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**HIGH TEMPERATURE PROPERTIES AND
HEAT TRANSFER PHENOMENA
FOR STEAM
AT TEMPERATURES UP TO 5000K**

by

ALEKSANDAR Ž. VASIĆ

A thesis
presented to the University of Ottawa
in August, 1993
in partial fulfillment of the
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MASTER of APPLIED SCIENCE
in
MECHANICAL ENGINEERING

Ottawa-Carleton Institute for
Mechanical and Aeronautical Engineering



Aleksandar Z. Vasic, Ottawa, Canada, 1993



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Abstract

High Temperature Properties and Heat Transfer Phenomena for Steam at Temperatures up to 5000K

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Thermodynamic and transport properties and heat transfer phenomena for steam in a high temperature region were examined. The phenomenon of thermal dissociation (transformation of steam from a single component gas to a six-component gas mixture) occurs in this temperature region. After a careful literature assessment of available sets of property tables and equations for high temperature steam, a set of high temperature steam properties was selected. First, a set of computer subroutines was developed - the Fraction code, for generating molar fractions of a dissociating steam and gas mixture for a given pressure and temperature. Second, a set of computer subroutines was developed for the computation of all possible combinations of binary diffusion coefficients and of the diffusion coefficient for the component through a gas mixture. Third, steam properties may be evaluated for an ideal gas mixture which includes no effects of chemical reactions - frozen state, or for a non-ideal solution at equilibrium state which includes maximal effects of chemical reactions - effective properties at equilibrium state. A set of computer subroutines was developed - the Frozen Properties code, for evaluating dissociated steam frozen properties for a given pressure and temperature. Finally, the effective properties recommended are those presented by Vargaftik (1983) using the prediction method of Kesselman and Blank (1968 i). A computer code, UODH2O (University of Ottawa Dissociated H₂O code), was developed using a look-up table and interpolation technique to generate effective properties at pressures from 0.01 to 100.00MPa and temperatures from 1000 to 5726.85°C.

Based on the semi-empirical model by Nesterenko et al. (1967 a) for dissociated nitrogen tetroxide ($\text{N}_2\text{O}_4 \rightleftharpoons 2\text{NO}_2$, a two-component gas mixture), a method was developed to determine the Nusselt number of a chemically reacting (dissociated) fluid flow. This method includes the effects of Lewis number (the former works assumed that Lewis number equals 1.0). The method proposed in this work was applied to dissociated steam (a six-component gas mixture). This method is a superposition model of the Nusselt number of the mixture of chemically non-reacting gases (frozen state) and the sum of the effects of all chemical reactions which occur in the gas mixture. The second term represents the contribution to heat transfer due to mass transfer of the species in the gas mixture. The High Temperature Steam Heat Transfer computer code (VASICA) was developed to predict heat transfer in a turbulent tube flow of steam. Predictions according to the proposed method are compared to the predictions of three typical correlations from the literature developed for low and moderate temperature conditions: Dittus and Boelter (1930), Petukhov et al. (1972) and Hadaller and Benerjee (1969).

Key words : Steam - Water Vapour - Thermodynamic Properties - Transport Properties -
High Temperature - Dissociation - Heat Transfer - Heat Transfer Coefficient

Dedication

To

Susanne

My best friend and life companion,
the special and very important person to me.
She demonstrated unfaltering faith in me,
continuous motivation and
assiduous support
which made this
work happen.

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Table of Contents

Abstract		i
Dedication		ii
Acknowledgements		iii
Table of Contents		iv
List of Figures		ix
List of Tables		xiii
List of Symbols		xiv
1 Introduction		1
1.1 Outline of the Problem		1
1.2 Dissociation		2
1.3 Effect of Dissociation on Heat Transfer		5
2 Prediction of High Temperature Properties for Pure Gases		7
2.1 General		7
2.2 Properties of Pure Gases which are Products of the Thermal Dissociation of Steam		7
2.3 Pure Gases		13
2.3.1 Hydrogen (H_2 and H)		13
2.3.2 Oxygen (O_2 and O)		18
2.3.3 Hydroxyl (HO)		19
3 Prediction of High Temperature Properties for Steam: Literature Review		20
3.1 General		20
3.2 Thermal Dissociation of Steam at High Temperature		20

3.3 Previous Studies	24
3.3.1 Literature review	24
3.3.2 Thermodynamic properties	29
3.3.2.1 Non-dissociated steam as an ideal gas	29
3.3.2.2 Non-dissociated steam as a real gas	30
3.3.2.3 Dissociated steam as an ideal mixture of ideal gases (ideal gas mixture)	30
3.3.2.4 Dissociated steam as an ideal mixture of real gases (ideal solution)	32
3.3.2.5 Dissociated steam as a real mixture of real gases (non-ideal solution)	33
3.3.3 Transport properties of steam	34
3.3.3.1 Non-dissociated steam as an ideal gas	34
3.3.3.2 Non-dissociated steam as a real gas	34
3.3.3.3 Dissociated steam as an ideal mixture of real gases (ideal solution)	35
3.3.3.4 Dissociated steam as a real mixture of real gases (non-ideal solution)	35
3.4 Review of Two Sources	36
3.4.1 R.A. Svehla	36
3.4.2 P.M. Kesselman et al.	39
3.5 Comparison of Predictions	53
4 Prediction of High Temperature Properties for Steam: Recommended Methods	54
4.1 General	54
4.2 Frozen Properties of Dissociated Steam: Mixture of Ideal Gases	55
4.3 Recommended Prediction Method for Mass Diffusion Coefficients	60
4.3.1 Binary mixture	60

4.3.2 Multi-component mixture	66
4.4 Effective Thermodynamic and Transport Properties of Dissociated Steam	69
4.5 Summary	78
5 Heat Transfer for Pure Gases and Steam at Moderate Temperatures.	79
5.1 General	79
5.2 Heat Transfer Correlations for Pure Fluids in Smooth Tubes	80
5.3 Heat Transfer Correlations for Superheated Steam in Smooth Tubes	86
5.4 Recommendation	86
6 Heat Transfer for Dissociated Steam at High Temperatures	89
6.1 Mechanism of Heat Transfer at High Temperatures	89
6.2 Previous Studies	98
6.2.1 Heat transfer for dissociated gases	98
6.2.1.1 Petukhov et al.'s model	99
6.2.1.2 Nesterenko et al.'s model	103
6.3 Heat Transfer by Radiation for Dissociated Steam	107
6.4 Effect of Dissociated Steam Compressibility on Heat Transfer	110
6.5 Summary	113
7 Prediction Method of Heat Transfer for Dissociated Steam	114
7.1 Introduction	114
7.2 Prediction Method of Heat Transfer for Dissociated Steam	115
7.3 Comparison of the Results	125
8 Conclusion and Discussion	131

References	134
Appendix	
A Method for Calculating Molar Fraction of Dissociated Steam as a Mixture of Chemically Reacting Gases	155
B Method for Calculating Steam Properties as a Mixture of Chemically Non-Reacting Gases (Frozen)	164
C Method for Calculating Steam Properties as a Mixture of Chemically Reacting Gases (Effective)	167
D Derivation of the Effective Nusselt Number for a Mixture of Chemically Reacting Gases	172
E Method for Calculating the Local Heat Transfer Coefficient and the Wall Temperature for a Turbulent Pipe Flow of Dissociated Steam with Constant Heat Flux at the Wall	179
F Programming Specifications for the Mole Fraction Calculation of Dissociated Steam	186
G Programming Specifications for Frozen Properties of Dissociated Steam for Pressure from 0.000101325 to 101.325MPa and Temperature from 726.85 to 4726.85°C	192
H Programming Specifications of UODH2O code for Effective Properties of Dissociated Steam for Pressure from 0.01 to 100.00MPa and Temperature from 1000. to 5726.85°C	211
I Programming Specifications of the High Temperature Steam Heat Transfer Code (VASICA)	253
J Table of Composition of Dissociated Steam at Pressure from 0.01 to 100.00MPa and Temperature from 1000 to 3000°C	273
K Table of Frozen Properties for Dissociated Steam at Pressure from 0.01 to 100.00MPa and Temperature from 1000 to 3000°C	279
L Table of Effective Properties for Dissociated Steam at Pressure from 0.01 to 100.00MPa and Temperature from 1000 to 3000°C	285

M	Look-up Table of Convective Heat Transfer Coefficients for High Temperature Dissociated Steam in Tube Flow at Pressure from 0.01 to 100.00MPa and Temperature from 1000 to 3000°C	291
N	Conversion of units and fundamental constants	296
O	Glossary	298
P	Manuscript of the paper, "A comparison of predictions of high-temperature steam properties" by Vasić et al. (1992).	300

List of Figures

1.1	Change of kinetic energy distribution for temperature increase from lower T_1 toward higher T_2 , according to Russell (1992).	4
1.2	Heat transfer coefficient in turbulent tube flow as a function of temperature. .	6
2.1	Molar fraction of dissociated steam as a function of temperature at a constant pressure. .	9
2.2	Effect of pressure on the molar fraction of steam.	11
2.3	The molar fractions of the mixture components at temperatures up to 3000°C and pressure 0.1MPa.	12
2.4	Thermal conductivity of the hydrogen-oxygen system for temperatures from 1000 to 15000K and pressure of 1 bar by Baronnet et al. (1985).	14
2.5	Dynamic viscosity of the hydrogen-oxygen system for temperatures from 1000 to 15000K and pressure of 1 bar by Baronnet et al. (1985).	15
2.6	The degree of hydrogen dissociation - α , density - ρ , thermal conductivity - λ , heat capacity - C_p , viscosity - μ and Prandtl number - Pr as a function of temperature and constant pressures by Petukhov and Popov (1964).	16
2.7	Variation of the hydrogen mole fractions with temperature at several pressures by Kubin et al. (1964).	17
3.1	The molar fractions of steam as a function of temperature from Baronnet et al.(1985)	22
3.2	Classification of the hypothesis for prediction properties of steam at high temperatures.	25
3.3	Comparison of viscosities of steam at high temperatures calculated by Svehla (1964) with experimental results by Bonilla et al. (1956), correction as proposed by Brokaw (1968) and experimental results of Latta (1965).	38
3.4	The shape of the Lennard-Jones intermolecular potential function.	40
3.5	Kesselman's method of determination of the parameters ϵ/k_B and b_0 by bringing the experimental data points (circles) and theoretical curve to graphical coincidence.	42
3.6	The experimental data on the second virial coefficient $B^*(T^*)$ by Lennard-Jones potential with variable $\epsilon(T)$ and $\sigma(T)$ by Kesselman (1964).	44

3.7	The Lennard-Jones potential parameters ϵ/k_B as a function of temperature by Kesselman and Blank (1968 i).	45
3.8	The Lennard-Jones potential parameters σ as a function of temperature by Kesselman and Blank (1968 i).	46
3.9	Comparison of experimental and theoretical viscosities at high temperature of argon by Reed and Gubbins (1973).	50
3.10	Comparison of several potential functions for the repulsion region of argon by Reed and Gubbins (1973).	51
3.11	Slope of the repulsion portion of the Lennard-Jones potential function for water vapour (H ₂ O) at high temperatures using data by Kesselman and Blank (1968 i).	52
4.1	Molar mass of dissociated steam as a function of temperature for a range of constant pressures, predicted by the Frozen Properties code.	56
4.2	Frozen enthalpy of dissociated steam as a function of temperature for a range of constant pressures, predicted by the Frozen Properties code.	57
4.3	Frozen heat capacity of dissociated steam as a function of temperature for a range of constant pressures, predicted by the Frozen Properties code.	58
4.4	Frozen thermal conductivity of dissociated steam as a function of temperature for a range of constant pressure, predicted by the Frozen Properties code.	59
4.5	Self-diffusion coefficients of steam dissociation components at pressure 0.1MPa.	63
4.6	Binary diffusion coefficients of species <i>l</i> through species <i>i</i> at 0.1MPa.	64
4.7	Binary diffusion coefficients of species <i>l</i> through species <i>i</i> at 0.1MPa.	65
4.8	Diffusion coefficients for components of steam dissociation through a mixture at a pressure of 0.1MPa.	68
4.9	Specific volume of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.	71
4.10	Density of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.	72
4.11	Entropy of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.	73

4.12	Enthalpy of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.	74
4.13	Heat capacity of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.	75
4.14	Viscosity of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.	76
4.15	Thermal conductivity of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.	77
6.1	Heat Transfer mechanism for the turbulent flow of dissociated steam in a round tube.	90
6.2	Schmidt number for the components of a gas mixture formed by steam dissociation as a function of temperature at constant pressure.	93
6.3	Prandtl number for a gas mixture formed by steam dissociation as a function of temperature at constant pressure.	94
6.4	Lewis number for the components of a gas mixture formed by steam dissociation as a function of temperature at constant pressure.	95
6.5	Reynolds number as a function of temperature for a range of constant pressures. .	97
6.6	Comparison of experimental and predicted heat transfer coefficients, applying the model by Nesterenko et al. (1968), including the kinetics of chemical reaction.	106
6.7	Water vapour (H ₂ O) emissivity at a constant total pressure of a dissociating steam gas mixture, for two mean beam length.	109
6.8	Maximal (critical) mass velocity as a function of temperature at constant pressure.	112
7.1	Heat effect of chemical reactions (during steam dissociation) as a function of temperature at constant pressure.	118
7.2	Sherwood number for components of steam dissociation as a function of temperature.	119
7.3	Change of Nusselt number as a function of temperature for each of the five terms that the proposed effective Nusselt number consists of.	121
7.4	Formation of the effective Nusselt number (sum of the five terms) as a function of temperature.	122

7.5	Formation of the effective heat transfer coefficients (sum of the five terms) as a function of temperature.	123
7.6	Difference between wall and bulk temperature during turbulent flow of dissociated steam in a tube as a function of bulk temperature at certain constant flow conditions.	124
7.7	Comparison of predictions from three sources and the present work, for heat transfer coefficients in high temperature steam during turbulent tube flow. . .	127
7.8	Difference between wall and bulk temperature during turbulent flow of dissociated steam in a tube as a function of bulk temperature at constant flow conditions.	129
7.9	Comparison of the wall temperature predictions with predictions from the present work.	130
C.1	Illustration of properties interpolation technique.	168

List of Tables

3.1	Combination of interactions between products of steam dissociation		23
3.2	Literature review for properties of non-dissociated steam		27
3.3	Literature review for properties of dissociated steam		28
5.1	Heat transfer correlations for turbulent flow of fluids in smooth tubes		81
5.2	Heat transfer correlations for turbulent flow of gases with large temperature differences in smooth tubes		84
5.3	Heat transfer correlations for turbulent flow of superheated steam in smooth tubes		87
A-1	The molar mass and the enthalpy of formation for components of water vapour dissociation at temperatures $T = 0^\circ\text{K}$ and $T = 298.15^\circ\text{K}$ (25°C) and pressure $P = 0.1\text{MPa}$ by Chase et al. (1985)		159
A-2	Multiplying factors for conversion between molar fractions, mass fractions, molar concentrations and mass concentrations		163
C-1	Intermolecular force parameters, $\epsilon(T)/k_B$ and $\sigma(T)$ for Lennard-Jones potential function, in temperature range from 1000 to 3400K for components of water vapour dissociation by Kesselman and Blank (1968 i)		170
C-2	Virial coefficients for components of water vapour dissociation in temperature range from 1000 to 3400K, by Kesselman and Blank (1968 i)		171
J-1	Table of dissociated steam composition at pressure range from 0.01 to 100.00MPa and temperature range from 1000 to 3000°C		274
K-1	Table of frozen properties for dissociated steam at pressure range from 0.01 to 100.00MPa and temperature range from 1000 to 3000°C		280
L-1	Table of effective properties for dissociated steam at pressure range from 0.01 to 100.00MPa and temperature range from 1000 to 3000°C		286
M-1	Look-up table for convective heat transfer coefficients on high temperature dissociated steam in tube flow at pressure range from 0.01 to 100.00MPa and temperature range from 1000 to 3000°C		292

List of Symbols

The following list of symbols is most commonly used. The less frequently referenced symbols are defined as they appear in the text.

<u>English letter symbols</u>	<u>Name</u>	<u>Units</u>
a	Adiabatic speed of sound	m s^{-1}
α	Thermal diffusivity = $k \rho^{-1} \text{Cp}^{-1}$	$\text{m}^2 \text{s}^{-1}$
C	Constant	dimensionless
C_i	Molar concentration of species i in a mixture m	$\text{mol}_i \text{m}_m^{-3}$
$\bar{C}_p$	Heat capacity at constant pressure per mole	$\text{J mol}^{-1} \text{K}^{-1}$
C_p	Heat capacity at constant pressure per unit mass	$\text{J kg}^{-1} \text{K}^{-1}$
C_v	Heat capacity at constant volume	$\text{J kg}^{-1} \text{K}^{-1}$
$D_{l,i}$	Mass diffusion coefficient of species l through species i	$\text{m}^2 \text{s}^{-1}$
$D_{l,m}$	Mass diffusion coefficient of species l through mixture m	$\text{m}^2 \text{s}^{-1}$
d	Internal pipe diameter	m
f, C_f	Fanning friction factor = $2 \tau_w \rho^{-1} u^{-2}$ (or skin-friction coefficient)	dimensionless
G	Fluid mass velocity = ρu	$\text{kg m}^{-2} \text{s}^{-1}$
g_i	Mass transfer coefficient of species i	m s^{-1}
h	Heat transfer coefficient	$\text{W m}^{-2} \text{K}^{-1}$
$\bar{H}$	Enthalpy per mol	J mol^{-1}
H	Enthalpy per unit mass	J kg^{-1}
$\bar{j}_i$	Molar flux of species i	$\text{mol}_i \text{m}^{-2} \text{s}^{-1}$
j_i	Mass flux of species i	$\text{kg}_i \text{m}^{-2} \text{s}^{-1}$

<u>English letter symbols</u>	<u>Name</u>	<u>Units</u>
J_l	The rate of generation of the species l due to the chemical reaction	$\text{kg}_l \text{ m}_m^{-3} \text{ s}^{-1}$
k, λ	Thermal conductivity	$\text{W m}^{-1} \text{ K}^{-1}$
k_B	Boltzmann constant	$\text{J K}^{-1} \text{ molecule}^{-1}$
$\bar{m}$	Amount of substance	mol
$\bar{M}_i$	Molar mass of species i	$\text{kg}_i \text{ kmol}_i^{-1}$
$\bar{M}_m$	Molar mass of gas mixture	$\text{kg}_m \text{ kmol}_m^{-1}$
N	Total number of molecules	dimensionless
n	Number of species in the mixture of gases	dimensionless
P	Absolute pressure	$\text{Pa} = \text{N m}^{-2}$
p	Pressure	$\text{Pa} = \text{N m}^{-2}$
$\tilde{R}$	Universal gas constant	$\text{J kmol}^{-1} \text{ K}^{-1}$
S	Entropy per unit mass	$\text{J kg}^{-1} \text{ K}^{-1}$
T	Absolute temperature of a fluid	K
t	Temperature	$^{\circ}\text{C}$
u	Velocity component of the flow in axial direction	m s^{-1}
$\langle u \rangle$	Mean axial velocity	m s^{-1}
v	Specific volume	$\text{m}^3 \text{ kg}^{-1}$
x_i	Mole fraction of component i in a liquid mixture m	$\text{mol}_i \text{ mol}_m^{-1}$
y_i	Mole fraction of component i in a gas mixture m	$\text{mol}_i \text{ mol}_m^{-1}$
Z	Compressibility factor	dimensionless

<u>Greek letter symbols</u>	<u>Name</u>	<u>Units</u>
α	Degree of dissociation	dimensionless
ϵ	Emissivity	dimensionless
γ	The specific heat ratio	dimensionless
ρ	Density	kg m^{-3}
ρ_i	Mass concentration of species i in a mixture m	$\text{kg}_i \text{m}_m^{-3}$
ρ_m	Density of gas mixture	$\text{kg}_m \text{m}_m^{-3}$
μ	Dynamic viscosity	N s m^{-2}
ν	Kinematic viscosity	$\text{m}^2 \text{s}^{-1}$
σ	Stefan-Boltzmann constant	$\text{W m}^{-2} \text{K}^{-4}$
τ	Shear stress between fluid layers	$\text{Pa} = \text{N m}^{-2}$
τ_w	Shear stress at the wall	$\text{Pa} = \text{N m}^{-2}$
ω_i	Mass fraction of component i in the mixture m	$\text{kg}_i \text{kg}_m^{-1}$
ξ	Darcy friction factor $= 8 \tau_w \rho^{-1} u^2 = 4 f$	dimensionless

<u>Dimensionless groups</u>	<u>Name</u>
-----------------------------	-------------

Cr_l	Reaction number, rate of generating the species l due to the chemical reaction in the mixture $= J_l \times G^{-1}$
--------	---

$Le_{l,m}$	Lewis number of the species l in the mixture $= k_l \rho_m^{-1} Cp^{-1} D_{l,m}^{-1}$
------------	---

Ma	Mach number $= u a^{-1}$
------	--------------------------

Nu	Nusselt number $= h d k^{-1}$
------	-------------------------------

Pe	Peclet number $= Re Pr = G d Cp k^{-1}$
------	---

Pr	Prandtl number $= Cp \mu k^{-1}$
------	----------------------------------

Re	Reynolds number $= G d \mu^{-1}$
------	----------------------------------

<u>Dimensionless groups</u>	<u>Name</u>
-----------------------------	-------------

$Sc_{t,m}$ Schmidt number = $\nu D_{t,m}^{-1}$

Sh_l Sherwood number = $g d_c D_{t,m}^{-1}$

St_T Stanton number = $Nu Pe^{-1} = Nu Re^{-1} Pr^{-1} = h G^{-1} Cp^{-1}$

<u>Overstrike</u>	<u>Name</u>
-------------------	-------------

~ Quantity of matter as expressed per mole

- Average value over time

<u>Brackets</u>	<u>Name</u>
-----------------	-------------

$\langle a \rangle$ Average value of an over cross section

$|=|$ Has the dimensions of ...

<u>Subscripts</u>	<u>Name</u>
-------------------	-------------

$_b$ Evaluated at bulk condition (T_b)

$_e$ Equivalent (diameter)

$_{eq}$ Equilibrium of the chemical composition in the mixture

$_{eff}$ Effective - properties of chemically reacting species

$_{fr}$ Frozen - properties of chemically non-reacting species

$_f$ Evaluated at film condition ($T_f = 0.5 (T_b + T_w)$)

$_H$ Defined as enthalpy difference

$_i$ Properties of species i

$_m$ Properties of the mixture of gases

$_r$ Reacting - properties due to chemical reaction

$_T$ Defined as temperature difference

SubscriptsName

- _w Evaluated at wall condition (T_w)
- ^o Condition at standard temperature ($T = 0K$)
- ²⁹⁸ Condition at standard temperature ($t = 25^\circ C$ or $T = 298.15K$)

SuperscriptsName

- ^o Condition at standard pressure ($P = 0.1MPa$)

Chapter 1

Introduction

1.1 Outline of the Problem

The use of a conventional steam system requires data on the properties of steam in a temperature region up to a maximum of 800°C. These properties are extensively investigated and documented in many books, in the form of steam tables and charts. Data presented in the steam tables represent the contributions and recommendations of qualified engineering organisations such as ASME¹ by Meyer et al. (1967), or governmental organisations such as NBS²/NRC³ by Haar et al. (1984). Applications in new technologies such as combustion, rocket propulsion, nuclear reactors, solar furnaces and arc plasma require the investigation of the properties of steam at much higher temperatures.

The specific needs for steam properties and heat transfer predictions at temperatures higher than 800°C are required in nuclear industry for Loss-of-Coolant-Accident (LOCA) analyzes in water-cooled reactors. The objective of this study can be divided into two parts. First, to survey available data for steam properties in high temperature regions, particularly at temperatures from 800 to 3000°C, and to recommend a method for predicting properties in that region. This data is needed to predict the local heat transfer coefficients. Second, to devise a method for the prediction of the heat transfer coefficient to steam for turbulent pipe flow with a constant wall heat flux for a high temperature region.

¹ ASME is an acronym for American Society of Mechanical Engineers.

² NBS is an acronym for National Bureau of Standards (U.S.A).

³ NRC is an acronym for National Research Council (Canada).

This thesis presents an analysis of the thermodynamic and transport properties of steam within the pressure range from 0.01 to 100MPa and the temperature range from 1000 to 5726.85°C (the region where phenomena of dissociation occur). The effect of high temperature properties on the convective heat transfer coefficient of turbulent flow is also examined.

1.2 Dissociation

Dissociation is a chemical term for the temporary, reversible decomposition of the molecules of a compound which occurs under certain conditions. This is the process by which a chemical compound splits into simpler constituents. These components are capable of recombining under other conditions. Dissociation can be electrolytic or thermal depending on the cause of dissociation (form of energy needed for breaking chemical bonds). In electrolytic dissociation, electrolytes are split into charged ions. In thermal dissociation, due to the effect of thermal energy molecules decompose into a number of specific components (molecules or atoms). The degree of dissociation is a function of temperature and pressure. After cooling, the products of dissociation will recombine. In this study, the term dissociation will always mean thermal dissociation.

One satisfactory method of understanding the mechanism of thermal dissociation is to analyze it on the molecular level. From the kinetic theory of gases, temperature is defined as the mean kinetic energy of all molecules. A temperature increase is then an increase of mean kinetic energy. Gas molecules are in continuous disorderly movement between collisions with other molecules. When two molecules collide they exchange kinetic energy. The molecule with the lower kinetic energy before the collision gains energy after the collision and the molecule with the higher kinetic energy before the collision loses part of its energy. If the energy exchanged between the molecules is less than required activation energy (energy needed to break their chemical structure), the two molecules bounce and continue chemically unchanged. Conversely, when the kinetic energy is greater than the needed activation energy, the colliding molecules break their chemical structure, absorbing part of the kinetic energy. After such a collision, three or more different molecules are produced. This is dissociation of the molecule into various fractions.

The degree of dissociation of a gas increases with temperature. Each molecule of a gas moves at different velocities. According to the statistical theory, the molecules have a normal velocity distribution. The majority of the molecular velocities border upon the mean velocity, hence a small percent have a velocity significantly greater than or smaller than the mean velocity.

At moderate temperatures of a gas, the mean kinetic energy and the mean velocity are relatively low, thus the number of molecules which have kinetic energy greater than the activation energy are comparatively few in the total number of molecules, as presented in Figure 1.1. Therefore, the degree of dissociation, though not zero, is negligibly small. However, at higher temperatures the mean kinetic energy is increased; accordingly, the number of molecules which have a kinetic energy larger than the activation energy is increased. As a result, an increase in temperature increases the degree of dissociation.

Conversely, the degree of dissociation decreases with pressure. At lower pressures the molar density of the gas is lower, hence the number of molecules which collide per unit time is less than at higher pressures. In a gas at the same temperature, which implies the same the mean kinetic energy, molecules at higher pressures collide more often than at lower pressures. Due to frequent collisions, the free path of a molecule between collisions is short and the velocity of the majority of molecules is close to the mean (average) velocity. The number of molecules which have velocity much greater than the mean velocity are comparatively few at higher pressure than at lower pressure. Therefore, deviation from the mean kinetic energy is smaller at higher pressures and the number of molecules which have a kinetic energy higher than the activation energy is smaller at higher pressures than at lower pressures. Thus, the degree of dissociation is smaller at higher pressures than at lower pressures.

