TRS, OUTPUT'
WRITE(*,*)
READ(*,*) INPUT0, INPUT1, INPUT2, OUTPUT
```

```
OPEN (5, FILE=INPUT0, STATUS='OLD')
OPEN (7, FILE=INPUT1, STATUS='OLD')
OPEN (8, FILE=INPUT2, STATUS='OLD')
OPEN (6, FILE=OUTPUT, STATUS='UNKNOWN')
```

! FILE UNIT # 5 CONTAINS THE NEURAL NETWORK DATA:

```
! NUMBER OF INPUT DATA POINTS INODE(1)
! NUMBER OF NODES IN LAYER 1 INODE(2)
! NUMBER OF NODES IN LAYER 2 INODE(3)
! NUMBER OF OUTPUTS 3 INODE(4)
```

```
READ(5,*)
READ(5,*)
READ(5,*) N LAYER, (INODE(I), I=1, N LAYER)
READ(5,*)
READ(5,*) DET, TMAX, TMIN
READ(5,*)
READ(5,*)
READ(5,*) (MEAN(J), J=1, INODE(1)+1)
READ(5,*)
READ(5,*) (DEV(J), J=1, INODE(1)+1)
READ(5,*)
```

```
READ(7,*)
READ(8,*) N ! NUMBER OF DATA POINT
```

```
DO I=2, N LAYER
  DO J=1, INODE(I)
    READ(5,*)
    READ(5,*) (W(I-1,J,K), K=1, INODE(I-1)+1)
```

```

        END DO
        READ(5,*)
    END DO

    DO I=1,N

        ! TRANSFORMATION OF THE DATA
        READ(7,*) KN, (DAT(J), J=1, 26)
        CALL DIMENS(DAT,B)
        DO J=1, INODE(1)
            A(J) = (B(J)-MEAN(J))/DEV(J)
        END DO
        A(INODE(1)+1) = 1.

        ! NEURAL NETWORK FEED FORWARD CALCULATION
        ! REPEAT FOR EACH LAYER: HIDDEN LAYER AND OUTPUT LAYER
        DO IK=2,NLAYER
            DO K=1,20
                SUMM(K) = 0.
            END DO

            DO J=1, INODE(IK)
                DO K = 1, INODE(IK-1)+1
                    SUMM(J) = SUMM(J) + W(IK-1,J,K)*A(K)
                END DO
            END DO

            DO J=1, INODE(IK)
                A(J) = (1-EXP(-DET*SUMM(J)))/(1+EXP(-DET*SUMM(J)))
                A(J) = 0.5*((TMAX-TMIN)*A(J) + (TMAX+TMIN))
            END DO
            A(INODE(IK)+1) = 1.
        END DO

        ! BACK TRANSFORMATION OF THE DATA TO NORMAL SCALE
        DO K=1, INODE(NLAYER)
            Y(K) = MEAN(INODE(1)+K) + DEV(INODE(1)+K) * A(K)
            Y(K) = Y(K) * DAT(16)*DAT(11)/DAT(17)
        END DO