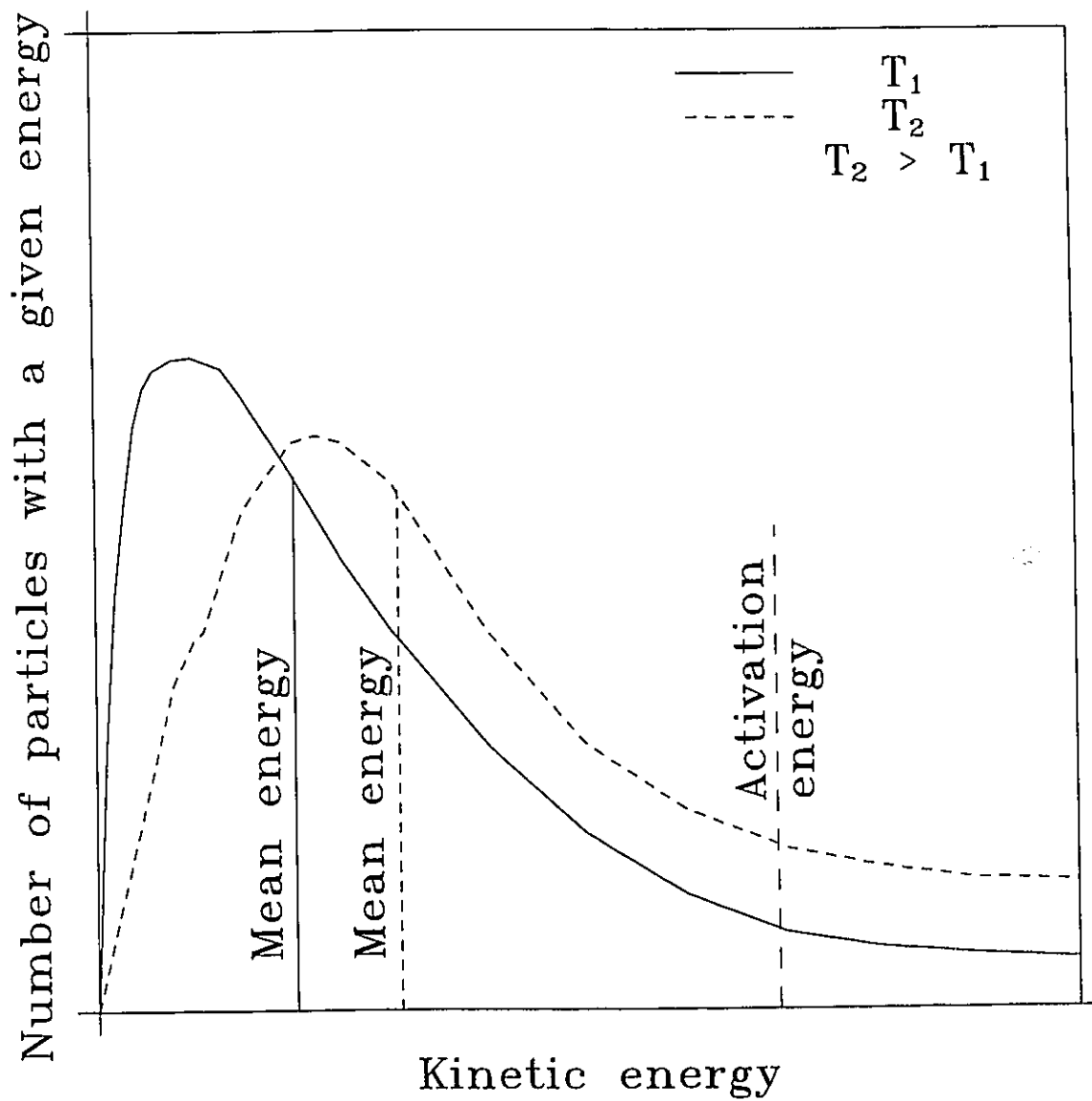


Figure 1.1: Change of kinetic energy distribution for temperature increase from lower T_1 toward higher T_2 , according to Russell (1992).

1.3 Effect of Dissociation on Heat Transfer

Extrapolation of steam-property equations to temperatures well beyond the upper limit of the range of their intended applications, or the use of ideal gas laws to predict steam properties at high temperatures, is a common practice. In Figure 1.2, the effect of such an extrapolation on the heat transfer coefficient is presented. The heat transfer coefficients are predicted using an extrapolation of non-dissociated steam property equations beyond the temperature limits (ASME $>1000^{\circ}\text{C}$ and IAPS⁴ $>2000^{\circ}\text{C}$) and the properties of dissociated steam⁵. Comparing the predictions based on the extrapolation with the actual data for dissociated steam, differences of up to an order of magnitude may be encountered. Such a practice thus can produce large inaccuracies, and become completely unacceptable in the temperature range where dissociation occurs.

Thermal dissociation is a heat absorbing process and recombination of fractions is a heat releasing process. The amount of heat absorbed or released, the heat of dissociation, is energy utilized by chemical reactions. Heat of steam dissociation is 6 to 7 times larger, per unit of mass, than the heat of water evaporation. Due to dissociation, the single component gas becomes a gas mixture. Composition gradients induce mass transfer in the gas mixture. Heat transport from one region to another takes place by mass diffusion and mass convection of gas mixture components. In addition to heat conduction, heat convection, and radiation, dissociated gas features the phenomena of transfer of heat by mass transfer.

⁴ IAPS is an acronym for International Association for the Properties of Steam.

⁵ Properties of steam are predicted using the UODH₂O (University of Ottawa Dissociated H₂O) code.

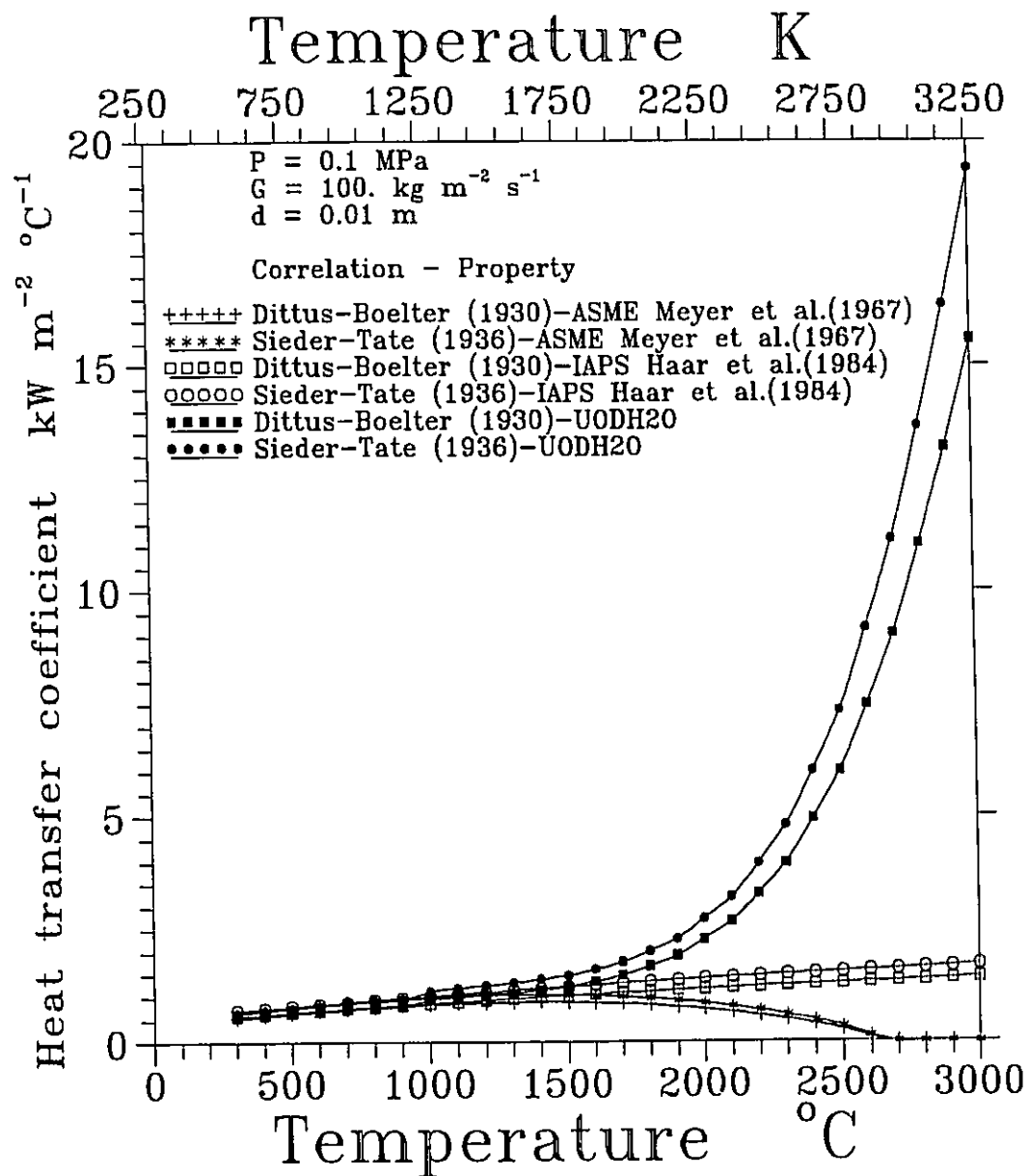


Figure 1.2: Heat transfer coefficient in turbulent tube flow as a function of temperature.

Chapter 2

Prediction of High Temperature Properties for Pure Gases

2.1 General

Pure gas is a single gas with a fixed composition and a fixed definite set of properties. Data for some thermodynamic properties of pure gases can be found in the general thermochemical tables of Chase et al. (1985), Gurvich et al. (1982), Barin and Knacke (1973) or McBride et al. (1963). The transport properties for pure gases have been reported by Vargaftik (1983), Keenan et al. (1980) and Vasserman et al. (1971). However, this chapter is concerned only with the properties of pure gases which are products of steam dissociation at high temperatures.

2.2 Properties of Pure Gases Which Are Products of the Thermal Dissociation of Steam

At moderate temperatures and pressures, steam (water vapour) is composed of water molecules alone. The water molecule consists of one oxygen atom (chemical symbol O) and two hydrogen (chemical symbol H) atoms. The degree of dissociation (α) is usually defined as the ratio of the number of molecules split by dissociation (n) to the total number of molecules present in gaseous phase (N) i.e.,

$$\alpha \equiv \frac{n}{N} \quad 0.0 \leq \alpha \leq 1.0 \quad (2.1)$$

Before dissociation ($\alpha = 0$), steam has only one component - H_2O molecules. However, with total dissociation ($\alpha = 1.0$), hypothetically it would become a mixture of two components, atomic

hydrogen and atomic oxygen. The molar fraction of the components in the gas mixture (y_i) is defined as the ratio of the number of moles of component (i) to the number of moles of the mixture (sum of the moles of all components).

$$y_i \equiv \sum_{i=1}^n \frac{n_i}{N} \quad (2.2)$$

The composition of the mixture after total dissociation ($\alpha = 1.0$) to atomic species can be expressed as

$$y_1 + y_2 = 1 \quad y_1 = y(H) = 2/3 = 0.666 \quad y_2 = y(O) = 1/3 = 0.333 \quad (2.3)$$

At temperatures up to 6000K, hydrogen and oxygen atoms may form nine components: H_2O (water vapour), H_2 , O_2 , HO (hydroxyl), H , O , HO_2 (hydrogen dioxide), H_2O_2 (hydrogen peroxide) and O_3 (ozone). The concentration of the last three components is negligible, according to Straub and Maidhof (1987 a), Baronnet et al. (1985) and Gefter et al. (1976). Baronnet et al. (1985) demonstrated that the molar fractions of the three components at pressure 0.1MPa are

$$y(HO_2) < 3 \cdot 10^{-5} \quad y(H_2O_2) < 2 \cdot 10^{-6} \quad y(O_3) < 3 \cdot 10^{-9} \quad (2.4)$$

and hence they can be neglected.

Thus, the product of steam dissociation at temperatures from 1500 to 3000°C is a mixture of the following six components: H_2O , H_2 , O_2 , HO , H and O .

The composition of the dissociated gas mixture may be determined according to several methods. The methods for calculating the molar fraction of dissociated water vapour as a mixture of chemically reacting gases are presented in Appendix A. According to the method by Ihara (1977), a set of computer subroutines, the Fraction code, written in FORTRAN77⁴ computer language, was developed for the prediction of the molar fraction of dissociated steam. The listing of the Fraction code is presented in Appendix F. The computation of the molar fractions for dissociated steam in a range of pressures and temperatures was performed. The results of molar fraction predictions generated for dissociated steam are presented in Appendix J as a table of dissociated steam composition at pressure range from 0.01 to 100.00MPa and temperature range from 1000 to 3000°C.

Thermal dissociation is temperature and pressure dependent. Figure 2.1 shows the molar

⁴ A problem-oriented high level programming language for scientific and mathematical use developed from American National Standard programming language FORTRAN, ANSI X3.9-1978, commonly referred to as FORTRAN77. FORTRAN is an acronym for FORMula TRANslation.

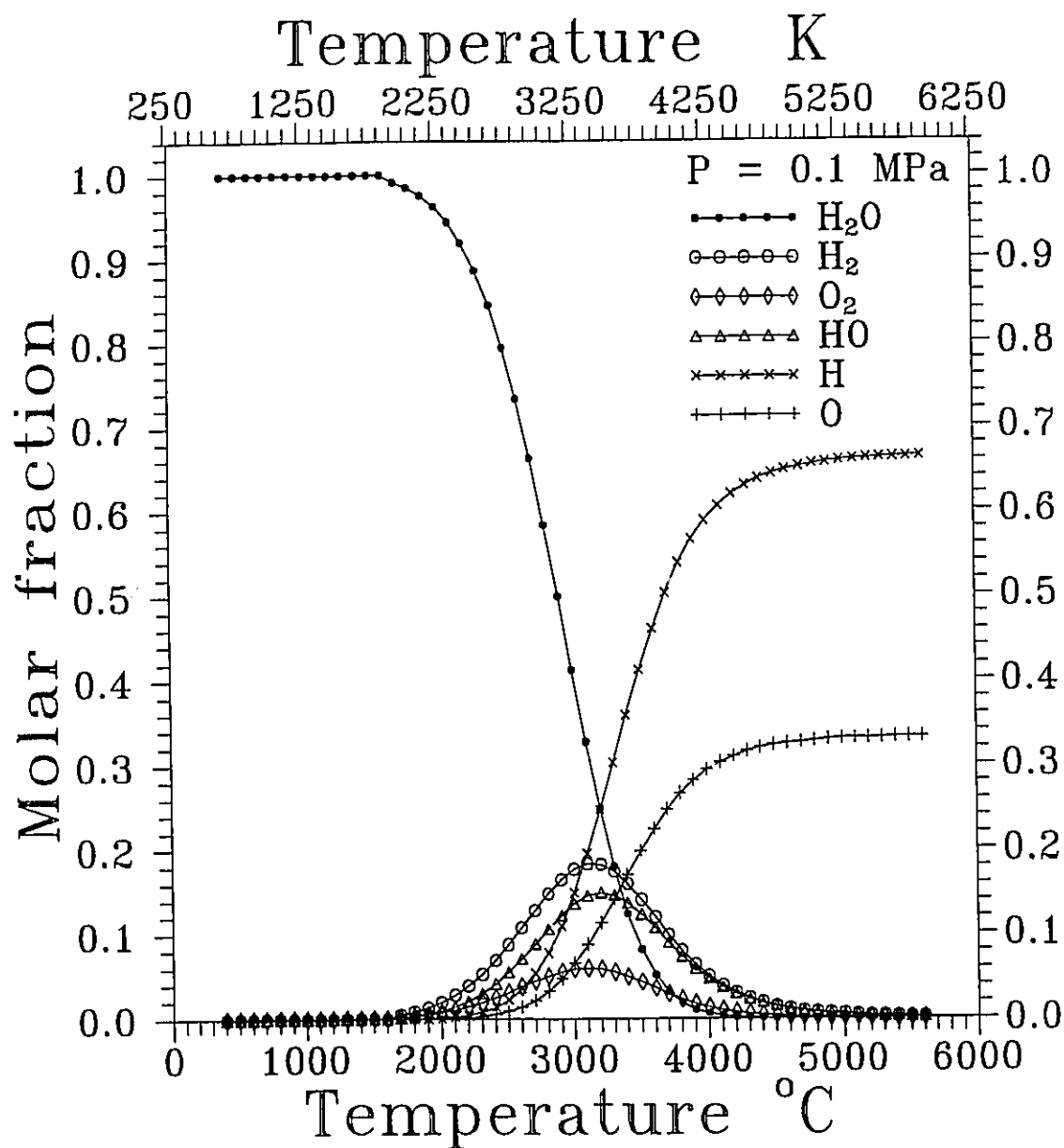


Figure 2.1: Molar fraction of dissociated steam as a function of temperature at a constant pressure.

fraction of dissociated steam as a function of temperature at a constant pressure of 0.1MPa. At atmospheric pressure (0.1MPa) and a temperature of 4200°C, the dissociation of the water molecule is practically complete.

The effect of pressure on the molar fraction of steam of the six component mixture is shown in Figure 2.2. At a constant temperature, the molar fraction of steam in the mixture is greater at higher pressures. Therefore, at higher pressures steam is less dissociated than at lower pressures. In other words, the same molar fraction of the steam occurs at higher pressures for a given higher temperature.

It is important to notice that the molar fraction of steam begins to change at any pressure and at temperatures higher than 1500°C, therefore, dissociation should be considered at any pressure and at temperatures higher than 1500°C.

The molar fractions of the mixture components at the temperature range of interest are shown in Figure 2.3. The following sections present available sources of information for the properties of the five subsidiary components (H_2 , O_2 , HO , H and O) as pure gases.

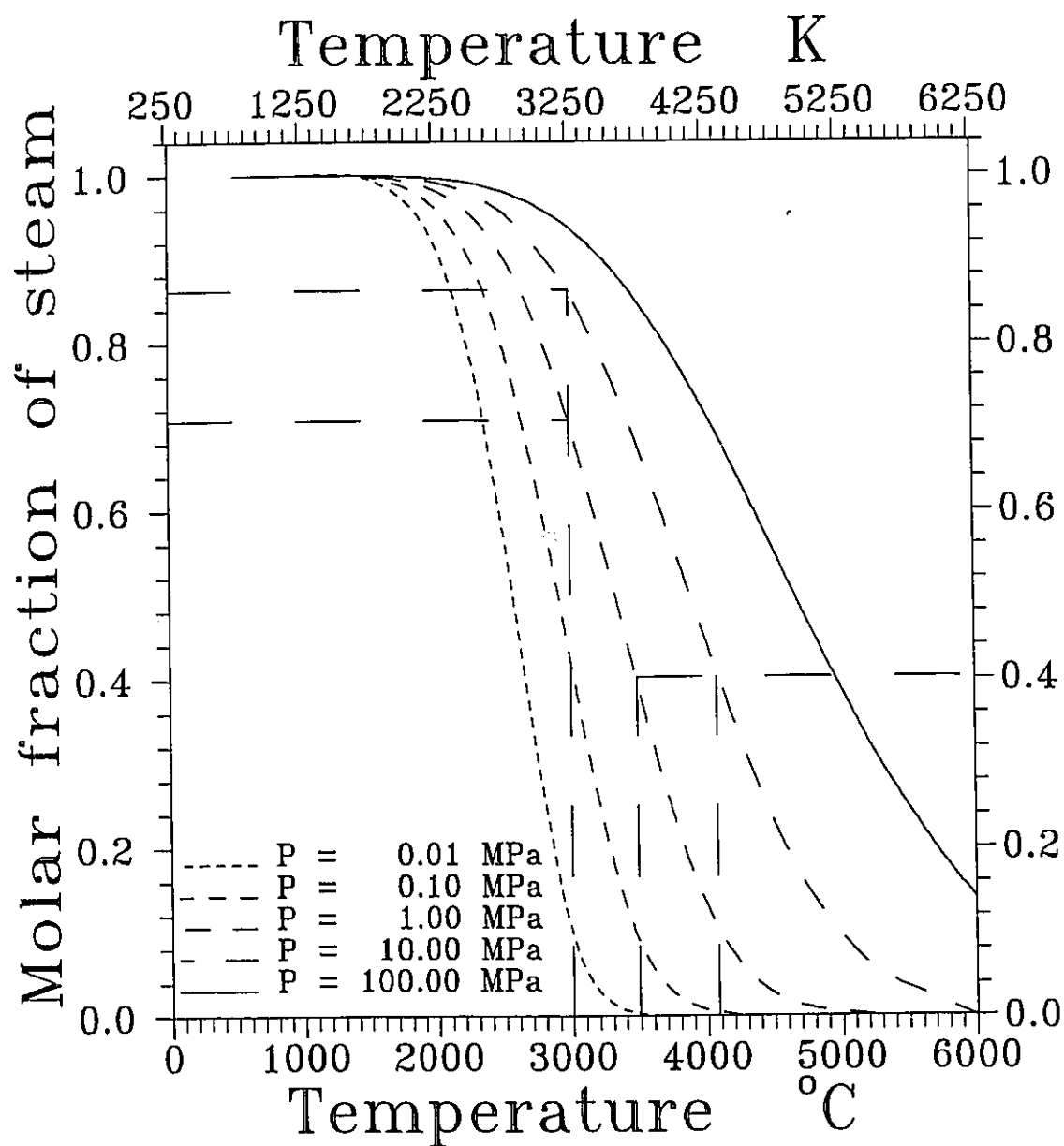


Figure 2.2: Effect of pressure on the molar fraction of steam.

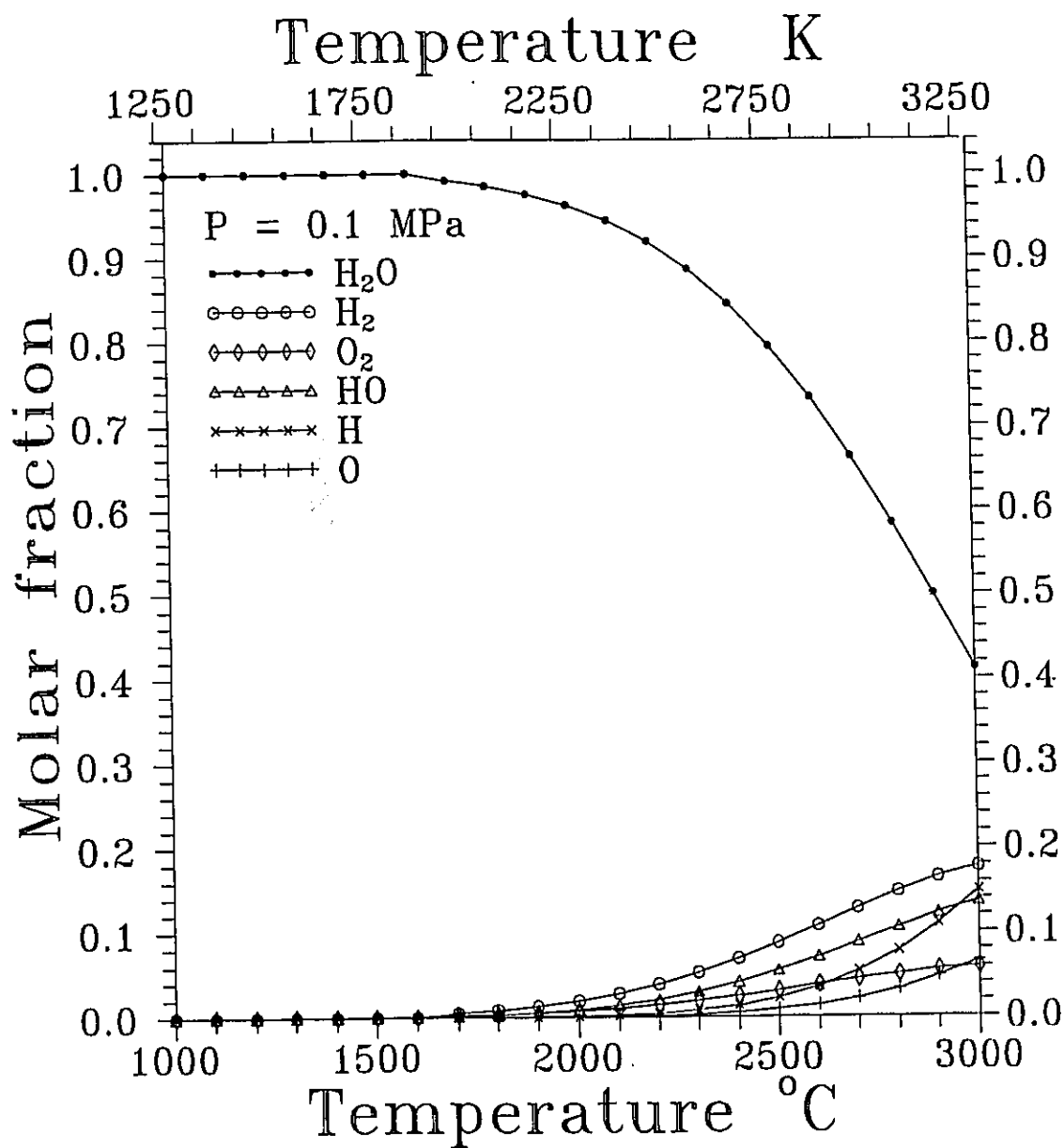


Figure 2.3: The molar fractions of the mixture components at temperatures up to 3000°C and pressure 0.1MPa.

2.3 Pure Gases

2.3.1 Hydrogen (H_2 and H)

The thermodynamic and transport properties of molecular hydrogen (H_2) are presented in the monograph by McCarty (1975). This monograph is a summary of all available data accumulated at the Cryogenic Data Centre of the National Bureau of Standards in Boulder, Colorado, U.S.A.. The properties are tabulated in the temperature range from the triple point to 3000K and the pressure range from 0.01 to 100MPa. The tables contain all properties of interest (e.g., v , ρ , S , H , c_v , c_p , μ , k , Pr , etc.).

In the works by Baronnet et al. (1985), Debbagh-Nour (1984) and Svehla (1964) the properties have been calculated for a hydrogen-oxygen system. Baronnet et al. (1985) presents the results in a graphical form, for example Figures 2.4 and 2.5 are reproduced from his paper; the thermal conductivity and dynamic viscosity of the hydrogen-oxygen system are given for temperatures from 1000 to 15000K and a pressure of 1bar. The curves labelled "1" represent properties of the pure molecular hydrogen (H_2). The physical properties of dissociating hydrogen at equilibrium ($H_2 \rightleftharpoons 2H$), are also reported in a graphical form by Petukhov and Popov (1964). Figure 2.6, reproduced from Petukhov and Popov's paper, presents the degree of hydrogen dissociation - α , density - ρ , heat capacity - c_p , viscosity - μ , thermal conductivity - k and Prandtl number - Pr as a function of temperature (from 2000 to 5000K) at constant pressures (1, 10 and 100atm).

The thermodynamic properties of hydrogen in the temperature range from 300K to 20000K are reported by Kubin et al. (1964). Figure 2.7 illustrates the temperature variation of hydrogen molar fractions at several pressures. At temperatures higher than 2000K, molecular hydrogen (H_2) dissociates to atomic hydrogen (H) which ionizes further to hydrogen ion (H^+). The atomic hydrogen is not a naturally occurring species; it is very reactive and its properties can be predicted by the molecular theory of gases.

A recent survey of the most accurate approximation methods for the estimation of physical properties of gases, including molecular and atomic hydrogen, is presented in the book by Reid et al. (1987).

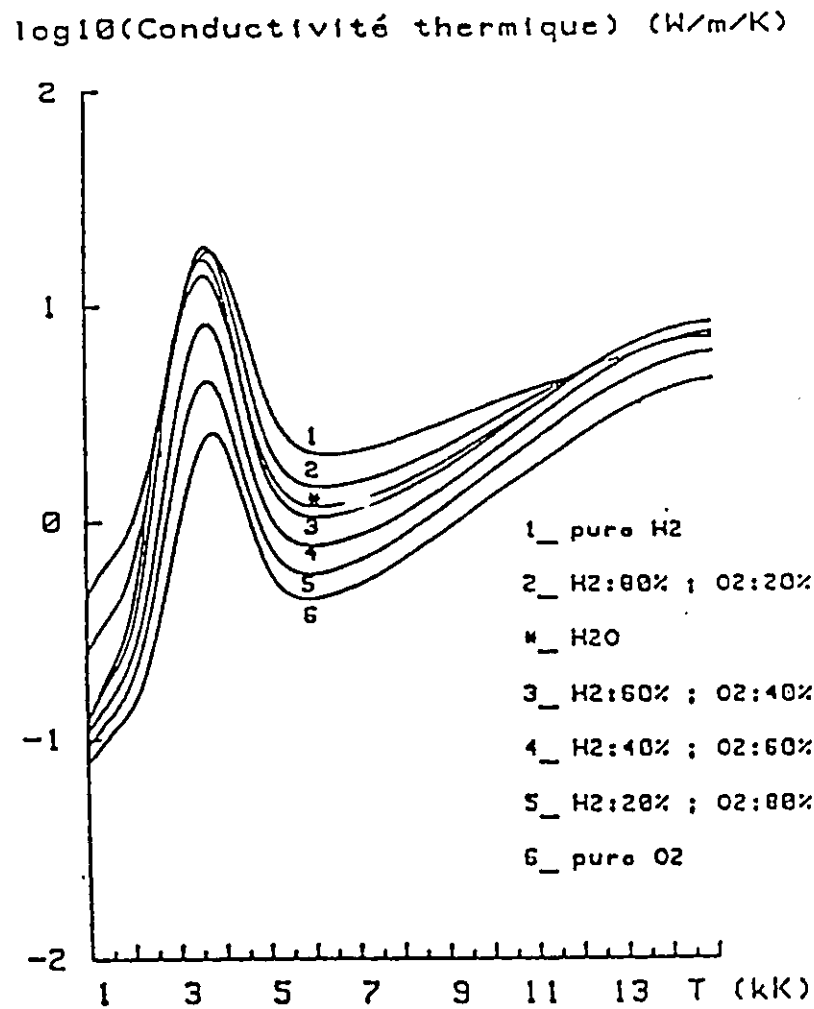


Figure 2.4: Thermal conductivity of the hydrogen-oxygen system for temperatures from 1000 to 15000K and pressure 1 bar by Baronnet et al. (1985).

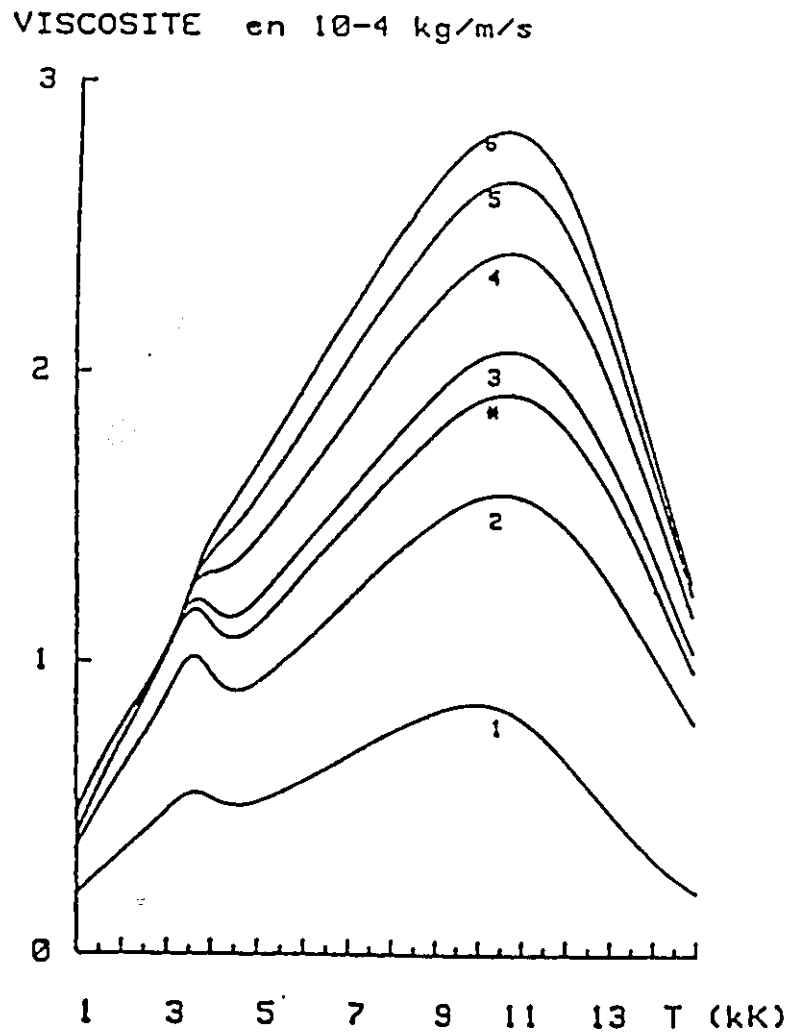


Figure 2.5: Dynamic viscosity of the hydrogen-oxygen system for temperatures from 1000 to 15000K and pressure 1 bar by Baronnet et al. (1985).

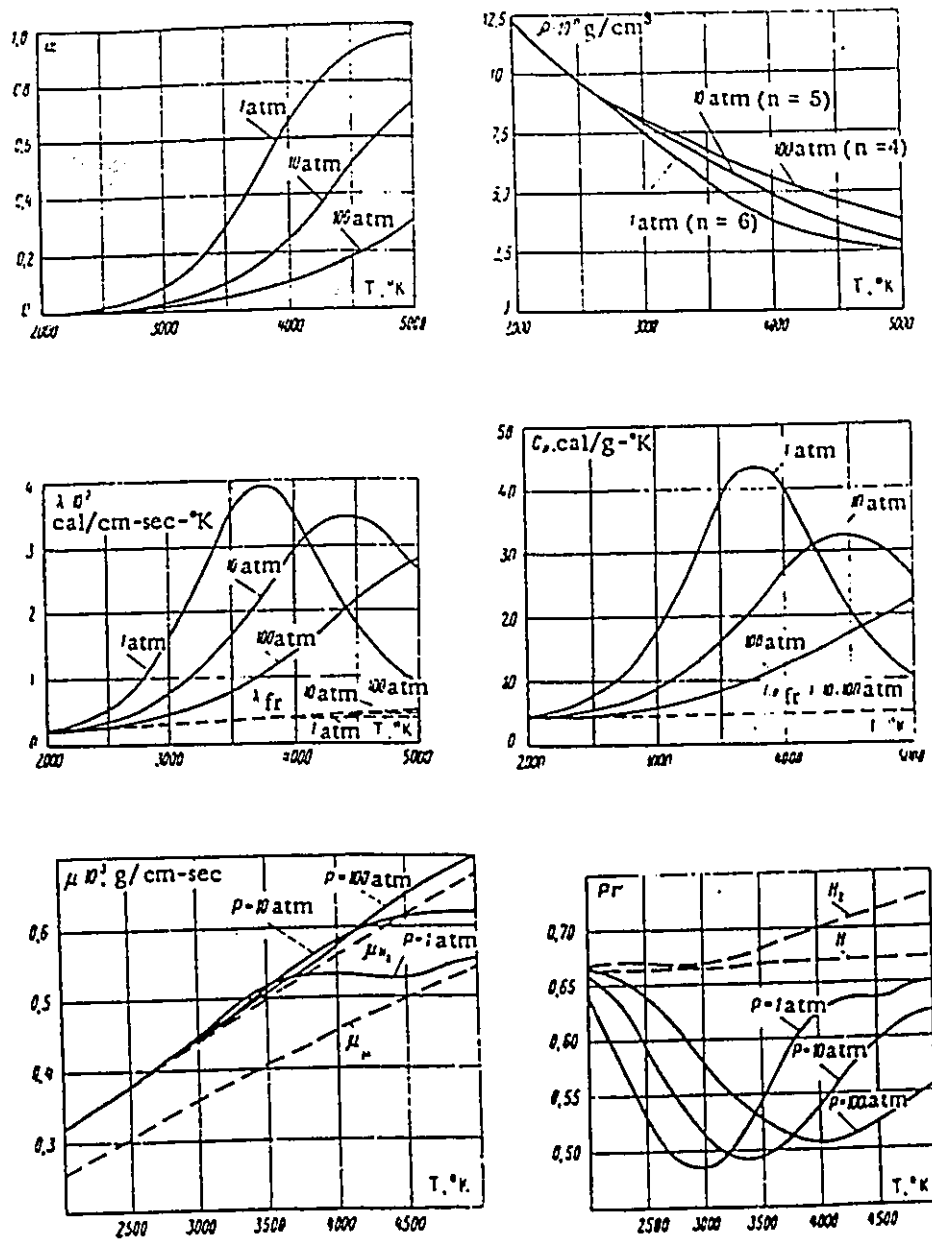


Figure 2.6: The degree of hydrogen dissociation - α , density - ρ , thermal conductivity - λ , heat capacity - C_p , viscosity - μ and Prandtl number - Pr as a function of temperature and constant pressures by Petukhov and Popov 1964

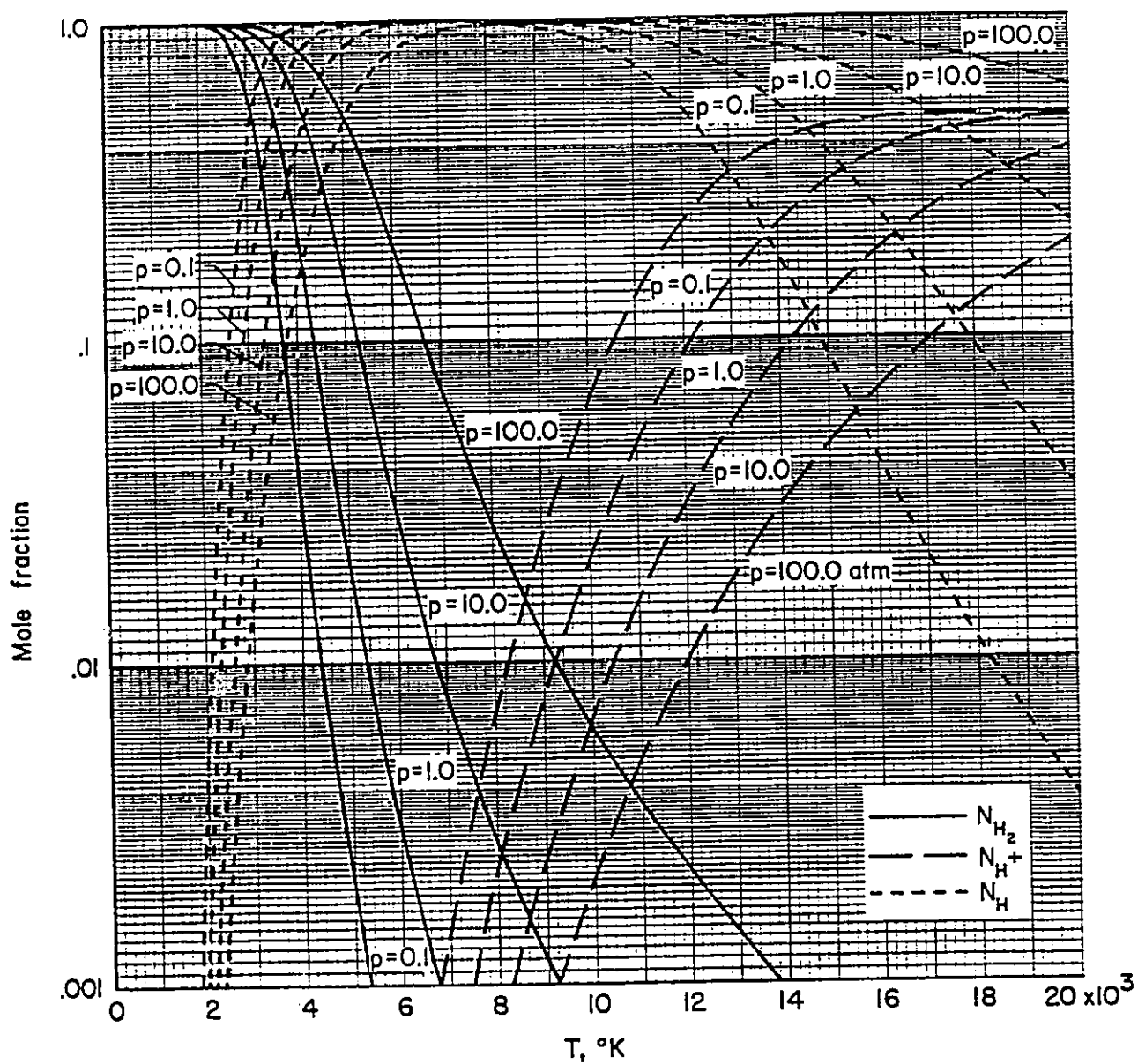


Figure 2.7: Variation of the hydrogen mole fractions with temperature at several pressures by Kubin et al. (1964).

2.3.2 Oxygen (O_2 and O)

The thermodynamic properties of molecular oxygen have been reported recently by Sychev et al. (1987). This is an English translation of the monograph published in 1981 by the National Standard Reference Data Service of the USSR for the properties (density, enthalpy, entropy and heat capacity) tabulated at the temperature range from 55 to 1500K and pressure range from 0.1 to 100.0MPa. The specific volume, enthalpy and entropy are also given at a temperature range from 1250 to 6000K and a pressure range from 0.01 to 100MPa. Transport properties (viscosity and thermal conductivity) of dissociated oxygen for the temperature range from 1600 to 6000K and pressure range from 0.0001 to 10MPa are tabulated by Vargaftik (1985).

As mentioned in section 2.3.1, Baronnet et al. (1985), Debbagh-Nour (1984) and Svehla (1964) have reported properties of the hydrogen-oxygen combination in general, and properties of the pure oxygen as a special case. Baronnet et al. (1985) presented his results in graphical form only. Thus, Figures 2.4 and 2.5 are reproduced from Baronnet et al. (1985), and the curves labelled "6" represent properties for the pure molecular oxygen (O_2). The transport properties for oxygen were evaluated from the work by Debbagh-Nour (1984), and were quoted by Baronnet et al. (1985).

Thermodynamic and transport properties of atomic oxygen are not available since atomic oxygen is so reactive. However, the properties can be predicted by the molecular theory of gases. As referred to in section 2.3.1, the approximation methods of Reid et al. (1987) for the estimation of the physical properties of gases can be used to predict the properties of pure molecular and atomic oxygen.

2.3.3 Hydroxyl (HO)

The water molecule can be divided into two electrically charged particles - a positively charged hydrogen ion (H^+) and a negatively charged hydroxide ion (OH^-). The pair of electrons that forms the bond between the hydrogen and oxygen atoms remains with the hydroxide ion. However, water can also be divided in another way - to produce electrically neutral fragments. The pair of electrons involved in bonding uncouples and one electron remains with the hydrogen atom ($H^\cdot$), while the other stays with the hydroxyl fragment to form a radical ($HO^\cdot$). The dot represents a single unpaired electron, which characterizes all radicals. Radicals are extremely reactive; they can react with each other to form new molecules, or they can react with a stable molecule to form a new molecule and a new radical. The new radical would then be free to react with another molecule, so continuing a chain reaction.

The thermodynamic properties of hydroxyl as an ideal gas are reported in the JANAF⁵ tables by Chase et al. (1985). The transport properties can be predicted using estimation methods presented by Reid et al. (1987) if the parameters of an intermolecular potential function for hydroxyl are known.

⁵ JANAF is an acronym for Joint Army Navy Air Force.

Chapter 3

Prediction of High Temperature Properties for Steam: Literature Review

3.1 General

The properties of steam are temperature and pressure dependant. In general, the temperature range can be split into two regions: a moderate temperature region, $T \leq 1000\text{K}$ and a high temperature region, $T > 1000\text{K}$.

The high temperature region can be further divided into three subregions. The first subregion is up to 2000K where no dissociation has yet occurred or it is negligible, the second subregion is from 2000 to 5000K where dissociation is dominant, and finally the third subregion, from 5000 to $20,000\text{K}$, where ionization occurs. Depending on the temperature range, steam may be evaluated, accordingly, as non-dissociated, dissociated or ionized. This work is concerned only with the first two subregions ($<5000\text{K}$).

The pressure range can be divided into subcritical pressures (below the critical point 22.064MPa , 373.99°C) and super-critical pressures (above 22.064MPa). This work considers temperatures much higher than the critical temperature (373.99°C), where water can only be in the super-heated vapour phase regardless the pressure being subcritical or super-critical.

3.2 Thermal Dissociation of Steam at High Temperature

The statistical thermodynamics of the working fluid, steam, in the high temperature region explain the mechanism of dissociation. Molecules of steam are in random continuous movement. Each molecule possesses a different velocity and from the theory of statistics, the velocity is distributed between the molecules according to a distribution function. Most of the molecules

have a velocity close to the mean velocity, while a small number of molecules have a velocity much higher or much lower than the mean velocity, as presented in Figure 1.1. Two colliding molecules require an activation energy to break their structure and form a new chemical structure. If the kinetic energy of the colliding molecules is less than the required activation energy, then these molecules will bounce and continue random movement. Water molecules with kinetic energy higher than the activation energy at collision have sufficient energy to break the chemical bonds between the hydrogen and oxygen atoms in a water molecule. After such a collision, instead of two water molecules, three new molecules ($(1 \text{ H}_2 + 2 \text{ HO})$ or $(2 \text{ H}_2 + 1 \text{ O}_2)$) are formed. The kinetic energy of these newly formed molecules is lower than the kinetic energy of the molecules which originally collided. A portion of the kinetic energy was consumed to break the chemical bonds. This process is called the thermal dissociation of molecules into components. Since the energy required to break the chemical bonds was extracted from thermal energy, this is thermal dissociation. Thus, the working fluid, which initially was one chemically neutral component, becomes a mixture of a few components.

Thermal dissociation occurs at all temperatures. At temperatures up to 1700°C (1973.15K - in the first subregion), the number of molecules with kinetic energy greater than the activation energy is very small. Consequently, the molar fraction of all other components is negligible. As the temperature increases, the mean kinetic energy of the molecules increases. The number of molecules with kinetic energy higher than the activation energy increases, hence the molar fraction of steam in the mixture decreases. Conversely, the molar fractions of the components of dissociation (y_i) are increasing. Figure 2.3 (see page 12) displays the molar fractions of mixture components at pressure 0.1MPa within the temperature range from 1000 to 3000°C . At temperatures higher than 1700°C the degree of dissociation (α) increases substantially, and can no longer be disregarded.

With a further temperature increase, all working fluids dissociate first into the atomic state of its components, and eventually, the gas becomes ionized. Figure 2.7, taken from Kubin et al. (1964), shows the mole fractions of hydrogen components during dissociation and ionization. A similar process occurs with steam; Figure 3.1, reprinted from the paper by Baronnet et al. (1985), presents the mole fraction of components formed from steam by dissociation and ionization.

Obviously the thermodynamic and transport properties of steam in the high temperature region must be calculated as properties of a mixture of chemically reacting (dissociating) gases. According to professor Straub (1987 b), it is not clear whether the dissociated mixture has to be treated as a mixture of ideal gases or real gases. A method for calculating the properties of

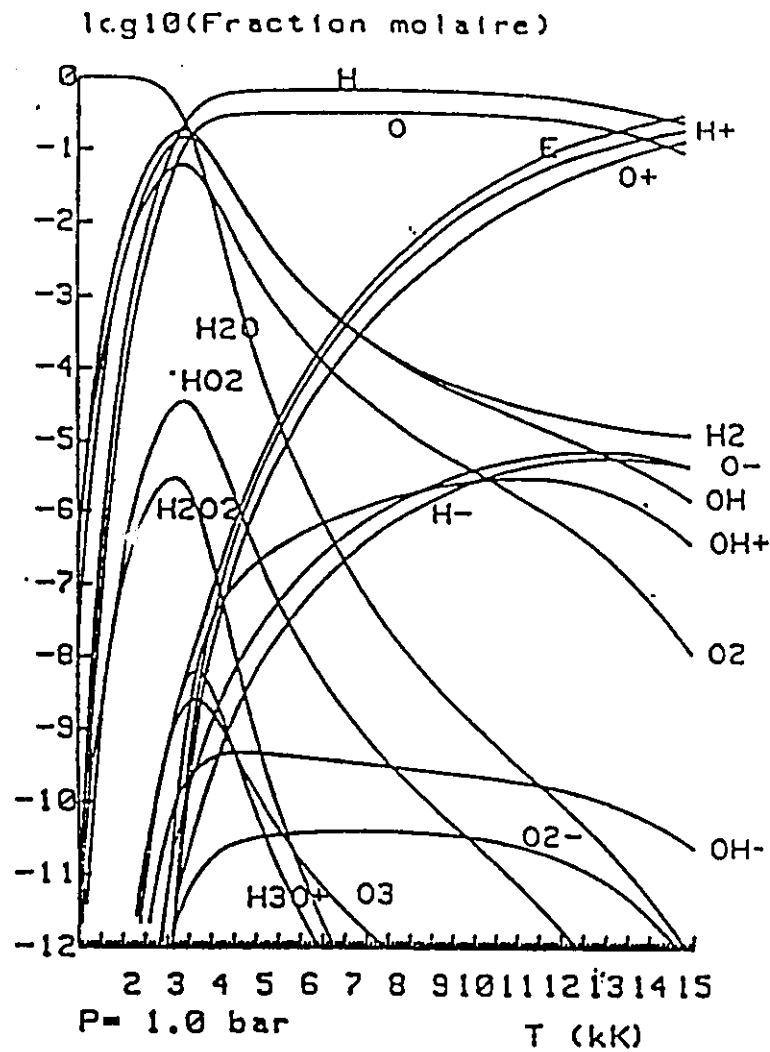


Figure 3.1: The molar fractions of steam as a function of temperature from Baronnet et al. (1985).

chemically reacting gases has been derived from the kinetic theory of gases by Hirschfelder et al. (1967). The method is not straightforward and requires many empirical constants. Intermolecular potential energy functions and collision integrals are required for all possible combinations of collisions between the molecules or atoms. Table 3.1 lists all combinations of interactions between the molecules and atoms in the mixture of the six components: 21 collisions are possible. Clearly, an intermolecular potential energy function is required to calculate the collision integral (21 in total) for each interaction at a specified temperature.

Table 3.1 **Combination of interactions between products of steam dissociation**

Components	H ₂ O	H ₂	O ₂	HO	H	O
H ₂ O	H ₂ O-H ₂ O					
H ₂	H ₂ O-H ₂	H ₂ -H ₂				
O ₂	H ₂ O-O ₂	H ₂ -O ₂	O ₂ -O ₂			
HO	H ₂ O-HO	H ₂ -HO	O ₂ -HO	HO-HO		
H	H ₂ O-H	H ₂ -H	O ₂ -H	HO-H	H-H	
O	H ₂ O-O	H ₂ -O	O ₂ -O	HO-O	H-O	O-O

3.3 Previous Studies

3.3.1 Literature review

This section considers temperatures higher than the limit of standard steam tables, 800°C (1073.15K). Assumptions for prediction of the thermodynamic properties of steam at a high temperature may be as indicated in the block diagram presented in Figure 3.2. First, steam may be postulated as either a non-dissociated or a dissociated gas. For a non-dissociated gas, it may be treated as an ideal or real gas. While, for a dissociated gas, it may be treated as an ideal mixture of ideal gases (ideal gas mixture) or an ideal mixture of real gases (ideal solution), a non-ideal (real) mixture of ideal gases (non-ideal gas mixture) or a non-ideal (real) mixture of real gases (non-ideal solution). Ideal mixture is mixture which does not show enthalpy change due to mixing. The total thermodynamic properties of an ideal mixture is the sum (in the mixing proportion) of the total properties of the individual species; however, transport properties for ideal mixture are not. Difference between the ideal-gas mixture and ideal solution is that properties of the individual species are either only properties of ideal gases or only properties of the components (gas, liquid or solid) of an solution. Time dependence (the rate of chemical reactions) is another consideration for evaluating the properties of gas mixture. Two extreme cases are usually analyzes: an infinite time of chemical reaction - frozen state, or an instantaneous time of chemical reaction - equilibrium state. Depending on the postulate, several studies may be found. The thermodynamic and transport properties of dissociated steam as non-ideal gas mixture are not found in the literature. Tables 3.2 and 3.3 summarize the list of up-to-date source references and give the properties of steam and the units for the properties published in these references. Earlier works by Rubakov (1963), Burhorn and Wienecke (1961) and Dorsey (1940) are not listed because they were preliminary attempts to study this complicated subject. On the other hand, works by Patel et al. (1990) and Artym et al. (1974) deal with properties of steam in the temperature region ($>5000\text{K}$) which is beyond the scope of this work.

The thermodynamic properties of non-dissociated steam as an ideal gas were tabulated in the JANAF tables by Chase et al. (1985, page 1274), Gurvich et al. (1978, Table 20, V.I, No.2, pp.45-46), Barin and Knacke (1973, page 383), and, for a real gas, by Chase et al. (1985, pp.1275-1279), Haar et al. (1984) and Vukalovitch (1967). The thermodynamic properties of dissociated steam as a ideal gas mixture were reported by Straub (1987 a), Ihara (1977),

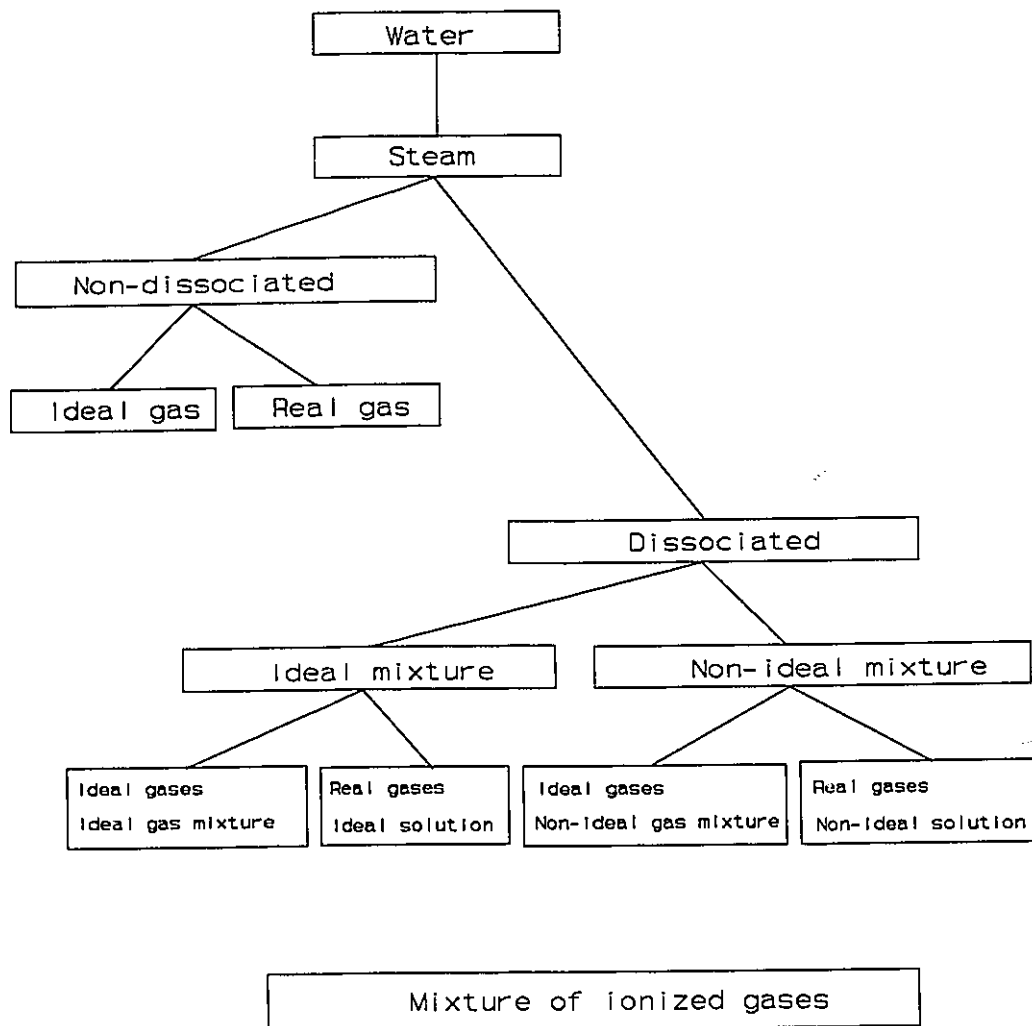


Figure 3.2: Classification of the hypothesis for prediction properties of steam at high temperatures.