        DO K=1,INODE(NLAYER)
            WRITE(6,100) NK, Y(K)
        END DO

100    FORMAT(14, 1X, E10.3)

    END DO
END PROGRAM

```

```

SUBROUTINE DIMENS(DATA,B)
DIMENSION DATA(30), BIM(20), B(20)
C
C   REL = BIM(1), REG = BIM(2), SCL = BIM(3), SCG = BIM(4)
C   FRL = BIM(5), FRG = BIM(6), WEL = BIM(7), WEG = BIM(8)
C   OM = BIM(9), ER = BIM(10), GAL = BIM(11), GAG = BIM(12)
C   TSL = BIM(13), TSG = BIM(14), SHF = BIM(15), SHL = BIM(16)
C   AS = BIM(17), HD = BIM(18), HAD = BIM(19), YAS = BIM(20)
C
DIM(1) = DATA(3)/DATA(16)/DATA(9)           ! REL = L/A/V
DIM(2) = DATA(4)/DATA(16)/DATA(10)          ! REG
DIM(3) = DATA(9)/DATA(7)/DATA(11)           ! SCL = V/RO/D
DIM(4) = DATA(10)/DATA(8)/DATA(12)          ! SCG
DIM(5) = DATA(16)*(DATA(3)/DATA(7))**2/9.81 ! FRL = A*L/RO
DIM(6) = DATA(16)*(DATA(4)/DATA(8))**2/9.81 ! FRG
DIM(7) = DATA(3)**2/(DATA(16)*DATA(14)*DATA(7)) ! WEL = L/A/SIG/RO
DIM(8) = DATA(4)**2/(DATA(16)*DATA(14)*DATA(8)) ! WEG
DIM(9) = DATA(15)/DATA(14)                  ! OM = SIG/SIG
DIM(10) = 1/DATA(16)/DATA(2)                 ! ER = 1/A/Z
DIM(11) = 9.81*(DATA(7)/DATA(9))**2/DATA(16)**3 ! GAL = RO/V/A
DIM(12) = 9.81*(DATA(8)/DATA(12))**2/DATA(16)**3 !
DIM(13) = DATA(9)**2*DATA(16)/DATA(7)/DATA(14) ! TSL = D*A/RO/SIG
DIM(14) = DATA(10)**2*DATA(16)/DATA(8)/DATA(14) !
DIM(15) = DATA(16)*DATA(17)                 ! SHF = D*A
DIM(16) = DATA(7)/(DATA(9)*9.81)            ! SHL = RO/D
DIM(17) = DATA(16)*DATA(17)                 ! AD = A*D
DIM(18) = DATA(2)/DATA(17)                  ! ZD = Z/D
DIM(19) = DATA(16)*DATA(17)**2/DATA(2)      ! ZAD = AD/Z
DIM(20) = DATA(23)*DATA(17)/(DATA(16)*DATA(11)) ! YAS = KLA*D/D/A

B(1) = DIM(1)
B(2) = DIM(2)
B(3) = DIM(3)
B(4) = DIM(4)
B(5) = DIM(5)
B(6) = DIM(7)
B(7) = DIM(17)
B(8) = DIM(18)

END SUBROUTINE

```

INPUT DATA FILE

NN DATA: 4 LAYERS: INPUT LAYER = 8, LAYER(2) = 3 LAYER(3) = 5, LAYER(4) = 1
N_LAYER IN_LAYER H_LAYER(1) H_LAYER(2) N_LAYER(N)
4 8 3 5 1
TRANSFER FUNCTION GAMA MAX MIN
0.01 11.000 -4.000

MEAN VALUES

9.69E+01 2.63E+02 1.04E+03 1.80E+00 4.02E-03 2.00E-02 6.56E+00 1.04E+02 1.74E+07

STANDARD DEVIATION VALUES

6.08E+01 2.73E+02 3.30E+02 1.43E-01 4.15E-03 2.01E-02 1.87E+00 5.25E+01 1.66E+07

LAYER(1)

-52.9158 10.2173 64.8027 -28.312 13.0119 -43.2943 -23.6880 34.3368 24.465542

LAYER(1)

-61.7820 -2.4606 -105.485 8.5049 108.1074 -6.4658 9.5473 154.3216 56.1444

LAYER(1)

80.7816 -5.0687 22.8984 -3.1711 -9.9195 -27.5760 -10.6312 -23.6447 -6.03

LAYER(2)

8.8658 -13.4570 -53.3897 -7.5133

LAYER(2)

101.6104 -7.7274 49.8860 11.2096

LAYER(2)

16.5340 62.5937 -18.6890 0.4384

LAYER(2)

-18.3272 -52.3305 15.2771 12.0818

LAYER(2)

42.1601 170.8592 97.8818 3.2192

LAYER(3)

-3.9176 -2.6876 14.2641 17.5710 -20.4170 34.5172