Svehla (1964)-(frozen⁶ and equilibrium⁷ state), Rybakov (1963) and Burnhorn and Wienecke (1961), and, for an ideal solution, by Artym et al. (1974) and Kmoníček (1967 a). Finally, Vargaftik (1983)⁸, Geftter et al. (1976) and Kesselman and Blank (1968 i) presented a non-ideal solution. Transport properties predictions for non-dissociated steam were published by Haar et al. (1984), Matsunaga et al. (1983), Kesselman (1966 c) and (1968 e) and Svehla (1962), and, for dissociated steam by Baronnet et al. (1985), Vargaftik (1983), Kesselman and Blank (1968 i) and Svehla (1964, frozen and equilibrium state).

Most of the aforementioned analyses are based on the following assumptions and theory:

- (i) Ideal gas or real gas assumption for the prediction of properties for individual pure components;
- (ii) Non-dissociated or dissociated gas assumption, the latter including the effect of chemical reactions;
- (iii) Ideal mixing or real mixing process, the latter includes the interactions of all components;
- (iv) Frozen or equilibrium state if rate of chemical reactions are considered;
and
- (v) Statistical thermodynamics.

⁶ The state of a multi-component gas mixture which requires infinite time for chemical reactions between components to occur (mixture of chemically non-reacting gases).

⁷ The state of a system in which a balance between the concentrations of reactants and products of the chemical reactions (under specific conditions) is reached.

⁸ The data presented in tables by Vargaftik (1983) are actually results obtained by Kesselman and Blank (1968 i), Kesselman et al. (1968 h) and Kesselman et al. (1968 f).

Table 3.2 Literature review for properties of non-dissociated steam

Author		Clase et al. (1985)	Haar et al. (1984)	Matsunaga et al. (1983)	Gurvich et al. (1978)	Barin et al. (1973)	Kesselman et al.(1968 i)	Vukalovitch (1967)	Svehla (1962)
Property	Sym								
Absolute pressure	P	0.1MPa	0-30000bar		0.1MPa	1atm		1-1000atm	
Absolute temperature	T	0-6000K	0-2000°C	0-2000K	100-20000K	298-2500K	1000-6000K	550-1000°C	600-5000K
Thermodynamic Properties									
Specific volume	v		m ³ kg ⁻¹					m ³ kg ⁻¹	
Density	ρ		kg m ⁻³						
Entropy	S	J mol ⁻¹ K ⁻¹	kJ kg ⁻¹ K ⁻¹		J mol ⁻¹ K ⁻¹	cal mol ⁻¹ K ⁻¹		kcal kg ⁻¹ K ⁻¹	
Enthalpy	H	kJ mol ⁻¹	kJ kg ⁻¹		kJ mol ⁻¹	kcal mol ⁻¹		kcal kg ⁻¹	
Free enthalpy	g	kJ mol ⁻¹			J mol ⁻¹	kcal mol ⁻¹			
Internal energy	u		kJ kg ⁻¹						
Second virial coefficient	B		m ³ kg ⁻¹	cm ³ mol ⁻¹					
Heat capacity	C _p	J mol ⁻¹ K ⁻¹	kJ kg ⁻¹ K ⁻¹		J mol ⁻¹ K ⁻¹	cal mol ⁻¹ K ⁻¹			
Equilibrium constant	K	log K(T)			log K(T)	β(T)			
Transport Properties									
Self-Diffusion coefficients	D ₁₁			m ² s ⁻¹					
Binary Diffusion coefficients	D ₁₂			m ² s ⁻¹					
Viscosity	η		μPa s	μPa s			N s m ⁻²		g cm ⁻¹ s ⁻¹
Thermal conductivity	k		mW m ⁻¹ K ⁻¹	mW m ⁻¹ K ⁻¹			kW m ⁻¹ K ⁻¹		cal cm ⁻¹ s ⁻¹ K ⁻¹
Prandtl number	Pr		nondim.						

Note: The symbol nondim. designates dimensionless properties, and no entry indicates that the property was not studied.

Table 3.3 Literature review for properties of dissociated steam

Author		Straub (1987)	Baronnet et al.(1985)	Ihara (1977)	Geffier et al.(1976)	Artym et al.(1974)	Kusončák (1967 a)	Kesselman et al.(1968 a)	Sveřbá (1964)
Property	Sym								
Absolute pressure	P	0,01 100,bar	0,1 10,bar	0,05 100atm	0,01 1000,bar	1, 1000,bar	0,001 100,bar	0,1 1000,bar	0,001 1000,atm
Absolute temperature	T	2000 6000K	1000 15000K	1000 6000K	1000 10000K	5000 20000K	1000 5000K	1000 6000K	600 5000K
Molar mass	M	g mol ⁻¹						kg mol ⁻¹	g mol ⁻¹
Number of mole	n	mol		mol					
Equilibrium constant	K _P	nondim.		nondim.					
Mole fractions	y _i	mol, mol ⁻¹		mol, mol ⁻¹	mol, mol ⁻¹			mol, mol ⁻¹	mol, mol ⁻¹
Thermodynamic Properties									
Specific volume	v					cm ³ g ⁻¹		m ³ kg ⁻¹	
Density	ρ				kg m ⁻³				
Entropy	S			cal mol ⁻¹ K ⁻¹	kJ kg ⁻¹ K ⁻¹	J g ⁻¹ K ⁻¹	kJ g ⁻¹ K ⁻¹	kJ kg ⁻¹ K ⁻¹	cal g ⁻¹ K ⁻¹
Enthalpy	H	cal mol ⁻¹		kcal mol ⁻¹	kJ kg ⁻¹	J kg ⁻¹	kJ g ⁻¹	kJ kg ⁻¹	cal g ⁻¹
Free enthalpy	g						kJ g ⁻¹		
Heat capacity	C _v	cal mol ⁻¹ K ⁻¹			kJ kg ⁻¹ K ⁻¹				
Heat capacity	C _p	cal mol ⁻¹ K ⁻¹		cal mol ⁻¹ K ⁻¹	kJ kg ⁻¹ K ⁻¹	J g ⁻¹ K ⁻¹		kJ kg ⁻¹ K ⁻¹	cal g ⁻¹ K ⁻¹
Specific heat ratio	γ				nondim.			nondim.	
Adiabatic speed of sound	a				m s ⁻¹	m s ⁻¹		m s ⁻¹	
Compressibility factor	Z				nondim.		nondim.		
Transport Properties									
Viscosity	μ		kg m ⁻¹ s ⁻¹					N s m ⁻²	poises
Thermal conductivity	k		W m ⁻¹ K ⁻¹					W m ⁻¹ K ⁻¹	cal cm ⁻¹ K ⁻¹
Prandtl number	Pr								nondim.
Lewis number	Le _m								nondim.
Electrical conductivity			K V ⁻¹ m ⁻¹						

Note: The symbol nondim. designates dimensionless properties, and no entry indicates that the property was not studied.

3.3.2 Thermodynamic properties

Thermodynamic properties may be predicted using the premise that a gas may be an ideal or real gas. The ideal (perfect) gas by definition is a gas where the molecular volume is negligible compared to the total volume of the gas, and where the forces of attraction between molecules approach zero. The equation of an ideal gas (a combination of Boyle's and Charles' law) may be written as

$$\frac{\tilde{M} P v}{\tilde{R} T} = Z = 1 \quad (3.1)$$

where Z is the compressibility factor.

For real (non-ideal) gases the compressibility factor is not equal to one, due to the finite dimensions of molecules and their intermolecular forces. Therefore, the compressibility factor for real gases is defined with the so called virial expansion (virial equation) as

$$Z = 1 + \frac{B}{v} + \frac{C}{v^2} + \frac{D}{v^3} + \dots \quad (3.2)$$

where, $B(T), C(T), D(T)$ etc. are the second, third, fourth, etc. virial⁹ coefficients and v is specific volume.

For a given gas, the virial coefficients are functions of the temperature (the mean of molecular kinetic energy) only. The virial coefficients have a physical meaning such that the second virial coefficient $B(T)$ indicates encounters of three particles, the third $C(T)$ of four particles, and so forth. The virial coefficients may be calculated from the theoretical consideration of the collision process for an equilibrium gas; they represent deviations from an ideal gas in terms of the intermolecular forces.

3.3.2.1 Non-dissociated steam as an ideal gas

The thermodynamic properties for an ideal gas according to statistical mechanics can be calculated when the total partition function (Q) of a fluid is known as follows:

⁹ "Virial" derived from latin vis (plural vires) meaning "force" (forces acting on the molecules).

$$\tilde{S} = \tilde{R} \ln Q + \tilde{R} T \left[\frac{\partial(\ln Q)}{\partial T} \right]_p + k_s \quad (3.3)$$

$$\tilde{H} = \Delta \tilde{H}_f^0 + \tilde{R} T^2 \left[\frac{\partial(\ln Q)}{\partial T} \right]_p + k_H \quad (3.4)$$

$$\tilde{C}_p = \left(\frac{\partial \tilde{H}}{\partial T} \right)_p \quad (3.5)$$

Constants k_s and k_H are used to assign the values of entropy and enthalpy readings at the reference point¹⁰. Using the expression for the partition function as a product of factors representing the translational, vibrational, rotational, coupling, etc., contributions to the total partition function, Friedman and Haar (1954) computed thermodynamic properties for water. Once more accurate data for the energy of rotational-vibrational states was available, the partition functions were corrected for temperatures less than 2000K by Woolley (1979). The computational results are presented in the JANAF tables by Chase et al. (1985).

3.3.2.2 Non-dissociated steam as a real gas

Properties for water as a real fluid were developed by Haar et al. (1979) and presented by Chase et al. (1985) and Haar et al. (1984). A three-term expression for the Helmholtz function was introduced as

$$A(\rho, T) = A_{ideal\ gas}(T) + A_{base}(\rho, T) + A_{residual}(\rho, T) \quad (3.6)$$

The first right-hand term represents the function in ideal gas state presented by Woolley (1979) while the second term is derived by rearranging terms in the Ursell-Mayer virial expansion and integrating with respect to density. Finally, the third term represents the residual part of the Helmholtz function. The forty coefficients for the residual function are generated by a correlation with experimental data for pressure, density, temperature, compressibility and entropy. Since A is an analytic function, all properties can be obtained by the evaluation of appropriate derivatives using the laws of thermodynamics.

3.3.2.3 Dissociated steam as an ideal mixture of ideal gases (ideal gas mixture)

Dissociated steam considered as an ideal mixture of ideal gases indicates that the

¹⁰ The reference point in this work is the zero value of entropy and enthalpy of water at triple point ($t=0.01^\circ\text{C}$, $P=611.73\text{Pa}$).

composition of the mixture is determined using conditions for chemical equilibrium and that the properties of pure components (species) are evaluated using ideal gas thermodynamic functions. Thus, the process of predicting thermodynamic properties can be divided in two parts: first, determination of the mixture composition, and second, generating the values of the properties by applying mixing rules employing certain values for the properties of pure components.

For dissociated steam in the temperature range up to 5000K, the following six components can be taken into consideration: H_2O , H_2 , O_2 , HO , H and O . To determine the composition (molar fraction of components y_i) of the mixture, two different approaches may be utilized: minimization of Gibbs free energy for components, Svehla (1964), or using the expression for the equilibrium constant, Straub (1987 a), Ihara (1977) and Rybakov (1963). For the second approach, a system of six algebraic equations must be solved. Four equations are obtained from the expressions for equilibrium constants for arbitrarily chosen chemical reactions; the other two equations are the law of partial pressure and an equation expressing the fact that the total number of hydrogen atoms is always twice that of oxygen. Most authors use numerical values for equilibrium constants, but Ihara (1977) used the relationship of the partition functions for the standard state at unit pressure.

Once the composition of the gas mixture is found, the thermodynamic properties are computed as

$$\tilde{M}_m = \sum_{i=1}^n y_i \tilde{M}_i \quad (3.7)$$

$$v_m = \frac{\tilde{R} T}{\tilde{M}_m P} \quad (3.8)$$

$$S_m = \frac{1}{\tilde{M}_m} \left(\sum_{i=1}^n y_i \tilde{S}_i - \tilde{R} \sum_{i=1}^n y_i \ln y_i \right) + k_s \quad (3.9)$$

$$\tilde{H}_m = \frac{1}{\tilde{M}_m} \left(\sum_{i=1}^n y_i \tilde{H}_i \right) + k_H$$

$$Cp_m = \left[\frac{\partial \left(\sum_{i=1}^n y_i \bar{H}_i \right)}{\partial T} \right]_{p=const.} \quad (3.11)$$

The last equation, after performing the derivation, may be written as

$$Cp_{m,eff,eq} = \left[y_i \sum_{i=1}^N \left(\frac{\partial H_i}{\partial T} \right) + \sum_{i=1}^N \left(\frac{\partial y_i}{\partial T} \right) H_i \right]_p = Cp_{fr} + Cp_r \quad (3.12)$$

The first term of Equation (3.12) is the frozen heat capacity (non-reacting gas mixture) and the second term is the reaction heat capacity (the effects of composition change with temperature due to chemical reactions in the gas mixture). Svehla (1964) presented Cp_{fr} (frozen) and $Cp_{m,eff,eq}$ (effective at equilibrium).

3.3.2.4 Dissociated steam as an ideal mixture of real gases (ideal solution)

If the components of a dissociated mixture are considered as real gases, then the equation of state would include virial expansion and the properties of pure components involving virial coefficients. Equations (3.8) to (3.10), modified by Kmoníček (1967 a), employ a second virial coefficient (B), and have the following form:

$$v_m = \left(\frac{\bar{R} T}{\bar{M}_m P} \right) \left[1 + \left(\sum_{i=1}^n y_i B_i \right) \frac{P}{\bar{R} T} \right] \quad (3.13)$$

$$S_m = \frac{1}{\bar{M}_m} \left[\sum_{i=1}^n y_i \bar{S}_i - \bar{R} \sum_{i=1}^n y_i \ln y_i - \bar{R} \ln \left(\frac{P}{P_o} \right) - P \sum_{i=1}^n y_i \left(\frac{dB_i}{dT} \right) \right] - 3.519 \quad (3.14)$$

$$H_m = \frac{1}{\bar{M}_m} \left\{ \sum_{i=1}^n y_i \bar{H}_i + P \sum_{i=1}^n y_i \left[B_i - T \left(\frac{dB_i}{dT} \right) \right] \right\} + 15\,955 \quad (3.15)$$

All terms from the Equations (3.8) to (3.10) for an ideal gas mixture are included in the Equations (3.13) to (3.15) for an ideal solution, additional terms are contributions due to the real behaviour of gases.

In the temperature range from 5000 to 20,000K, the mixture of gases consists mainly of atoms of hydrogen and oxygen. Artym et al. (1974) calculated the thermodynamic properties by applying exact methods of statistical mechanics and also employing second virial coefficients.

Baronnet et al. (1985) reported that thermal properties have been calculated, considering the gas as a mixture of nine components (the six mentioned above and a free electron (e), and ions (H⁺ and O⁺)), using partition functions and the method of Gibbs free energy minimization for composition. However, the results of the calculation are not published in numerical form other than as graphs.

3.3.2.5 Dissociated steam as a real mixture of real gases (non-ideal solution)

Vargaftik (1983) presented tables of properties, referring to Kesselman and Blank (1968 i) and Kesselman et al. (1968 h) as a source of these data. Kesselman assumed that all interactions between components in the mixture may be described using the Lennard-Jones potential function. This potential function has two constants, ϵ/k_B and σ , characteristic for each gas. However, in a reference from (1964), Kesselman developed a method to determine the temperature-dependent parameters $\epsilon(T)/k_B$ and $\sigma(T)$ for this potential. These parameters are determined from the second virial coefficient $B(T)$ using experimental data for the compressibility factor Z . Once these parameters are known, the second $B(T)$ and third $C(T)$ virial coefficients can be calculated theoretically as described by Hirschfelder et al. (1967). The principle that a gas mixture is a non-ideal solution was introduced by using the equilibrium constant (K_p) as a ratio of the equilibrium constant of the ideal gas mixture (K_{po}) and the constant (K_q) obtained from activities of the components in the reaction

$$K_p = \frac{K_{po}}{K_q} \quad (3.16)$$

$$\ln K_q = \sum_{i=1}^n (a_i \ln q_i) \quad (3.17)$$

where a_i are the stoichiometric numbers for the components in the reaction. The chemical activity of the components using virial coefficients is

$$\ln q_i = \left[B_i + \left(C_i - B_i^2 \right) \frac{P}{R T} \right] \frac{P}{R T} \quad (3.18)$$

Geftter et al. (1976) presented foundations of the cluster expansion theory and the methods

for calculating composition, and the thermodynamic properties for the mixture of real chemically-reacting gases. Applying these methods, thermodynamic properties of dissociated steam were evaluated in his paper.

3.3.3 Transport properties of steam

3.3.3.1 Non-dissociated steam as an ideal gas

From the definition of an ideal gas, the intermolecular forces approach zero, thus, an ideal gas cannot have transport properties.

3.3.3.2 Non-dissociated steam as a real gas

Transport properties were evaluated by Haar et al. (1984) who used Equation (3.6) to calculate density at a given pressure and temperature, and IAPS Release on Dynamic Viscosity of Water Substance (from 1975, revised 1983) and IAPS Release on Thermal Conductivity of Water Substance (from 1977, revised 1983). Conversely, Matsunaga and Nagashima (1983), Kesselman (1966 c) and Svehla (1962) used the Chapman-Enskog viscosity equation:

$$\mu = 26.69 \frac{\sqrt{\bar{M}_m T}}{\sigma^2 \Omega_v} \quad (3.19)$$

$$\Omega_v = f(T^*) \quad (3.20)$$

$$T^* = \frac{T}{\frac{\epsilon}{k_B}} \quad (3.21)$$

To determine σ and the collision integral Ω_v , an intermolecular potential function $\phi(r)$ must be defined. Matsunaga and Nagashima (1983) chose the modified Stockmayer potential developed by Monchick and Mason (1961) with parameter $\sigma = 2.595 \text{ \AA}$, $\epsilon/k_B = 470 \text{ K}$ and $w = 1.5$. Collision integrals are tabulated by Monchick and Mason (1961) as a function of reduced temperature T^* . Kesselman (1966 c) calculated viscosity using the temperature-dependent parameters $\epsilon(T)/k_B$ and $\sigma(T)$ for the Lennard-Jones potential. These parameters, developed by Kesselman (1964), are determined from the second virial coefficient using compressibility experimental data. However, Svehla (1962) calculated viscosity using the same potential with the parameters from the viscosity data by Bonilla et al. (1956). Bonilla's experimental data are systematically lower due to the incorrect reference viscosity data for nitrogen used for calibrating

the apparatus, as reported by Brokaw (1968).

Using the above parameters thermal conductivity was predicted by employing various methods: Matsunaga and Nagashima (1983) used that of Thoen-Hellemans and Mason (1973), Kesselman (1968 e) used the theory of Mason and Monchick (1962), and Svehla (1962) used the modified Eucken approximation.

3.3.3.3 Dissociated steam as an ideal mixture of real gases (ideal solution)

An ideal mixture is a mixture of gases which has mixture properties dependent only on the properties of the pure gases which comprise the mixture.

Baronnet et al. (1985) calculated viscosity and thermal conductivity by applying the most recently published data for interaction potentials. The Chapman and Enskog method has been used for computing viscosity. Thermal conductivity is calculated as

$$k = k_e + k_h + k_{intern.} + k_{react.} \quad (3.22)$$

The terms represent the contributions due to translation of electrons, translation of all other components, internal energy (vibration-rotation) and chemical reaction. The first two terms are calculated by the Chapman and Enskog method, the third by the Eucken method, and the fourth term by the general theory of Butler and Brokaw (1956) and Brokaw (1960).

3.3.3.4 Dissociated steam as a real mixture of real gases (non-ideal solution)

When the actual value of the property of a mixture and the value it would have as an ideal mixture are not equal, then that mixture is a real mixture.

Although Vargaftik (1983) quoted Kesselman and Blank (1968 i), Kesselman et al. (1968 h) and (1968 f) as the sources for the transport property tables, the numerical values are not the same and the reasons for these changes are not known. It may be assumed that the data were revised due to some calculation errors. Hence, the data for viscosity and thermal conductivity from the paper by Kesselman and Blank (1968 i) were not used in this analysis; but, a description of the method for prediction of the transport properties presented in these papers were used. The viscosity of the gas mixture Kesselman calculated using the formula listed by Hirschfelder et al. (1967), and the viscosity of all components, are calculated in the same manner as was explained for non-dissociated steam using the temperature-dependent parameters $\varepsilon(T)/k_B$ and $\sigma(T)$ for the Lennard-Jones potential.

3.4 Review of Two Sources

3.4.1 R.A. Svehla

The monograph by Svehla (1964) presents the results of calculating the thermodynamic and transport properties of the hydrogen (H) - oxygen (O) system. The hydrogen weight percent varies from 0.0 (pure oxygen) to 100.0 (pure hydrogen). Steam is stoichiometrically only one of the fourteen calculated cases, and has 11.1901 weight percent of hydrogen. The theoretical basis for the above calculations is from Hirschfelder et al. (1967). The calculations were made using a computer program developed at the Lewis Research Center by Zeleznik and Sanford (1962) and Svehla. In the calculations, Svehla did not incorporate one single intermolecular force law, but rather a variety of potentials appropriate to each interaction. For the H₂O-H₂O interaction, the Stockmayer intermolecular potential function by Monchick and Mason (1961) was used:

$$\phi(r) = 4 \epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 - g w \left(\frac{\sigma}{r} \right)^3 \right] \quad (3.23)$$

$$g = 0.5 [2 \cos(R_a) \cos(R_b) - \sin(R_a) \sin(R_b) \cos(C)] \quad (3.24)$$

$$w = \frac{m_a m_b}{2 \epsilon \sigma^3} \quad (3.25)$$

where:

- r - intermolecular separation, [=] nm;
- ϵ - the maximum energy of attraction;
- σ - the value of r for which $\phi(r) = 0$, [=] nm;
- R_a, R_b - the angles of inclination of the dipole axes to the line joining the centers of the molecules;
- C - the azimuthal angle between them;
- m_a, m_b - the dipole moment of molecules a and b (1.85Debye for H₂O);
- k_B - Boltzmann constant.

If in the above Equation (3.25) one of the molecules is non-polar, which means ($m = 0.0$), then the Stockmayer intermolecular potential function Equation (3.23) becomes the Lennard-Jones intermolecular potential function.

To determine constants for the Stockmayer function ($\sigma = 0.271\text{nm}$, $\epsilon/k_B = 506\text{K}$, $m = 1.83\text{debye}$ and $w = 1.2$), the experimental data for steam viscosity by Bonilla et al. (1956) were

used by Svehla (1964). The experimental apparatus by Bonilla et al. (1956) was calibrated with nitrogen, using viscosities from Vasilescu (1945). However, later, more accurate measurements showed that Vasilescu's (1945) data were not correct. Since the Bonilla et al. (1956) experimental data were not correct, the results of viscosity and thermal conductivity predictions by Svehla (1964) are also not correct. Bonilla also measured the viscosity of argon on the same apparatus and in the same temperature range. Brokaw (1968) suggested that the steam viscosity data from Bonilla can be corrected by using Bonilla's viscosity for argon and recent more accurate data for viscosity of argon. Figure 3.3¹¹ illustrates comparisons between the viscosities of steam at high temperatures calculated by Svehla (1964) and experimental results by Latta (1965) and Bonilla et al. (1956). The experimental results of Bonilla et al. (1956) are corrected according to the Brokaw (1968) suggestion using the Dymond and Alder (1969) potential for viscosity of argon. The experimental results by Latta (1965) and corrected results of Bonilla et al. (1956) are higher than the values calculated by Svehla (1964). The experimental results for viscosity have relative deviation from the corrected results in the range from -3.07% to -8.37%, while the root mean square error is -5.48%.

The prediction of thermal conductivity by Svehla (1964) involves the viscosity data for components in the gas mixture. Inaccuracy of the experimental data for steam viscosity reproduce inaccuracy of thermal conductivity predictions. The predictions of thermal conductivity by Svehla (1964) are lower than should be. The estimated inaccuracy of the predictions is in order of -10%.

¹¹ A discussion of the lines representing predictions of viscosity by Aleksandrov et al. (1975) and Vargaftik (1983) is in the next section.

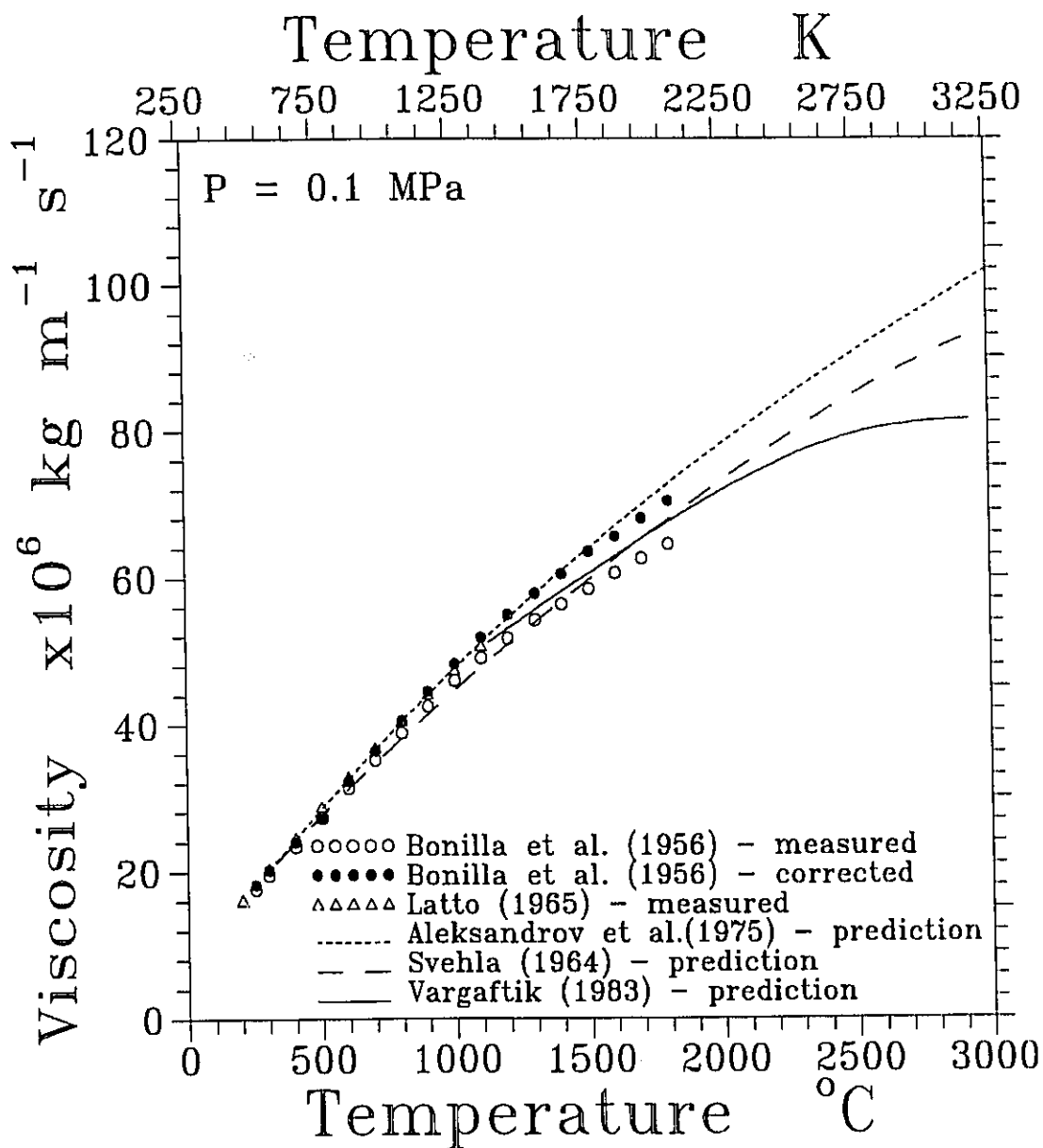


Figure 3.3: Comparison of viscosities of steam at high temperatures calculated by Svehla (1964) with experimental results by Bonilla et al. (1956), correction as proposed by Brokaw (1968) and experimental results of Latto (1965).

3.4.2 P.M. Kesselman et al.

The results of all the calculations of Kesselman et al. are reported in the book by Vargaftik (1983) and the theoretical explanations of the method may be found in a number of papers. The basic concept of the method is described by Kesselman (1964), (1966 c), (1968 f), (1968 g) and (1968 h). The method for the calculation of properties has been presented at the Seventh International Conference on the Properties of Steam (1968 i) and (1968 j). The computed data were calculated by treating steam as a thermally dissociated real gas (a mixture of six components: H₂O, H₂, O₂, HO, H and O). The effect of being a real gas (non-ideal), was taken into consideration by the second and third virial coefficients for the components H₂O, H₂ and O₂.

Virial coefficients are calculated by the method described in Kesselman's papers from (1964) and his doctoral thesis (1966 a). The method employs experimental data obtained from measurements of compressibility for the second $B(T)$ and the third $C(T)$ virial coefficients. The values of second and third virial coefficients are applied to determine the temperature-dependent parameters $\epsilon(T)$ and $\sigma(T)$ for the Lennard-Jones intermolecular interaction potential (single potential to be used for all interactions). The Lennard-Jones potential is

$$\phi(r) = 4 \epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (3.26)$$

where:

$\phi(r)$ is a potential function;

r is the intermolecular separation, [=] nm;

ϵ is the maximum energy of attraction;

σ is the value of r for which $\phi(r) = 0$, [=] nm.

The shape of the potential function is shown in Figure 3.4. The interactions of heterogeneous particles are calculated using the well-known empirical combination rules

$$\left(\frac{\epsilon}{k_B} \right)_{l,i} = \sqrt{\left(\frac{\epsilon}{k_B} \right)_l \left(\frac{\epsilon}{k_B} \right)_i} \quad (3.27)$$

$$\sigma_{l,i} = \frac{\sigma_l + \sigma_i}{2} \quad (3.28)$$

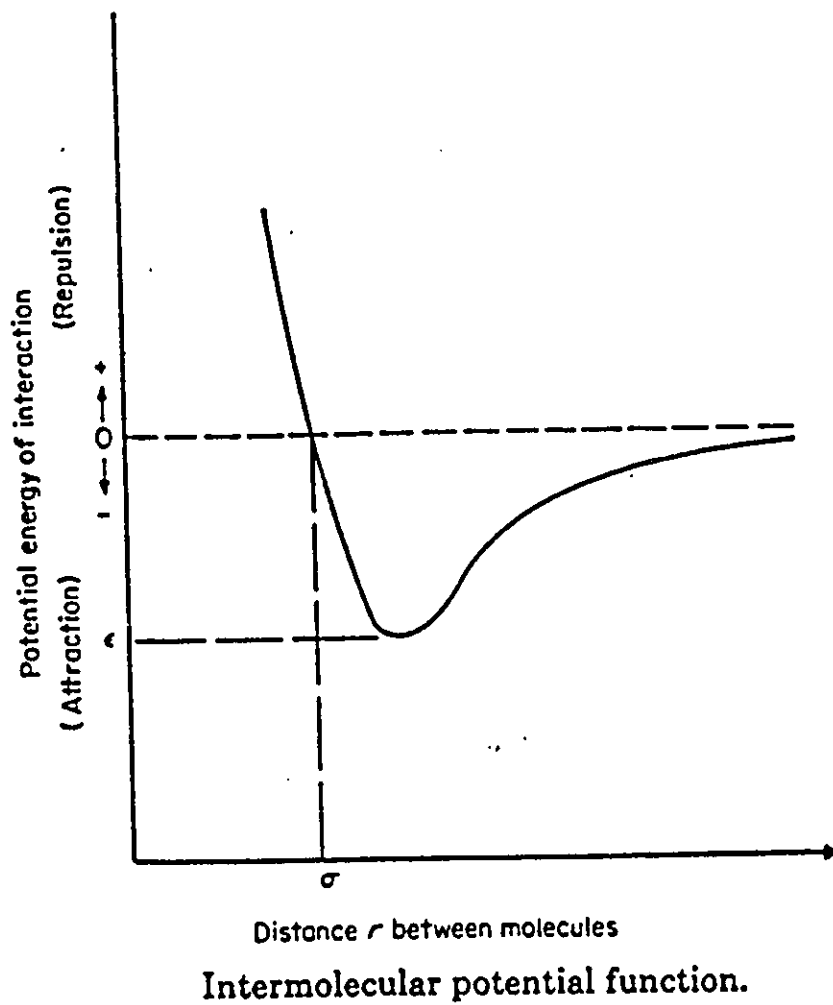


Figure 3.4: The shape of the Lennard-Jones intermolecular potential function.

Theoretical correlations between the virial coefficients and the constants of the Lennard-Jones potential are

$$B(T) = b_o B^*(T^*) \quad (3.29)$$

$$C(T) = b_o^2 C^*(T^*) \quad (3.30)$$

$$b_o = \frac{2}{3} \pi N_A \sigma^3 \quad (3.31)$$

$$T^* = \frac{T}{\frac{\epsilon}{k_B}} \quad (3.32)$$

where:

B^*, C^* are theoretically calculated virial coefficients and are tabulated by Hirschfelder et al. (1967, pp.1114-1117);
 $\pi = 3.14159...$;
 N_A is Avogadro's number;
 k_B is the Boltzmann constant;
 T is absolute temperature in K.

Kesselman's method for determination of the parameters ϵ/k_B and b_o is to bring the experimental data points (the circles) and the theoretical curve (the continuous curve) to graphical coincidence as shown in Figure 3.5. The first step was to plot data points of the second and third virial coefficients as a function of temperature from the compressibility experimental data in the logarithmic coordinates $\log B - \log T$ or $\log C - \log T$, and a theoretical curves in the coordinates $\log B^* - \log T^*$ or $\log C^* - \log T^*$. The second step was to combine theoretical curves (the continuous curve) with experimental data points (the circles) by placing one over the other. The third step was to bring them to graphical coincidence by making a parallel shifts and rotation, mindful of the following:

$$\log[B(T)] = \log(b_o) + \log[B^*(T^*)] \quad (3.33)$$

$$\log[C(T)] = 2 \log(b_o) + \log[C^*(T^*)] \quad (3.34)$$

$$\log(T^*) = \log(T) - \log\left(\frac{\epsilon}{k_B}\right) \quad (3.35)$$

Knowing the angles of rotation and the distance of shifting the coordinate systems, values for

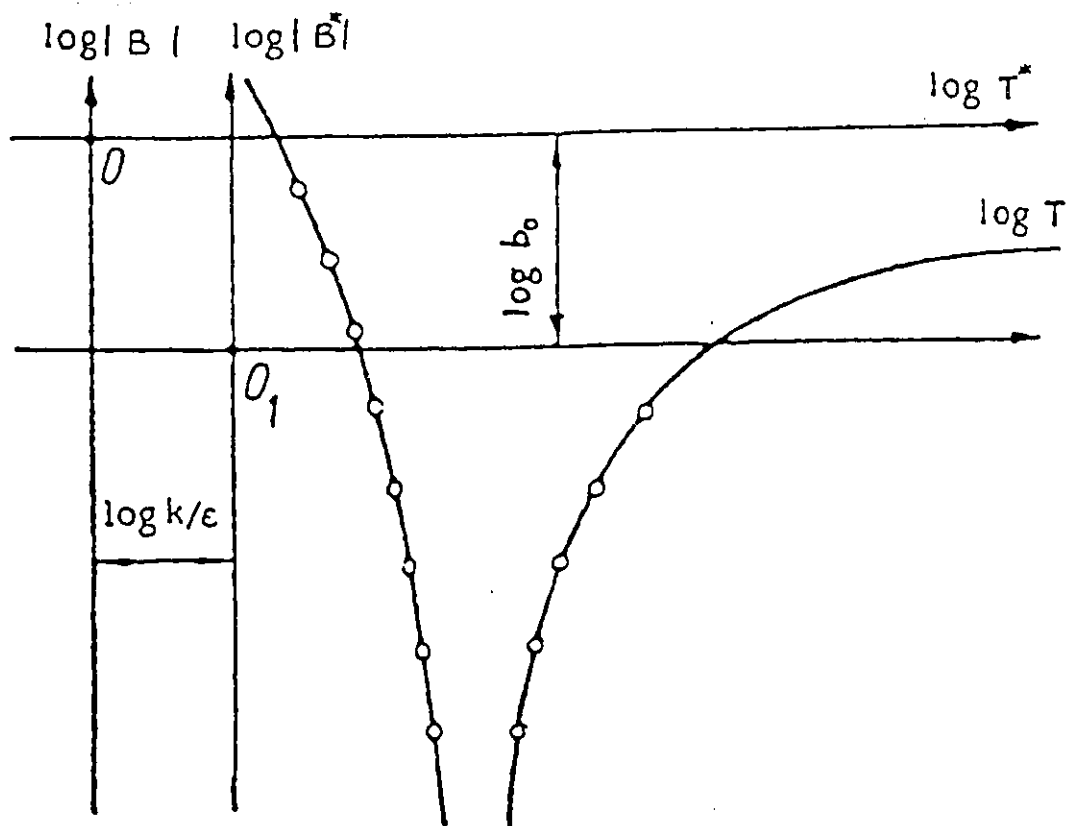


Figure 3.5: Kesselman's method of determination of the parameters ϵ/k_B and b_0 , by bringing the experimental data points (circles) and theoretical curve to graphical coincidence.

$\epsilon(T)$ and $\sigma(T)$ can be calculated for each temperature as following:

$$\log\left(\frac{\epsilon}{k_B}\right) = \log(T) - \log(T^*) \quad (3.36)$$

$$\log(b_o) = \log[B(T)] - \log[B^*(T^*)] \quad (3.37)$$

$$\log(b_o) = \frac{1}{2}\{\log[C(T)] - \log[C^*(T^*)]\} \quad (3.38)$$

$$\sigma = \left(\frac{3}{2\pi N_A} b_o\right)^{\frac{1}{3}} \quad (3.39)$$

Figure 3.6 exhibits a very good agreement of the second virial coefficient $B^*(T^*)$ from theoretical calculation (the continuous curve), and the experimental data points (the symbols) obtained using Lennard-Jones potential with variable $\epsilon(T)$ and $\sigma(T)$ from Kesselman (1964).

The same procedure for determining parameters $\epsilon(T)$ and $\sigma(T)$ were performed for the second and third virial coefficient $C(T)$. For each temperature the values of the parameters obtained from the second virial coefficient or third virial coefficient are observed to be the same. Parameters $\epsilon(T)$ and $\sigma(T)$ for components of steam dissociation are given in Appendix C (Tables C-1 and C-2), from Kesselman and Blank's (1968 i) paper. In Figures 3.7¹² and 3.8, Kesselman and Blank (1968 i) demonstrated that the Lennard-Jones potential parameters $\epsilon(T)$ and $\sigma(T)$ for components of steam dissociation are a function of temperature.

¹² Deviations of the $\epsilon/k_B(T)$ values for line three (O₂) and six (O) are so small that the curves visually coincide.

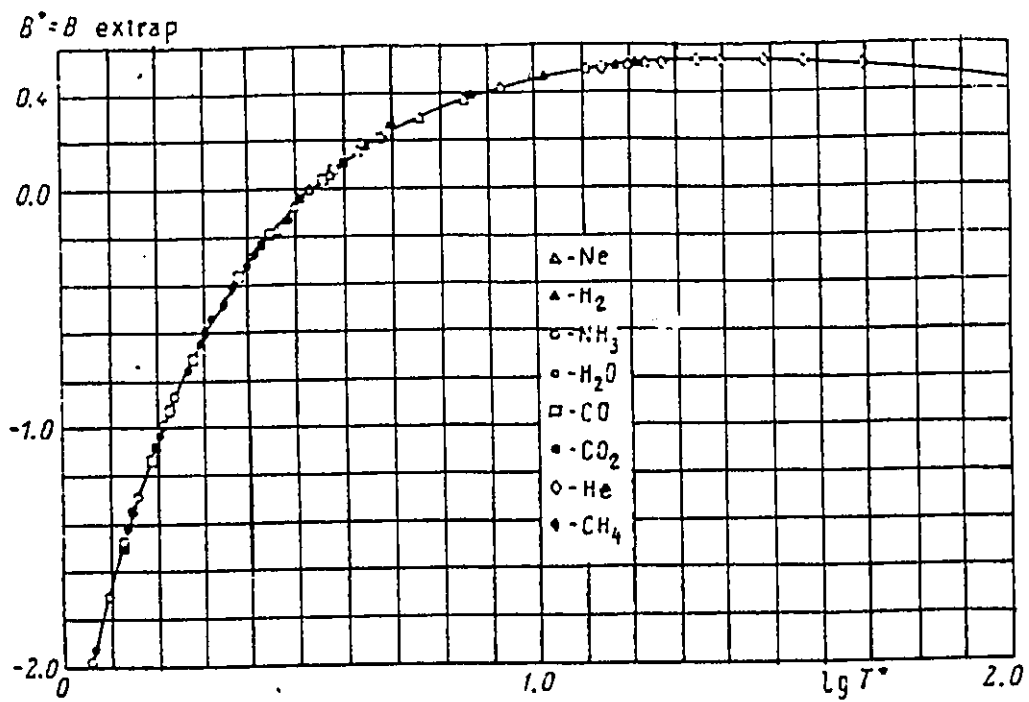


Figure 3.6: The experimental data on the second virial coefficient $B^*(T^*)$ by the Lennard-Jones potential with variable $\epsilon(T)$ and $\sigma(T)$, by Kesselman (1964).

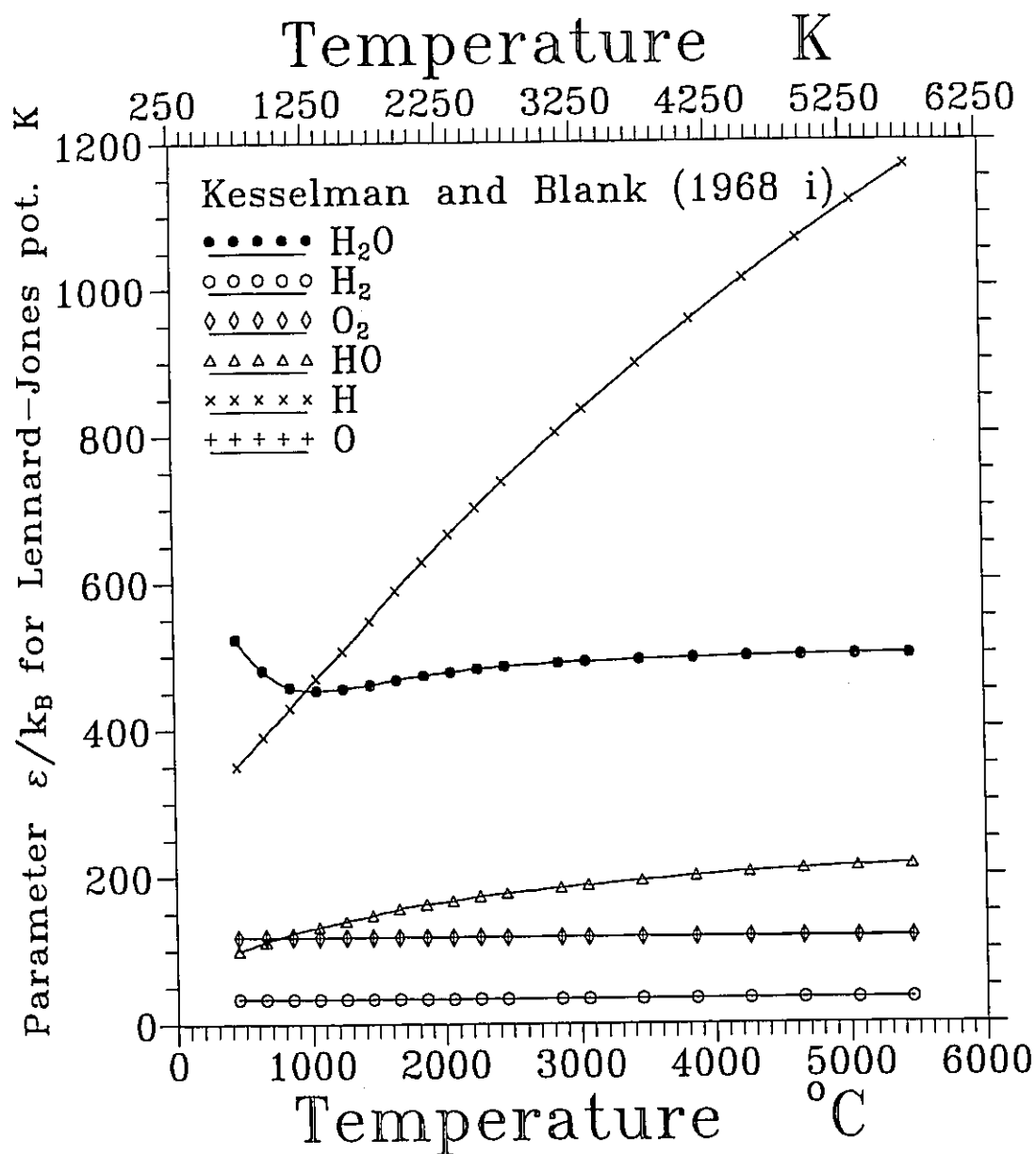


Figure 3.7: The Lennard-Jones potential parameter ϵ/k_B as a function of temperature by Kesselman and Blank (1968 i).

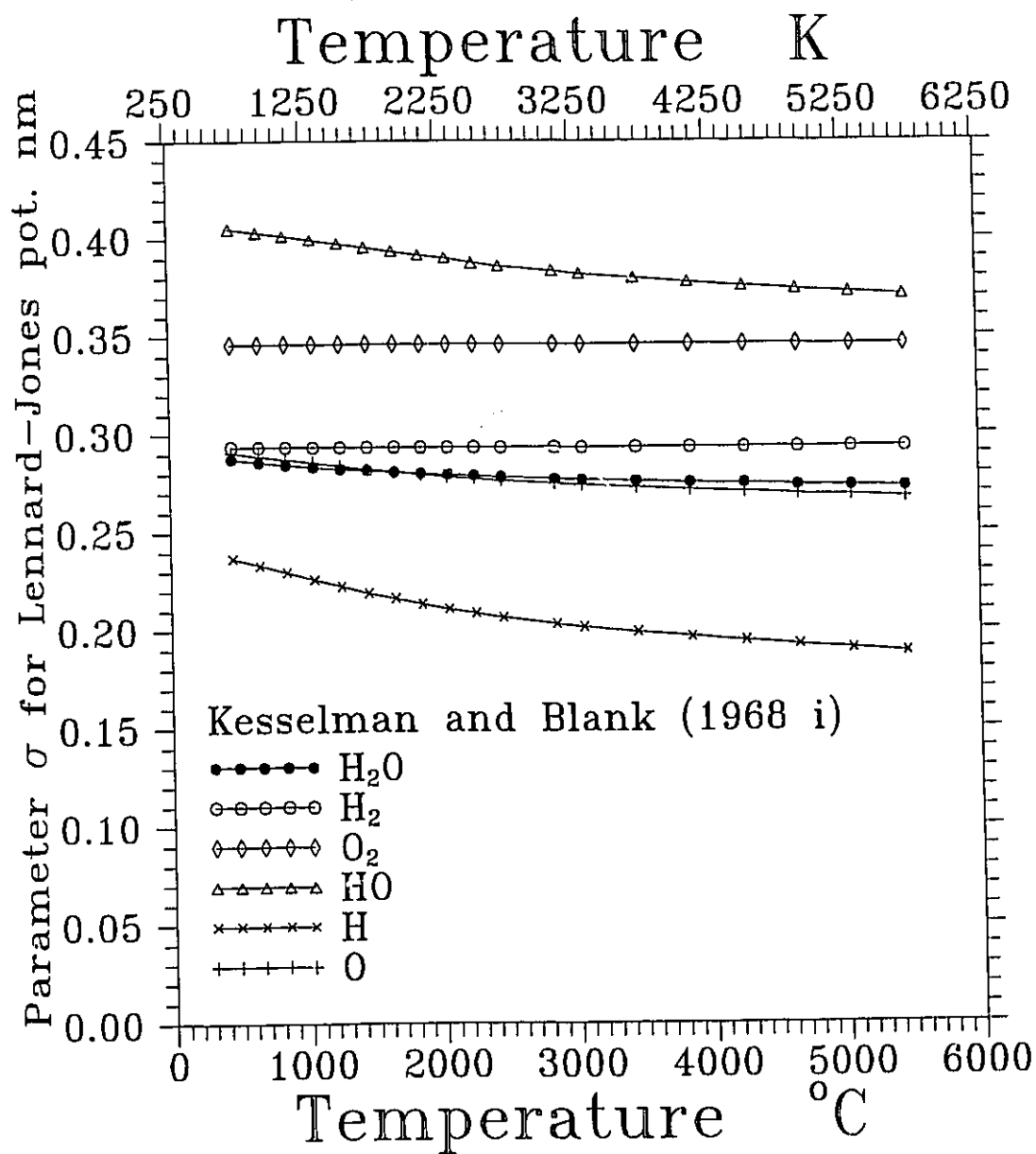


Figure 3.8: The Lennard-Jones potential parameter σ as a function of temperature by Kesselman and Blank (1968 i).

This method was used by Kesselman and his co-workers to determine potential parameters and to calculate properties of steam and other fluids: some hydrocarbons (1965 b), lithium (1968 c), krypton (1968 d), products of organic fuel combustion (1968 e) and dissociated air (1968 f).

For the other three components (HO, H and O) of a dissociated steam mixture, only the second virial coefficient was calculated according to the theoretical method presented in papers (1968 a) and (1968 b).

Once the potential function parameters and virial coefficients are determined for all components, then the properties of pure components may be calculated. The properties of pure components are calculated in terms of the virial equations of state (including third virial coefficients)

$$Z_i = \frac{\bar{M}_i P v_i}{\bar{R} T} = 1 + \frac{B_i}{v_i} + \frac{C_i}{v_i^2} \quad (3.36)$$

According to Kmoníček (1967 a) Equation (3.36) may be re-arranged to take the form of

$$Z_i = 1 + \left(\frac{P}{\bar{R} T} \right) B_i - \left(\frac{P}{\bar{R} T} \right)^2 (B_i^2 - C_i) - 2 \left(\frac{P}{\bar{R} T} \right)^3 B_i C_i \quad (3.37)$$

Kmoníček (1967 a) in his analyses included only two terms from the right-hand side of Equation (3.37). The last term in the above equation is a product of two virial coefficients and so may be neglected. Using such a form of virial equation, Kesselman derived the following:

$$v_i = \left[\frac{\bar{R} T}{P} + B_i + (C_i - B_i^2) \frac{P}{\bar{R} T} \right] \frac{1}{\bar{M}_i} \quad (3.38)$$

$$\bar{S}_i = \bar{S}_{o,i} - \bar{R} \ln \left(\frac{P}{P_o} \right) - \bar{R} \left\{ \frac{1}{v_i} \left[T \left(\frac{dB_i}{dT} \right) \right] + \frac{1}{2 v_i^2} \left[B_i^2 - C_i + T \left(\frac{dC_i}{dT} \right) \right] \right\} \quad (3.39)$$

$$\bar{H}_i = \bar{H}_{o,i} + \bar{R} T \left\{ \frac{1}{v_i} \left[B_i - T \left(\frac{dB_i}{dT} \right) \right] + \frac{1}{2 v_i^2} \left[2 C_i - T \left(\frac{dC_i}{dT} \right) \right] \right\} \quad (3.40)$$

where $\bar{S}_{o,i}$ and $\bar{H}_{o,i}$ are entropy and enthalpy of the ideal gas at the standard state tabulated by Gurvich et al. (1962). To calculate the properties of the mixture, the following mixture equation

is used:

$$v_m = \left(\sum_{i=1}^N y_i v_i + \sum_{i=1}^N \sum_{j=1}^N y_i y_j \Delta v_{ij} \right) \frac{1}{\bar{M}_m} \quad (3.41)$$

$$\Delta v_{ij} = w_{ij} + (B_i - B_j)^2 \frac{P}{R T} \quad (3.42)$$

$$w_{ij} = 2 B_{ij} - B_i - B_j \quad (3.43)$$

where:

- v_m - specific volume of the dissociating mixture;
- v_i - specific volume of pure component calculated in terms of the virial equation;
- y_i, y_j - mole fractions of the components in the mixture;
- B_i, B_j - second virial coefficients of the components in the mixture;
- B_{ij} - second virial coefficient of heterogeneous interactions calculated using the rules of combination of potential parameters;
- P - absolute pressure of the dissociating mixture;
- $\bar{R}$ - universal gas constant;
- T - absolute temperature of the dissociating mixture.

With the use of thermodynamical differential relations, the formulas for thermodynamic properties (entropy, enthalpy, heat capacity, specific heat ratio and velocity of sound) were obtained. Thermodynamic properties of the mixture are

$$S_m = \left(\sum_{i=1}^n y_i \tilde{S}_i - \bar{R} \sum_{i=1}^n y_i \ln y_i + \sum_{i=1}^n \sum_{j=1}^n y_i y_j \Delta S_{ij} \right) \frac{1}{\bar{M}_m} + k_s \quad (3.44)$$

$$\Delta \tilde{S}_{ij} = -P \frac{dw_{ij}}{dT} + \left[(B_i - B_j) \frac{P^2}{2 R T} \right] \left[\left(\frac{B_i}{T} - 2 \frac{dB_i}{dT} \right) - \left(\frac{B_j}{T} - 2 \frac{dB_j}{dT} \right) \right] \quad (3.45)$$

$$H_m = \left(\sum_{i=1}^n y_i \tilde{H}_i + \sum_{i=1}^n \sum_{j=1}^n y_i y_j \Delta \tilde{H}_{ij} \right) \frac{1}{\bar{M}_m} + k_H \quad (3.46)$$

$$\Delta \tilde{H}_{ij} = \left[w_{ij} - T \left(\frac{dw_{ij}}{dT} \right) \right] P + \left[(B_i - B_j) \frac{P^2}{R T} \right] \left\{ \left[B_i - T \left(\frac{dB_i}{dT} \right) \right] - \left[B_j - T \left(\frac{dB_j}{dT} \right) \right] \right\} \quad (3.47)$$

Terms from Equations (3.13) to (3.15) for ideal solution are included in Equations (3.41) to (3.47) for non-ideal solution and supplementary terms are due to interaction of mixture components.

The transport properties (viscosity and thermal conductivity) are calculated according to the rigorous kinetic theory of a multi-component gas mixture. The viscosity is calculated according to Hirschfelder et al. (1954, page 531, equation (8.2-25)). The thermal conductivity is calculated as the sum of the thermal conductivities of a constant composition mixture (according to Hirschfelder et al. (1954) formula) and the conductivities due to chemical reaction, using the formula by Brokaw (1960).

According to the arguments presented by Reed and Gubbins (1973), high temperature transport data are sensitive to the shape of the repulsion portion of the potential function. The potential function which utilizes potential function parameters obtained at a low temperature region is steeper in the repulsion region than the potential function which is in good agreement with experimental data at high temperature region. Figures 3.9 and 3.10 from the book by Reed and Gubbins (1973) support this argument using data for argon. The Dymond and Alder (1969) potential has better agreement with the experiments as shown in Figure 3.9, because that potential does not have a steep gradient in the repulsion region as other potentials have, as shown in Figure 3.10. Kesselman's method employed temperature-dependent potential function parameters $\epsilon(T)$ and $\sigma(T)$. As shown in Figure 3.11, the slope of the repulsion part of the Lennard-Jones potential function for steam (H_2O) decreases at higher temperatures. It can be expected that such an approach will give better results than the potential function with constant parameters based on low temperature measurements (up to $1800^\circ C$). The results of predictions for viscosity using temperature-dependent parameters in the Lennard-Jones potential function applying Kesselman's method by Vargaftik (1983), are presented in Figure 3.3. The solid curve follows the path of the experimental data by Lato (1965) (the triangles) and is parallel to the data by Bonilla et al. (1956) (the circles). The predictions by Svehla (1964) (the broken curve) are based on inaccurate experimental data by Bonilla et al. (1956) (the empty circles), however, if the parameters for predictions by Svehla (1964) were based on the corrected data by Bonilla et al. (1956) (the full circles), the broken line would almost coincide with the predictions using from the equation by Aleksandrov et al. (1975) (the dotted curve).

$$\mu = T_r^{1/2} \left(\sum_{i=0}^3 a_i T_r^{-i} \right)^{-1} [=] \mu Pa s \quad T_r = \frac{T}{T_{cr}} \quad T_{cr} = 647.27K \quad (4.21)$$

$$a_0 = 0.0181583 \quad a_1 = 0.0177624 \quad a_2 = 0.0105287 \quad a_3 = -0.0036744$$

Legend:

The broken line - Lennard-Jones potential ($\epsilon/k_B = 124.9\text{K}$, $\sigma = 0.341\text{nm}$)

The continuous line - Dymond and Alder (1969) numerical tabulated potential ($\epsilon/k_B = 138.2\text{K}$, $\sigma = 0.328\text{nm}$)

The circles - experimental data of Dawe and Smith

The triangles - experimental data of Guevera et al.

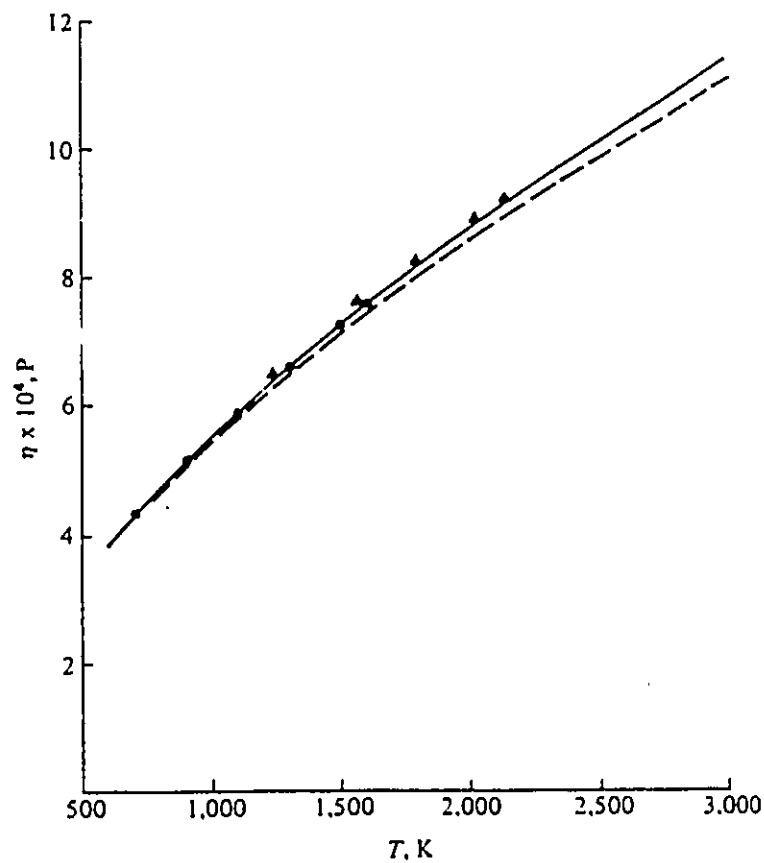


Figure 3.9: Comparison of experimental and theoretical viscosities of argon at high temperature by Reed and Gubbins (1973).

Legend:

- The dotted line - Lennard-Jones potential ($\epsilon/k_B = 124.9\text{K}$, $\sigma = 0.341\text{nm}$)
- The broken line - Kihara potential ($\epsilon/k_B = 139.8\text{K}$, $\sigma = 0.335\text{nm}$, $d/\sigma = 0.1$)
- The continuous line - Dymond and Alder (1969) numerical tabulated potential ($\epsilon/k_B = 138.2\text{K}$, $\sigma = 0.328\text{nm}$)

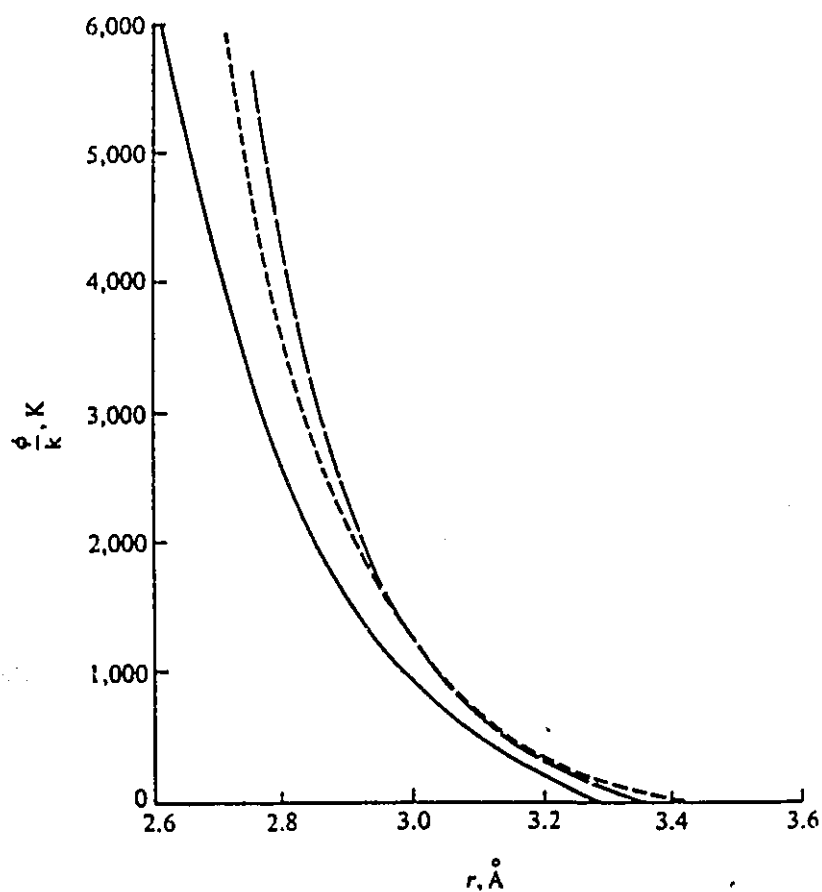


Figure 3.10: Comparison of several potential functions for the repulsion region of argon by Reed and Gubbins (1973).

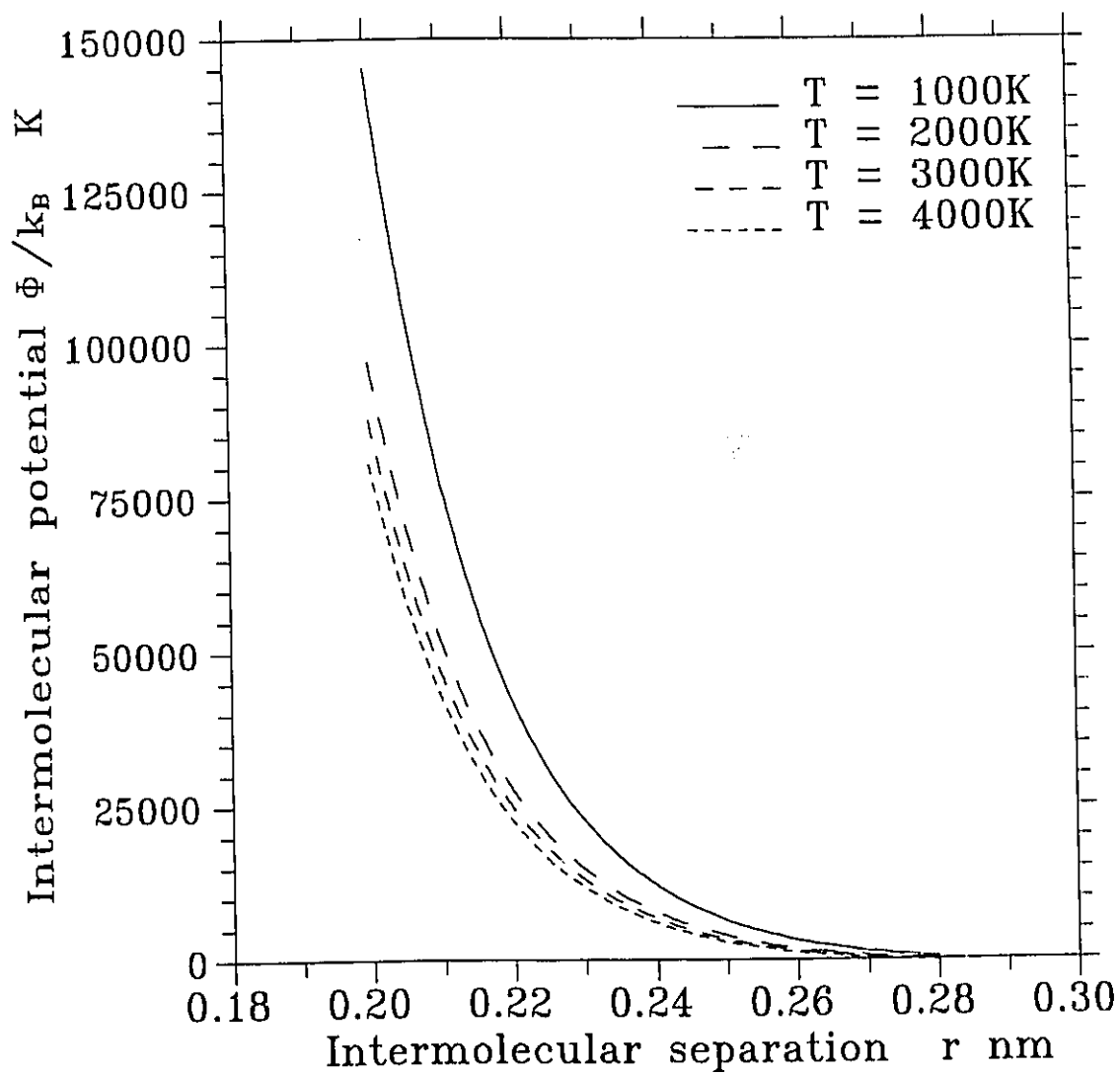


Figure 3.11: Slope of the repulsion portion of the Lennard-Jones potential function for water vapour (H_2O) at high temperatures using data by Kesselman and Blank (1968 i).

The equation by Aleksandrov et al. (1975) is developed from experimental data at low temperatures and according to the authors the extrapolation of this equation is valid for temperatures up to 1500°C. Consequently, predictions by Vargaftik (1983) would be more accurate provided that the predictions by Svehla (1964) were based on the corrected data by Bonilla et al. (1956).

3.5 Comparison of Predictions

All available data sets and equations for high temperature steam properties have been extracted from the literature, converted to the same units (SI¹³), changed to the same reference state¹⁴, and analyzed. A comparison of predictions of high-temperature steam properties was published by Vasić et al. (1992); the manuscript of the paper is presented in Appendix P. Predictions of thermodynamic properties for dissociated steam from all analyzed sources are in reasonable good mutual agreement. Choice of the recommended source, Vargaftik (1983) is based on the large number of data points and widest range of pressure and temperature since predictions are at list equally accurate then from the other sources. However, predictions of transport properties in numerical form are available only from two sources Svehla (1964) and Vargaftik (1983) using the prediction method of Kesselman and Blank (1968 i). There are three arguments which make doubt about accuracy of predictions by Svehla (1964). First, viscosity predictions by Svehla (1964) apply parameters determined using experimental data by Bonilla et al. (1956) which have systematic error. Second, if that error is corrected prediction by Svehla (1964) would almost coincide with the predictions based on non-dissociated steam low temperature measurements by Aleksandrov et al. (1975) but not corrected high temperature measurements by Bonilla et al. (1956). Finally, according to argument in last section it can be expected that predictions of viscosity which use the potential function which have lover slope at the repulsion part at higher temperatures, Kesselman and Blank (1968 i) will give better results than the potential function with constant parameters based on low temperature measurements, Svehla (1964). Transport properties for the dissociated steam presented by Vargaftik (1983) using the prediction method of Kesselman and Blank (1968 i) are more accurate then data by Svehla (1964), hence they were adopted in this study.

¹³ The system of units identified internationally as SI (Le Système international d'unités).

¹⁴ The zero value of entropy and enthalpy of water at triple point ($t = 0.01^{\circ}\text{C}$, $P = 611.73\text{Pa}$).

Chapter 4

Prediction of High Temperature Properties for Steam: Recommended Methods

4.1 General

A number of different properties may be determined for steam; however, the concern of this work is the steam properties required for heat transfer evaluation: thermodynamic properties (molar mass, specific volume, entropy, enthalpy and heat capacity) and transport properties (mass diffusion coefficient, viscosity and thermal conductivity). At high temperatures, steam is dissociated, hence, a gas mixture may be evaluated as ideal or non-ideal. Another consideration for evaluating the properties is the rate of chemical reactions as an infinite time of chemical reaction - frozen state, or an instantaneous time of chemical reaction - equilibrium state. The two methods of predicting the properties of steam recommended here represent two extreme cases: an ideal gas mixture in a frozen state and a non-ideal solution in an equilibrium state. Evaluating properties by the first method does not include the effect of chemical reactions (properties are named frozen properties), and by the second method includes maximal effect of chemical reaction (properties are named effective properties in equilibrium).

The first section will consider the frozen properties of dissociated steam. In the following section the recommended prediction method for mass diffusion (binary and multi-component mixture) coefficients will be presented. Finally, the effective properties of dissociated steam will be presented in the last section. Each section includes a description of the properties evaluated and the pressure and temperature dependence of the properties are demonstrated in a number of figures.

4.2 Frozen Properties of Dissociated Steam: Mixture of Ideal Gases

The properties of a multi-component mixture of chemically neutral ideal gases, or, a mixture of gases with an infinite time required for a chemical reaction, are properties formed by an ideal mixing of gas components, proportional to composition, without residue. The hypothetical mixture of gases in the same composition proportion but without the effect of chemical reaction, or with the rate of chemical reaction so small that they need an infinite time to complete, is called the frozen state. Thus, properties of such a mixture are called "frozen properties". The mixture of gases formed by steam dissociation is not a mixture of chemically neutral gases. However, the frozen properties may be evaluated with the intent to separate the effect of chemical reaction on the properties of the gas mixture.

The method for calculating dissociated steam (water vapour) properties as a mixture of chemical non-reactive gases (frozen) is presented in Appendix B. It includes the method for computation of molar mass, enthalpy, heat capacity and thermal conductivity¹⁵ - properties required for further analyses. A set of computer subroutines was developed for generating dissociated-water-vapour frozen properties. The listing of the subroutines (The Frozen Properties code) for predicting frozen properties of high temperature steam is presented in Appendix G.

Computation of the dissociated steam frozen properties, for a wide range of pressures and temperatures, was performed to test the predictions. The generated results of frozen properties predictions for dissociated steam are presented in Appendix K.

Figures 4.1 to 4.4 present the molar mass, enthalpy, heat capacity and thermal conductivity as a function of temperature for a range of constant pressures. The molar mass changes, as temperature increases, from the value of water ($18.01528 \text{ kg kmol}^{-1}$) to the molar mass ($6.005 \text{ kg kmol}^{-1}$) of the gas mixture (the mixture of atomic hydrogen (H) and atomic oxygen (O) in proportion 2:1). As temperature increases, all other frozen properties - enthalpy, heat capacity and thermal conductivity - undergo a modest change as the effect of chemical reaction is not included.

¹⁵ Prediction of the frozen thermal conductivity employ data generated by Svehla (1964). According to discussion in Chapter 3 predictions of viscosity and thermal conductivity by Svehla (1964) are not accurate. Since, this are the only data available in literature for frozen thermal conductivity, they are adapted in this work.

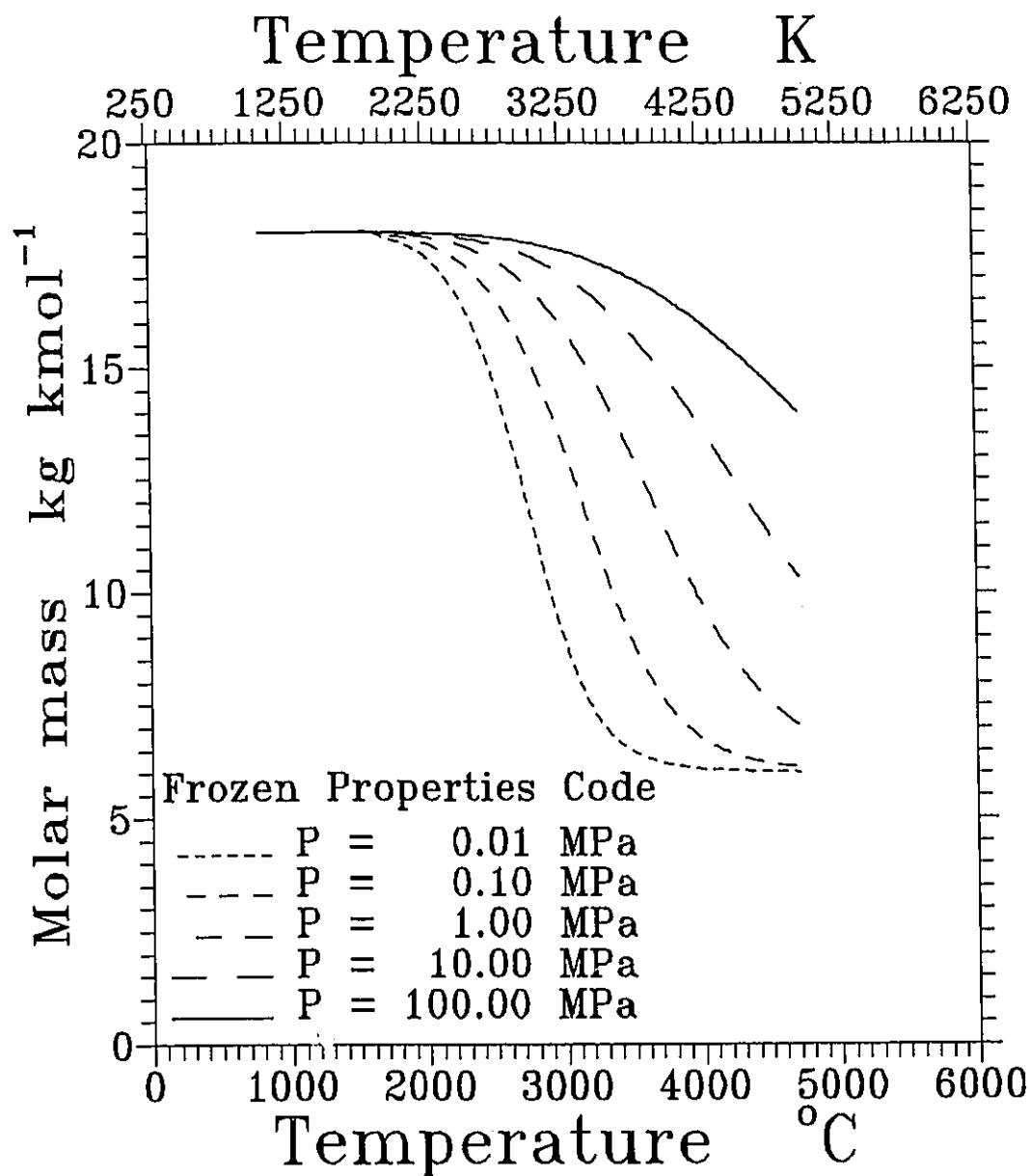


Figure 4.1: Molar mass of dissociated steam as a function of temperature for a range of constant pressures, predicted by the Frozen Properties code.

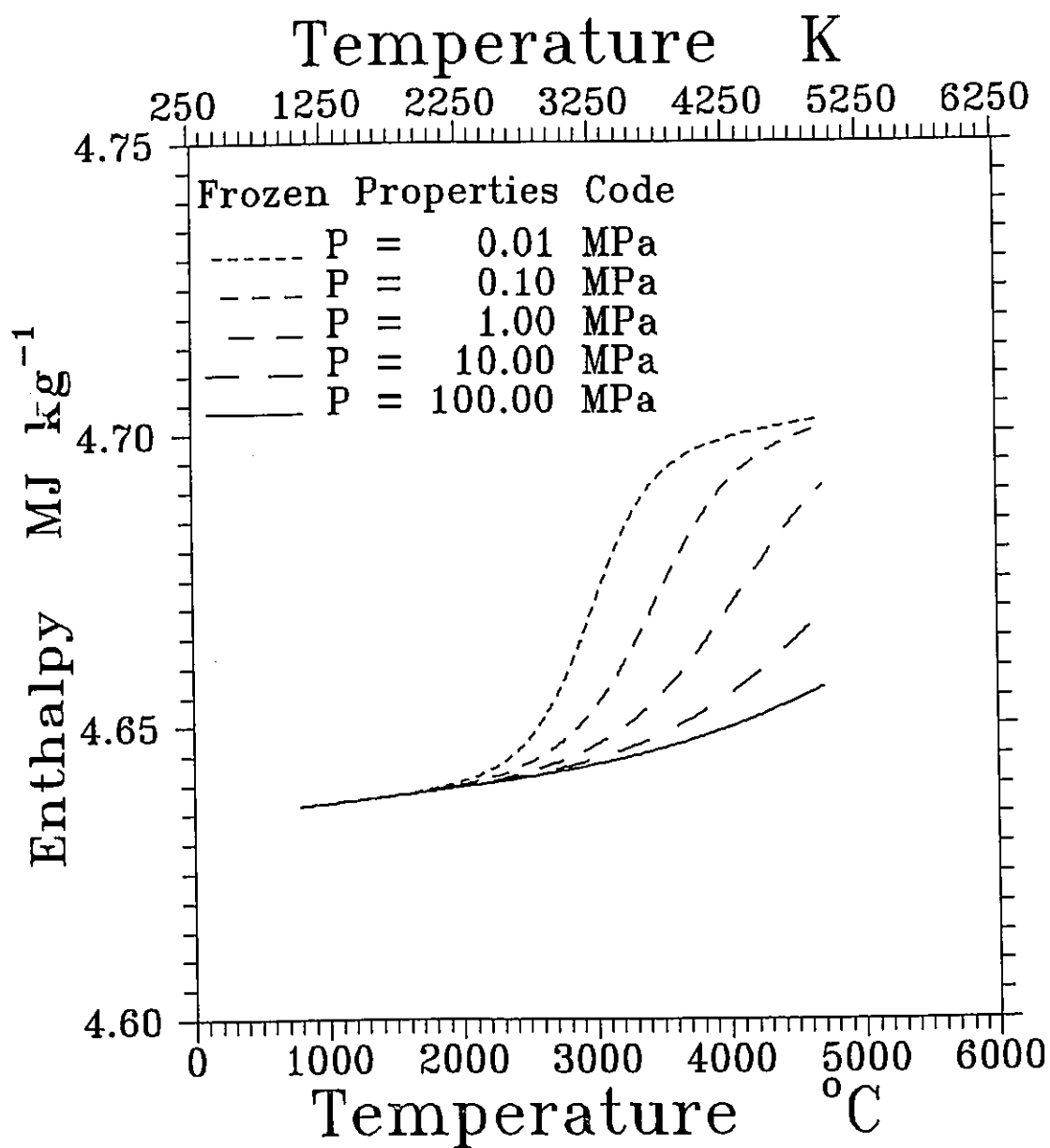


Figure 4.2: Frozen enthalpy of dissociated steam as a function of temperature for a range of constant pressures, predicted by the Frozen Properties code.

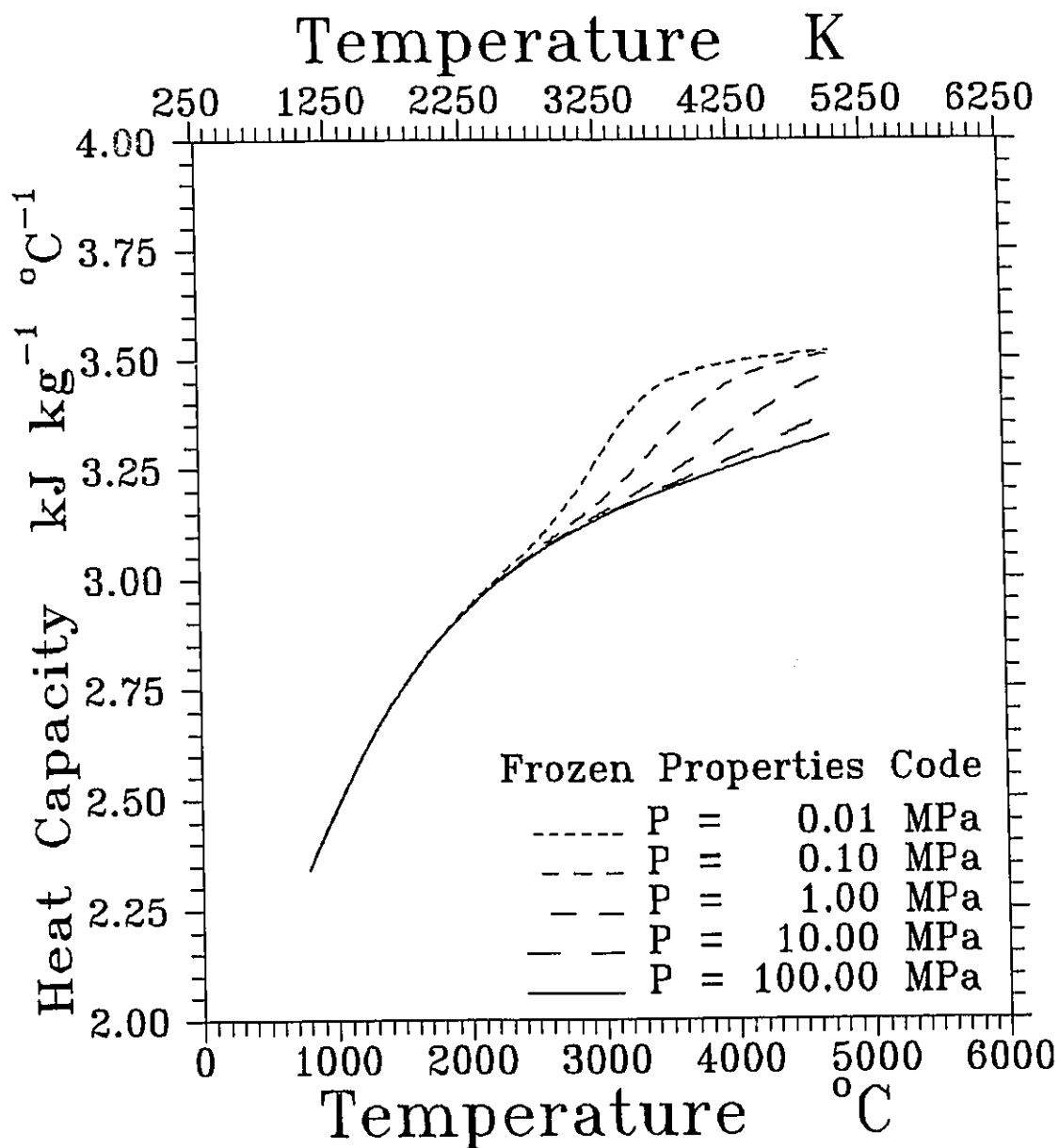


Figure 4.3: Frozen heat capacity of dissociated steam as a function of temperature for a range of constant pressures, predicted by the Frozen Properties code.

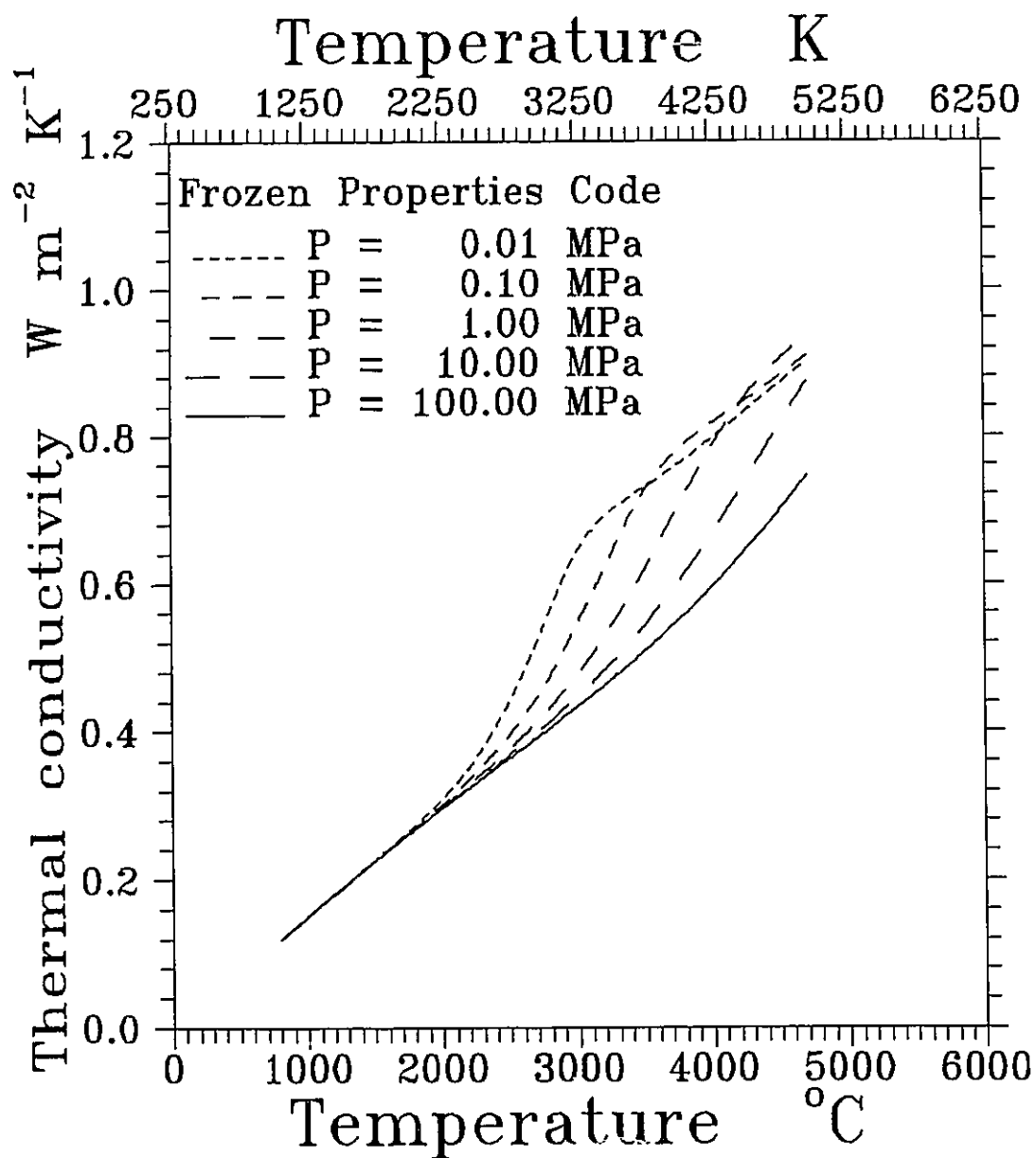


Figure 4.4: Frozen thermal conductivity of dissociated steam as a function of temperature for a range of constant pressures, predicted by the Frozen Properties code.

4.3 Recommended Prediction Method for Mass Diffusion Coefficients

4.3.1 Binary mixture

Mass diffusion coefficients for a binary mixture of gases are most commonly calculated using the formula developed by Chapman and Enskog kinetic theory, Chapman et al. (1939). This formula has often been cited by Hirschfelder et al. (1957), Bird et al. (1962), Cussler (1984), Reid et al. (1987), etc. All of these authors used different units, such that the numerical coefficient in the formulas differ even though all have same origin. After converting to the SI system of units, the formula becomes

$$D_{l-i} = \frac{0.1882899 \cdot 10^{-9} T^{1.5}}{\tilde{M}_{l,i}^{0.5} \sigma_{l,i}^2 \Omega_{D,l,i} P} [=] m^2 s^{-1} \quad (4.1)$$

where:

- l, i - species l diffuses through species i ;
- T - absolute temperature [=] K;
- $1/\tilde{M}_{l,i} = (1/\tilde{M}_l) + (1/\tilde{M}_i)$ - reduced mass of the system [=] kmol kg⁻¹;
- $\tilde{M}_l, \tilde{M}_i$ - molecular mass of the species l and i [=] kg kmol⁻¹;
- $\sigma_{l,i}$ - characteristic length, [=] nm;
- $\Omega_{D,l,i}$ - diffusion collision integral, [=] dimensionless;
- P - pressure, [=] MPa.

The characteristic length σ is a molecular property and it may be computed from the parameters of individual species using the arithmetic average equation

$$\sigma_{l,i} = \frac{\sigma_l + \sigma_i}{2} \quad (4.2)$$

The collision integral $\Omega_{D,l,i}$ is dependant on the integration of the interaction between two species. It was tabulated for the Lennard-Jones potential function by Hirschfelder et al. (1967) or it may be calculated very accurately using the following approximation from Neufield et al. (1972):

$$\Omega_{D,l,i} = \frac{1.06036}{(T_{li}^*)^{0.15610}} + \frac{0.19300}{\exp(0.47635 T_{li}^*)} + \frac{1.03587}{\exp(1.52996 T_{li}^*)} + \frac{1.76474}{\exp(3.89411 T_{li}^*)} \quad (4.3)$$

and,

$$T_{li}^* = \frac{T}{\left(\frac{\epsilon_{l,i}}{k_B}\right)} \quad (4.4)$$

The value of $(\epsilon_{l,i}/k_B)$ is the energy of interaction of two different molecules. Though without any theoretical support, a geometric average of the energy of interaction of each species is usually used,

$$\left(\frac{\epsilon_{l,i}}{k_B}\right) = \sqrt{\left(\frac{\epsilon_l}{k_B}\right)\left(\frac{\epsilon_i}{k_B}\right)} \quad (4.5)$$

It should be noted that an inconsistency occurs in the derivation of the formula in Equation (4.1). Intermolecular forces are considered by exploiting the potential function, yet on the other hand, to include the pressure effects, the ideal gas law was used. An ideal gas is a gas with no intermolecular forces. For consistency with the initial assumptions, i.e. that in the gas mixture intermolecular forces exist, the virial equation has to be employed. Thus Equation (4.1) becomes

$$D_{l-i} = \frac{0.1882899 \cdot 10^{-9} T^{1.5}}{\tilde{M}_{li}^{0.5} \sigma_{li}^2 \Omega_{pl,i} P} Z_{li} [=] m^2 s^{-1} \quad (4.6)$$

The term Z is the compressibility factor of binary mixtures, and can be calculated using the combination rules as follows

$$Z_{li} = 1 + B_{li}(T) \rho_{li} + C_{li}(T) \rho_{li}^2 \quad (4.7)$$

$$\rho_{li} = \rho_l + \rho_i \quad (4.8)$$

$$\tilde{B}_{li}(T) = b_o B^*(T_{li}^*) \quad (4.9)$$

$$C_{li}(T) = b_o^2 C^*(T_{li}^*) \quad (4.10)$$

$$b_o = \frac{2}{3} \pi N_A \sigma_{li}^3 \quad (4.11)$$

$B^*(T_{li}^*), C^*(T_{li}^*)$, the theoretically calculated virial coefficients as a function of T_{li}^* in the range $0.30 < T_{li}^* < 400.0$, are tabulated by Hirschfelder (1954, Table I-C, pp.1114-1117) or can be calculated with formulas presented by the same author in Table I-E (p.1119).

The values of $\epsilon_i(T)/k_B$, $\sigma_i(T)$, $B_i(T)$ and $C_i(T)$ for the components of dissociated steam as a function of temperature are presented in Tables C-1 and C-2 in Appendix C, determined by Kesselman and Blank (1986 i). Most of the values in the tables come directly from Kesselman and Blank's (1986 i) data. Additional values are added (extrapolated) to cover the whole parametric range. Dissociated steam is a mixture of six components, accordingly, thirty-six (36) binary diffusion coefficients can be evaluated. The main terms or self-diffusion coefficients represent the binary diffusion of each component through itself (6 coefficients). The cross terms of the binary diffusion coefficients (30 coefficients) for two components j and i are equal.

$$D_{j-i} = D_{i-j} \quad (4.12)$$

Therefore, fifteen (15) binary diffusion coefficients are required.

A set of computer subroutines was developed for the computation of all possible combinations of binary diffusion coefficients, according to Equation (4.1) and Table C-1, in dissociated steam (21 coefficients). A listings of the subroutines is presented in Appendix I, as part of the High Temperature Steam Heat Transfer code (VASICA¹⁶). A main program calls the subroutine BINDCO(P,T), with entering parameters absolute pressure P(MPa), and temperature T(°C) in the range from 726.85°C (1000K) to 5726.85°C (6000K). Accompanying subroutines are PARAMET, REDMAS, SIGMABIN, EPSILBUN, NEUFD, MASDIF and BLOCK DATAES. Results of the calculations are stored in COMMON BLOCK /BINDIF/ as DBIN.

Some typical self-diffusion (6) and binary diffusion coefficients (15) for dissociated steam components, as a function of temperature at a pressure of 0.1MPa, are presented in Figures 4.1 to 4.3. The lighter the components (smaller molar mass), the larger the self-diffusion coefficient. Hydroxyl (HO) is the only component which deviates from that observation; it has a slightly smaller self-diffusion coefficient than expected. The molar mass of hydroxyl is smaller than that of H₂O, thus it is expected to have a larger self-diffusion coefficient than that of H₂O. Hence, though the largest binary diffusion coefficient is for the lightest interaction (H₂ - H), the smallest is for the (O₂ - HO) interaction, and not for the heaviest interaction, (H₂O - O₂).

¹⁶ VASICA is an acronym for VASIĆ Aleksandar computer code.

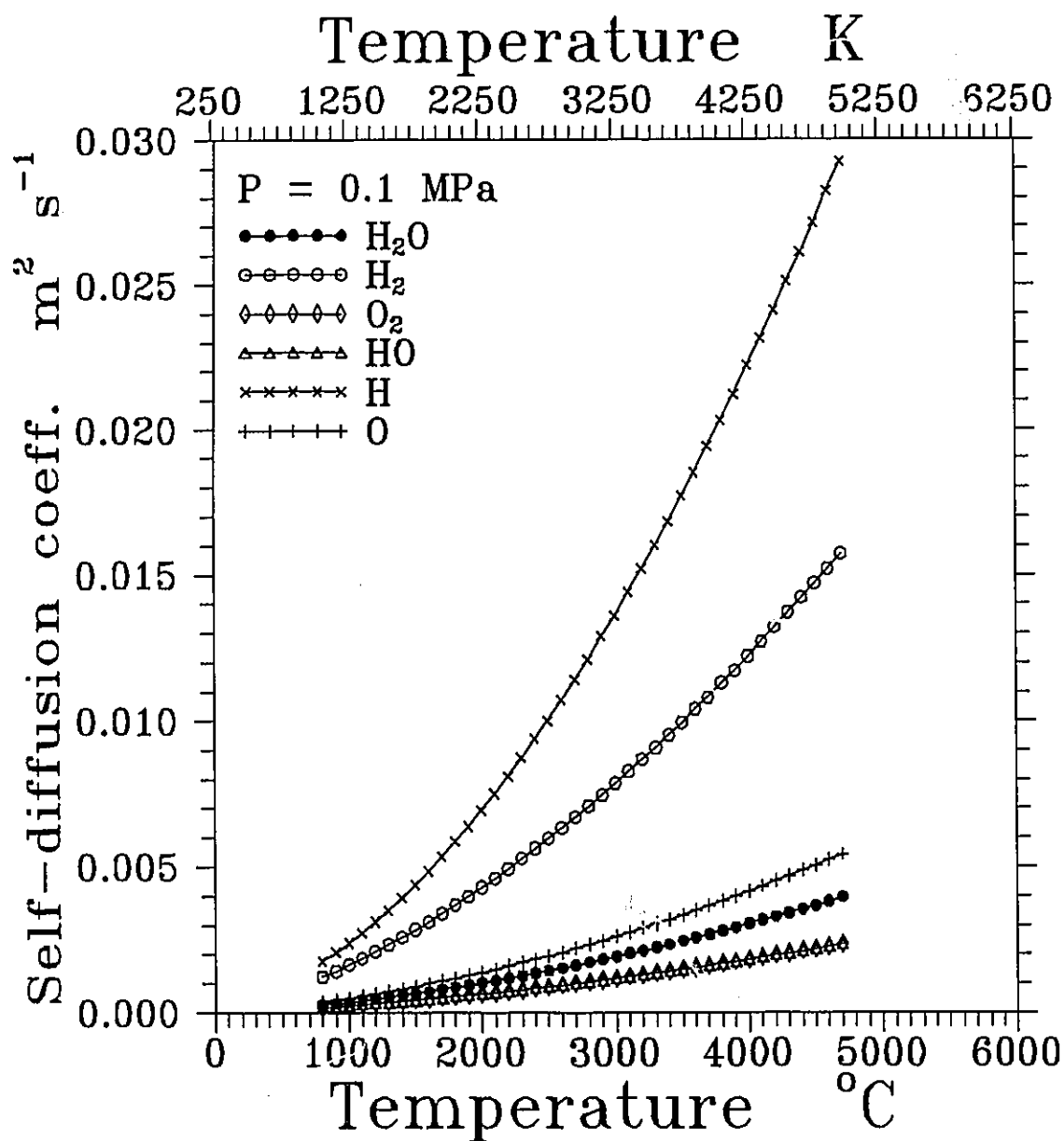


Figure 4.5: Self-diffusion coefficients of steam dissociation components at pressure 0.1MPa.

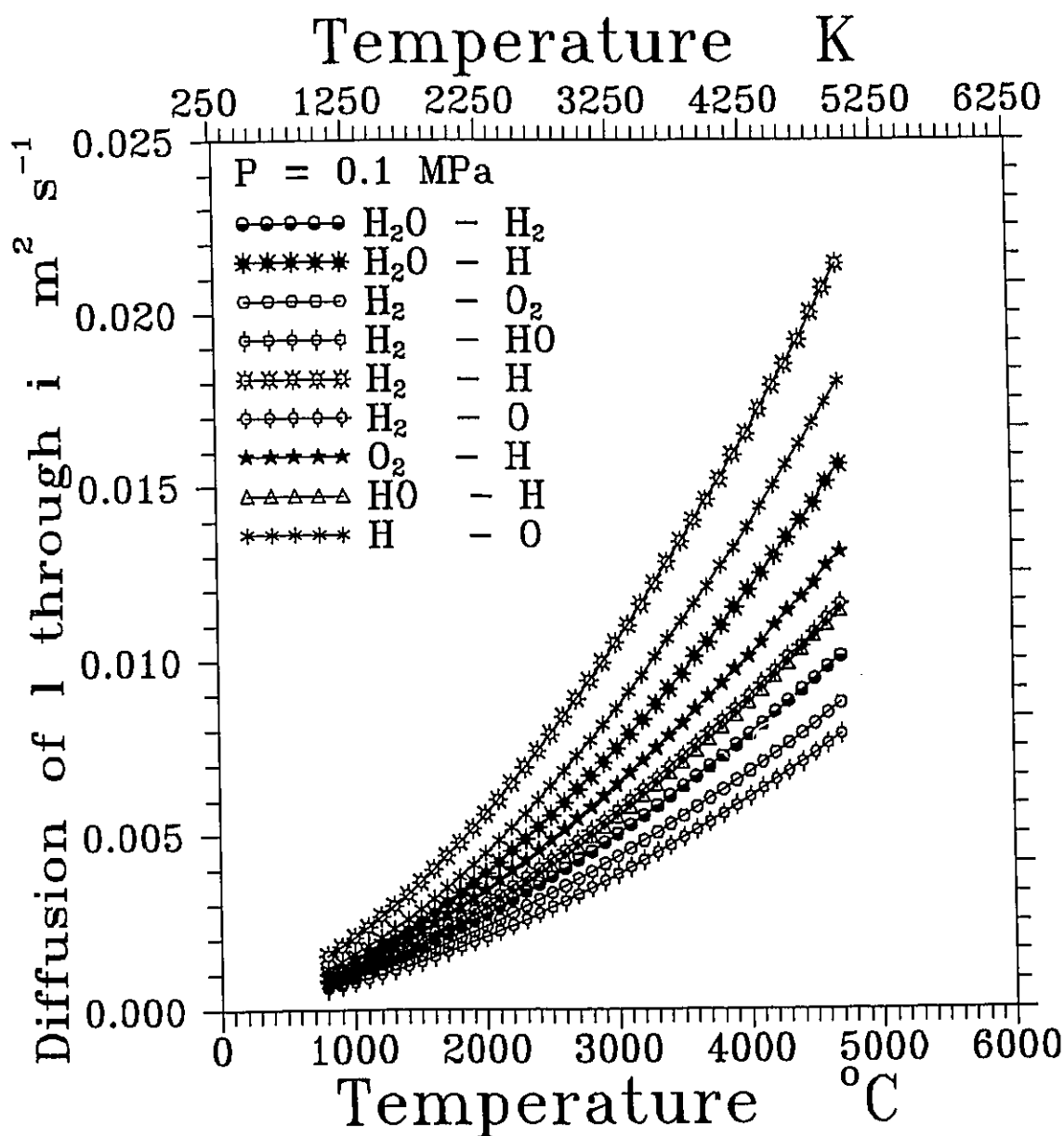


Figure 4.6: Binary diffusion coefficients of species l through species i at 0.1MPa.

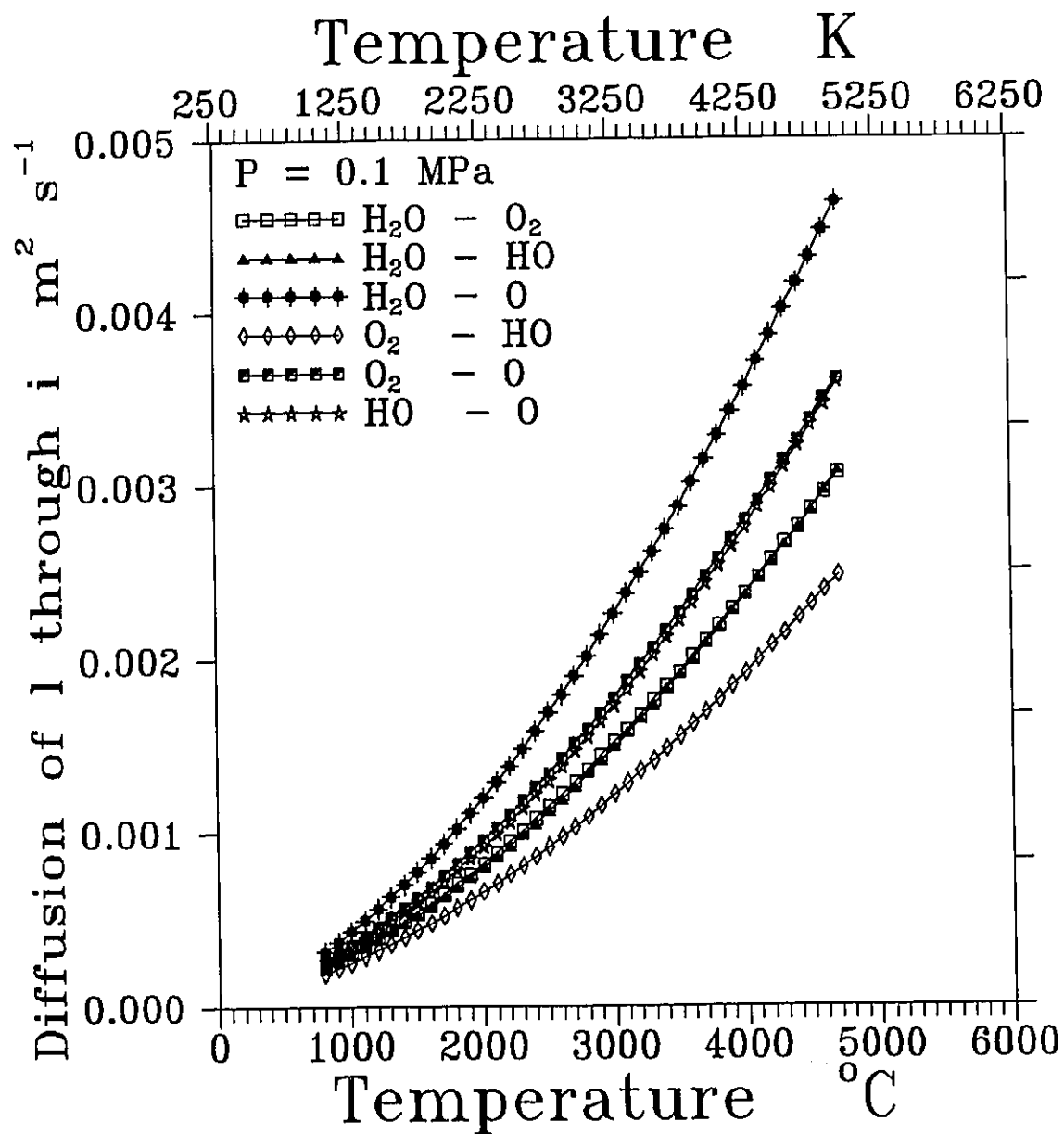


Figure 4.7: Binary diffusion coefficients of species l through i at 0.1MPa.

4.3.2 Multi-component mixture

Multi-component diffusion is described by generalizing the equation for binary diffusion. The general relation between binary diffusion coefficients and multi-component coefficients is not known, except for a few special systems:

1. For a system with a nearly pure species $i = 1$ and all other components, $i = 2, 3, \dots, n$, as trace components, then

$$D_{1-m} = D_{1-1} \quad (4.13)$$

2. For a system in which all binary diffusion coefficients are the same, then

$$D_{1-m} = D_{1-i} \quad (4.14)$$

3. For a system in which all components $i = 1, 2, \dots, n$, $i \neq 1$ move with the same velocity (or are stationary), then Blanc's law can be applied

$$D_{1-m} = \frac{1 - y_1}{\sum_{i=1 \atop (i \neq 1)}^n \frac{y_i}{D_{1-i}}} \quad (4.15)$$

A multi-component system of dissociated steam is dependent upon temperature and pressure. The process of dissociation can be divided into four regions:

- a region where steam is the predominant component of the mixture ($y(\text{H}_2\text{O}) \approx 1$) and the remaining components are trace components (system 1);
- a region where the molar fractions of all components in the mixture are of the same magnitude ($y(\text{H}_2\text{O}) < 0.5$), (system 3);
- a transition region ($0.5 < y(\text{H}_2\text{O}) < \approx 1$);
- a region where the gas mixture is an almost pure binary mixture of atomic hydrogen (H) and oxygen (O) ($y(\text{H}_2\text{O}) \approx 0$).

It is assumed that in the transitional region, the diffusion coefficient of component l through the mixture may be computed as proportional to system 1 and 3 according to following equation:

$$D_{l-m} = D_{l-1} + \left[\frac{1 - y_l}{\sum_{i=1 \atop (i \neq l)}^6 \frac{y_i}{D_{l-i}}} - D_{l-1} \right] \frac{1 - y_l}{1 - 0.5} \quad (4.16)$$

The computer subroutine MIXDIFF(L,DMIX) was developed for the computation of the diffusion coefficient for the component l through a gas mixture according to the method described above. A listing of the subroutines is presented in Appendix I, as part of the High Temperature Steam Heat Transfer code (VASICA). A main program must first call the Fraction code for evaluating the composition of the gas mixture, then call subroutine BINDCO(P,T), to determine all the binary diffusion coefficients, and finally call subroutine MIXDIFF(L,DMIX). For a given component L , the subroutine evaluates the diffusion coefficient of that component through the six-component mixture of dissociated steam (results are presented as variable DMIX).

Typical diffusion coefficients, for the components of steam dissociation through gas mixture as a function of temperature at a pressure of 0.1MPa, are presented in Figures 4.8. The lighter the component (smaller molar mass), the larger the diffusion coefficient through mixture. Hydroxyl (HO) is the only component which deviates from this observation; it has at higher temperatures a slightly smaller diffusion coefficient than expected. However, the same observation can be made for the case of self-diffusion coefficients as shown in Figure 4.5.

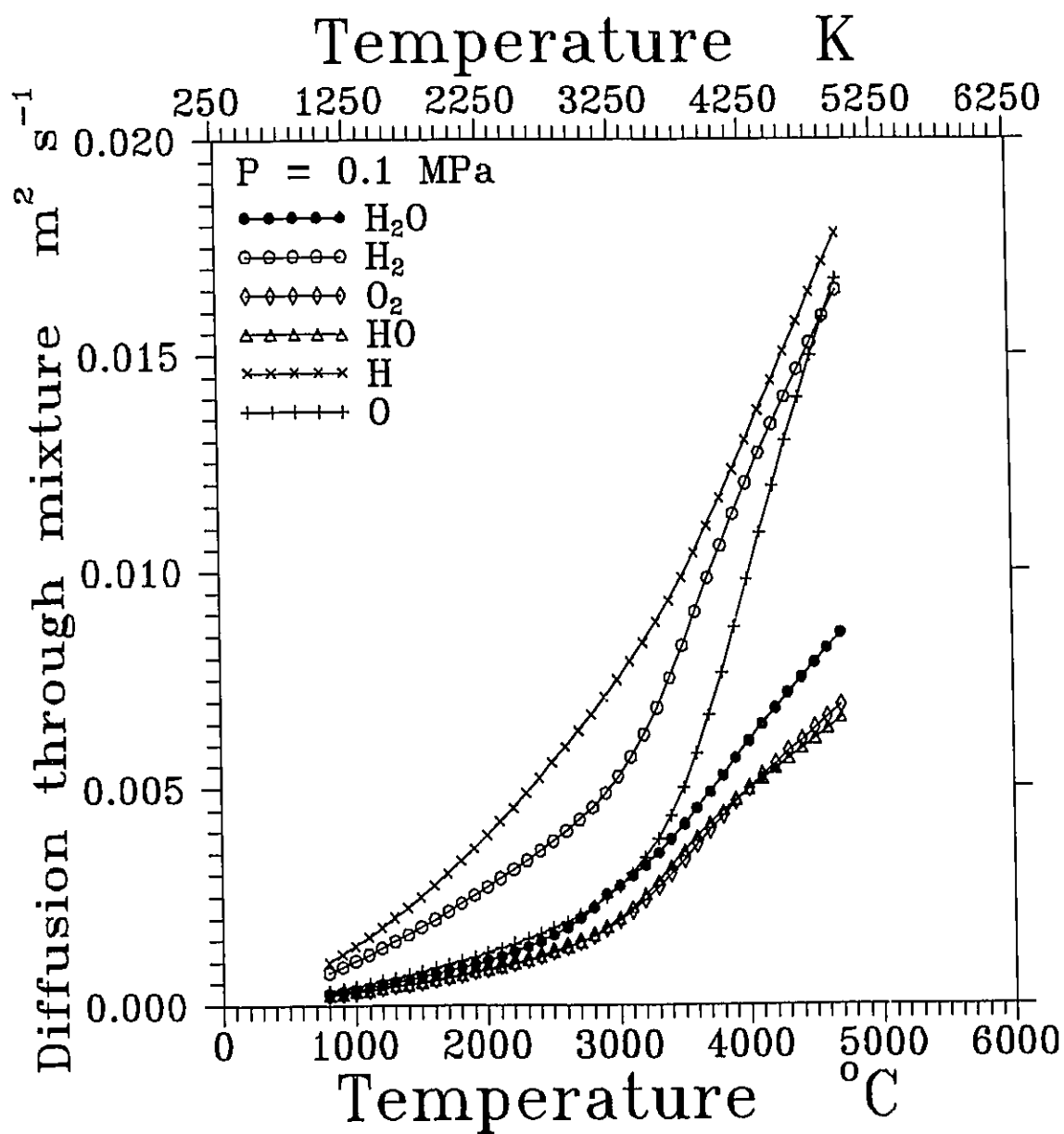


Figure 4.8: Diffusion coefficients for the components of steam dissociation through a mixture at a pressure of 0.1MPa.

4.4 Effective Thermodynamic and Transport Properties of Dissociated Steam

After a careful assessment, analysis and comparison of all available sources for the prediction of steam properties at high temperature, Vasić et al. (1992) concluded that the prediction method by Kesselman and data presented by Vargaftik (1983) are reliable for general use. As a result, they were recommended for industrial application.

The method for computing high temperature steam properties using a look-up table and an interpolation technique is presented in Appendix C. Most of the entries in the look-up table were constructed from data tabulated by Vargaftik (1983). Additional entries for viscosity and thermal conductivity were extrapolated and added at pressure of 100MPa by the author to expand the parametric range. Extrapolation were performed using graphical method.

Consequently, a set of computer subroutines was developed for generating steam properties via a linear interpolation technique using data tabulated by Vargaftik (1983). A set of computer subroutines, for generating steam thermodynamic¹⁷ and transport properties, is presented. A listing of the program specifications of the UODH2O code, for effective properties of dissociated steam in the range of pressure from 0.01 to 100.00MPa and temperature from 1000 to 5726.85°C, is presented in Appendix H. The UODH2O code presented here is connected with the IAPS Property code listed by Haar et al. (1984) and makes possible an evaluation of the properties of liquid water, steam and dissociated steam at a pressure ranging from 0.01MPa to 100.00MPa and a temperature ranging from triple point temperature 0.01°C to 5726.85°C.

The UODH2O code was used to predict dissociated steam effective thermodynamic and transport properties. The predicted results are presented in the table of effective properties for dissociated steam, at a pressure ranging from 0.01 to 100.00MPa and a temperature ranging from 1000 to 3000°C, in Appendix L.

Some typical thermodynamic and transport property values, as a function of temperature at a range of pressures, are shown in Figures 4.9 to 4.15, as predicted by the UODH2O code. Comparing the frozen and effective enthalpy from Figures 4.2 and 4.12 respectively, one can conclude that frozen and effective enthalpy have same values at temperature lower then 1500°C.

¹⁷ The reference point is defined as the zero value of entropy and enthalpy in this case. The water triple point ($t = 0.01^\circ\text{C}$, $P = 611.73\text{Pa}$) is chosen as the reference point.

At high temperature and low pressure effective enthalpy is many times larger than frozen enthalpy. This is due to effects of chemical reactions. The same conclusion may be reached for heat capacity and thermal conductivity. However, at high temperature and low pressure when steam is completely dissociated heat capacity and thermal conductivity have same values again. Effective properties are more dependent on pressure than are frozen properties.

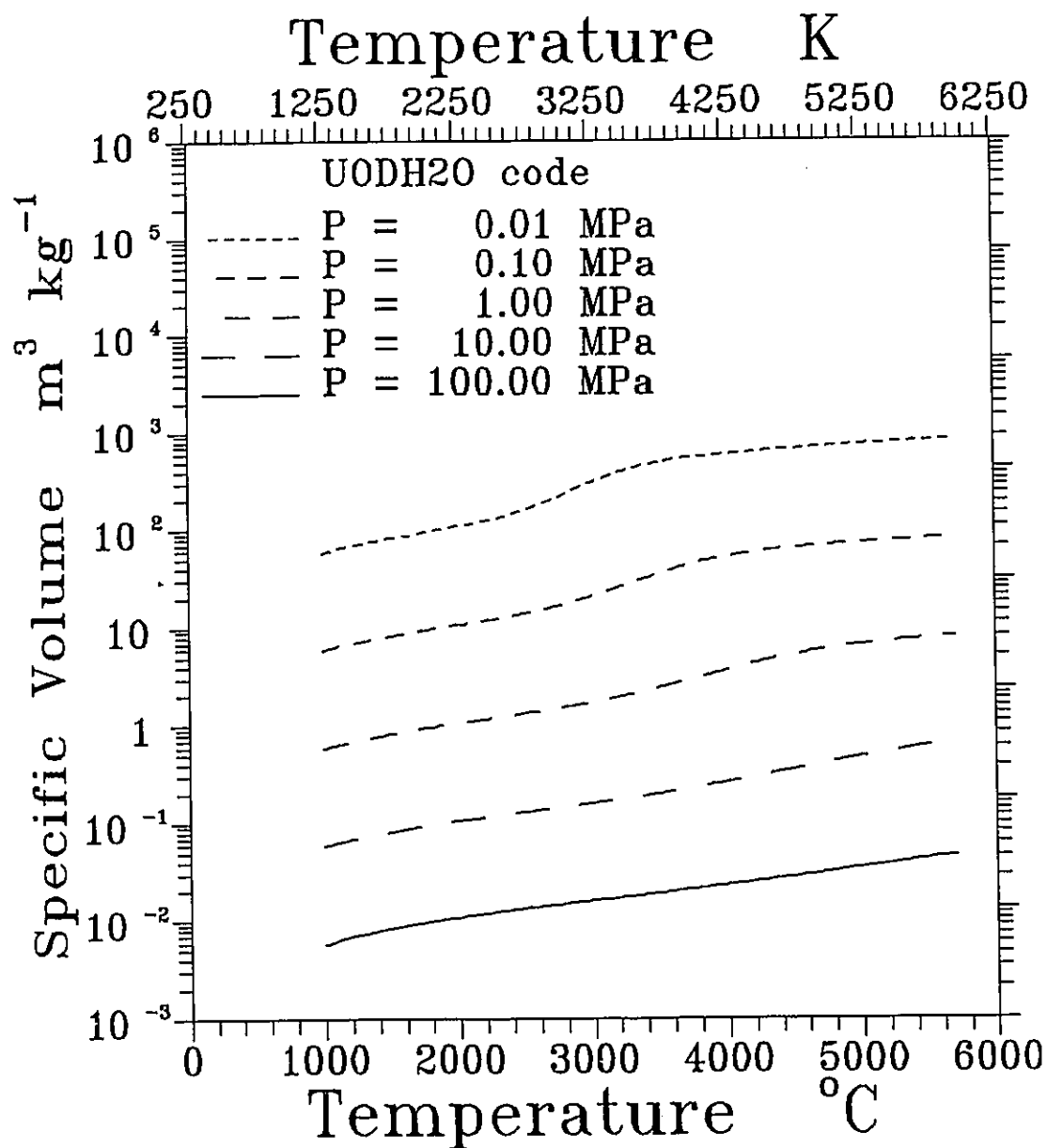


Figure 4.9: Specific volume of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH20 code.

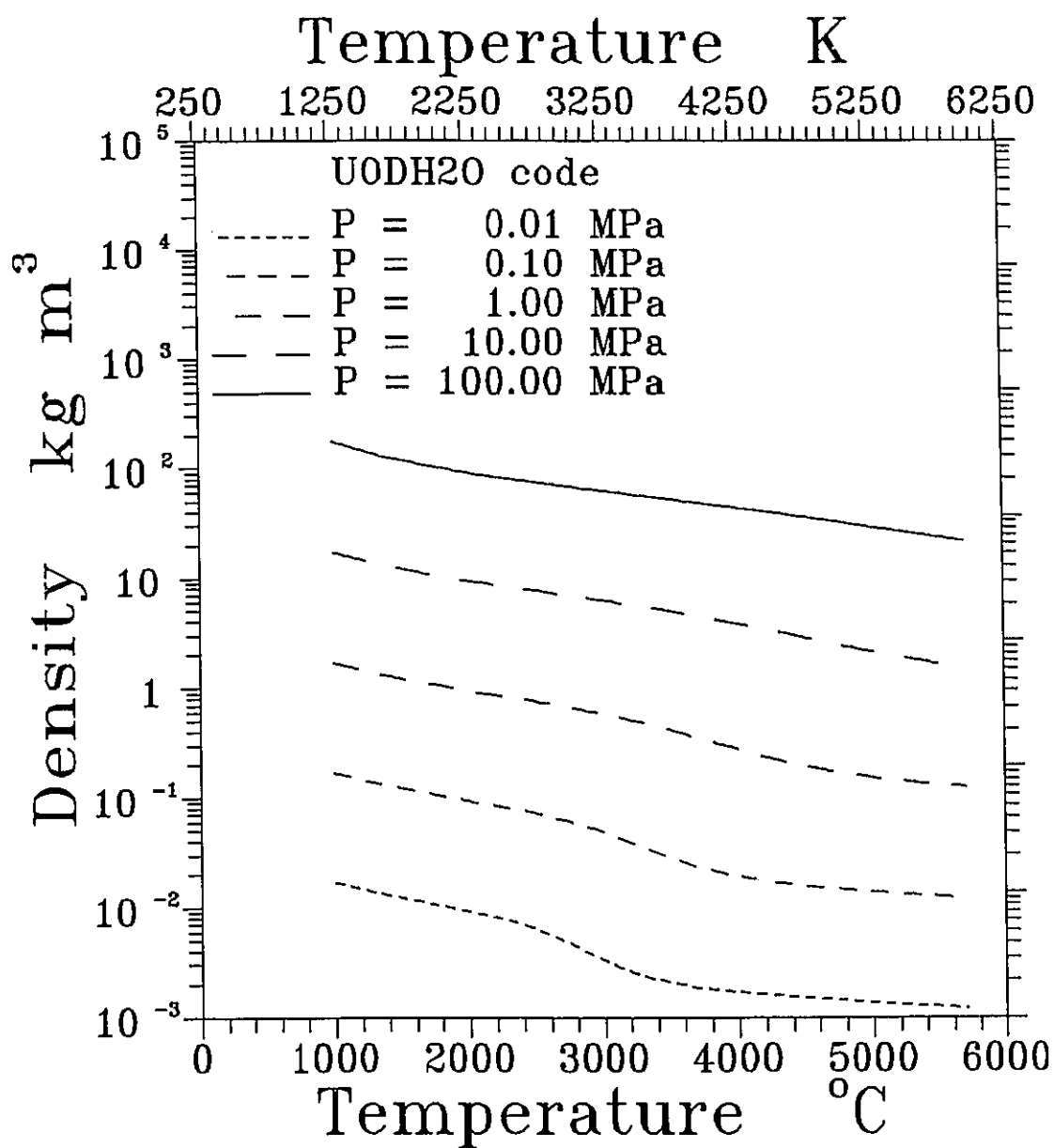


Figure 4.10: Density of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.

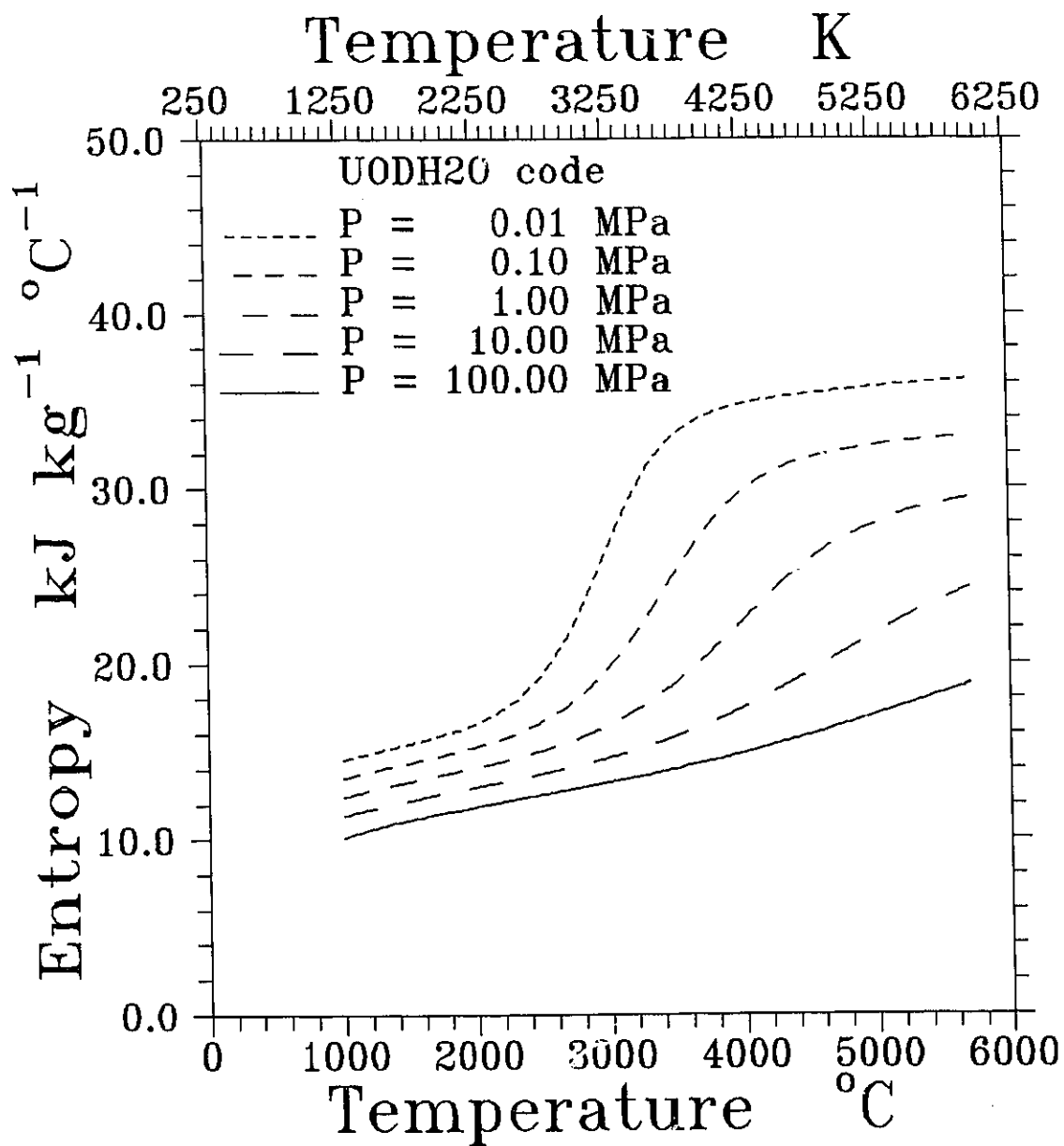


Figure 4.11: Entropy of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH20 code.

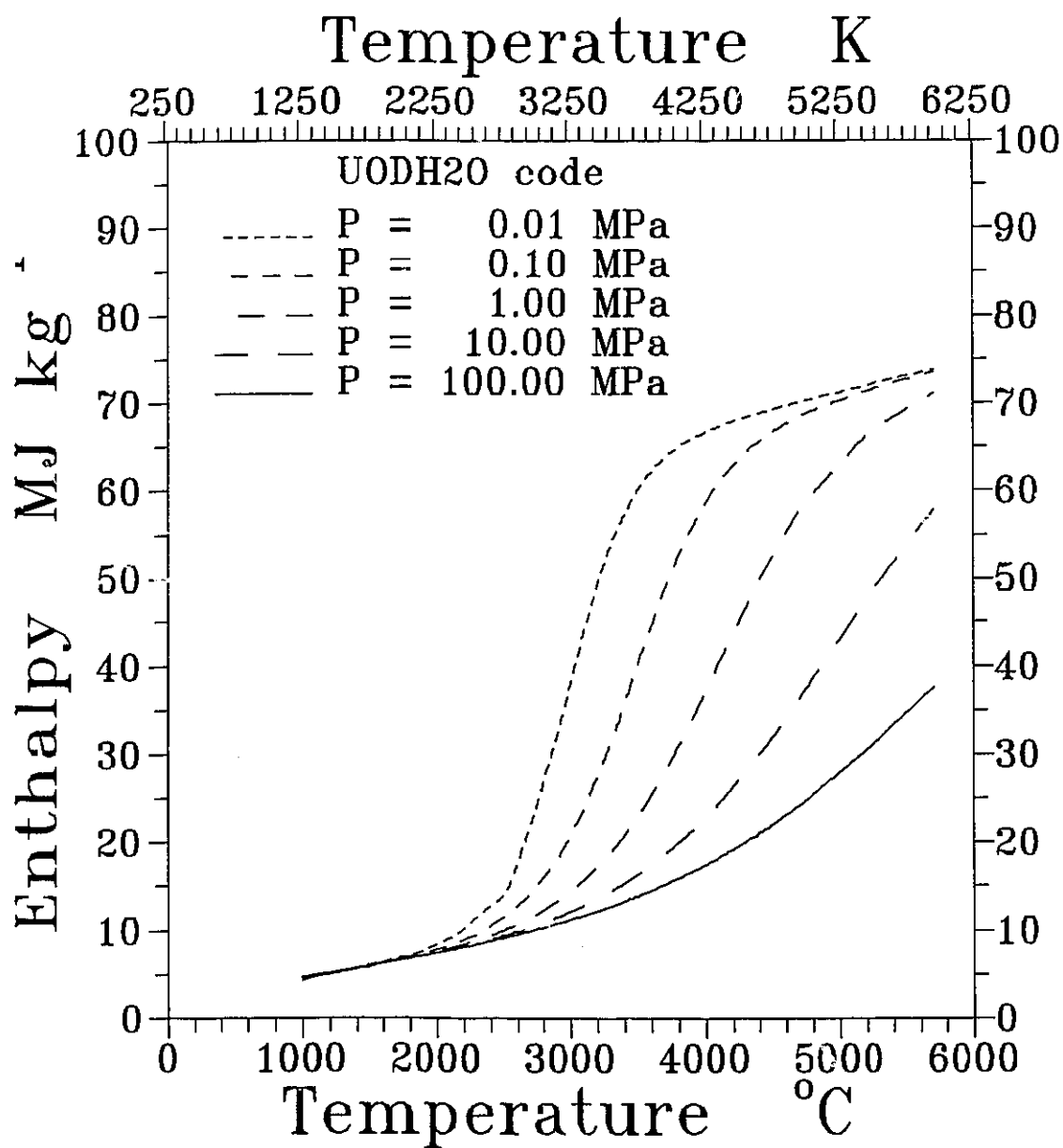


Figure 4.12: Enthalpy of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH20 code.

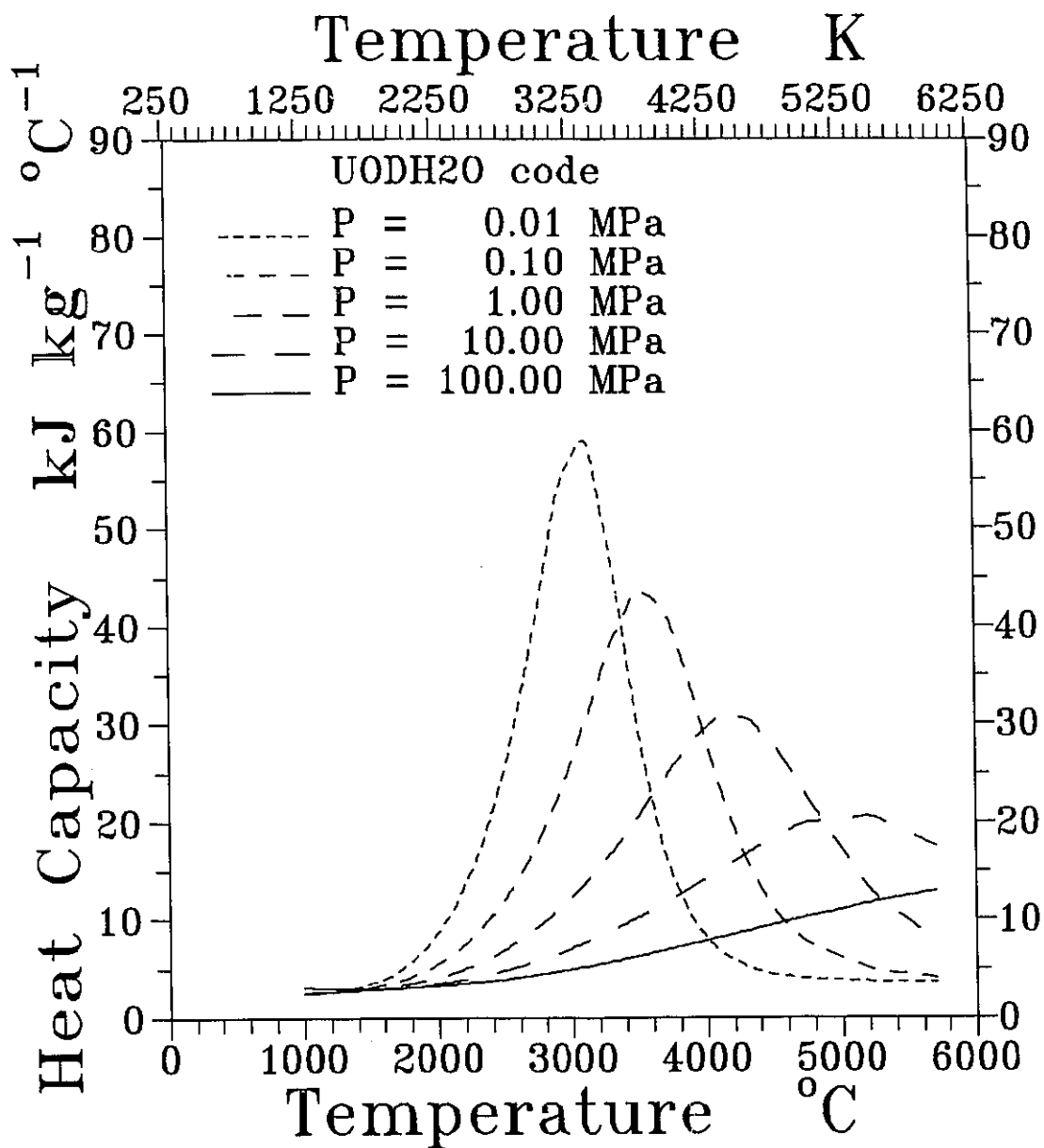


Figure 4.13: Heat capacity of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH20 code.

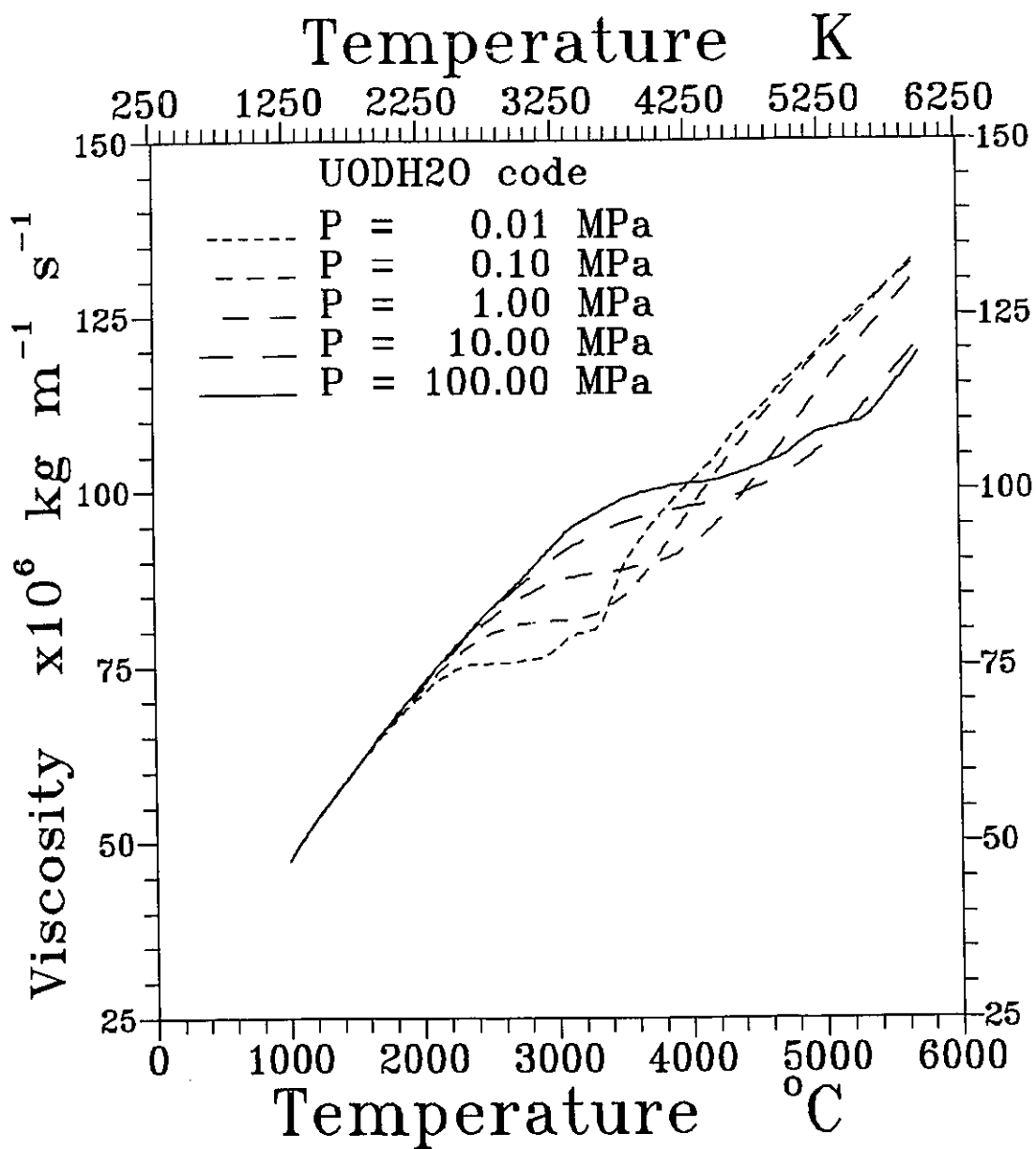


Figure 4.14: Viscosity of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.

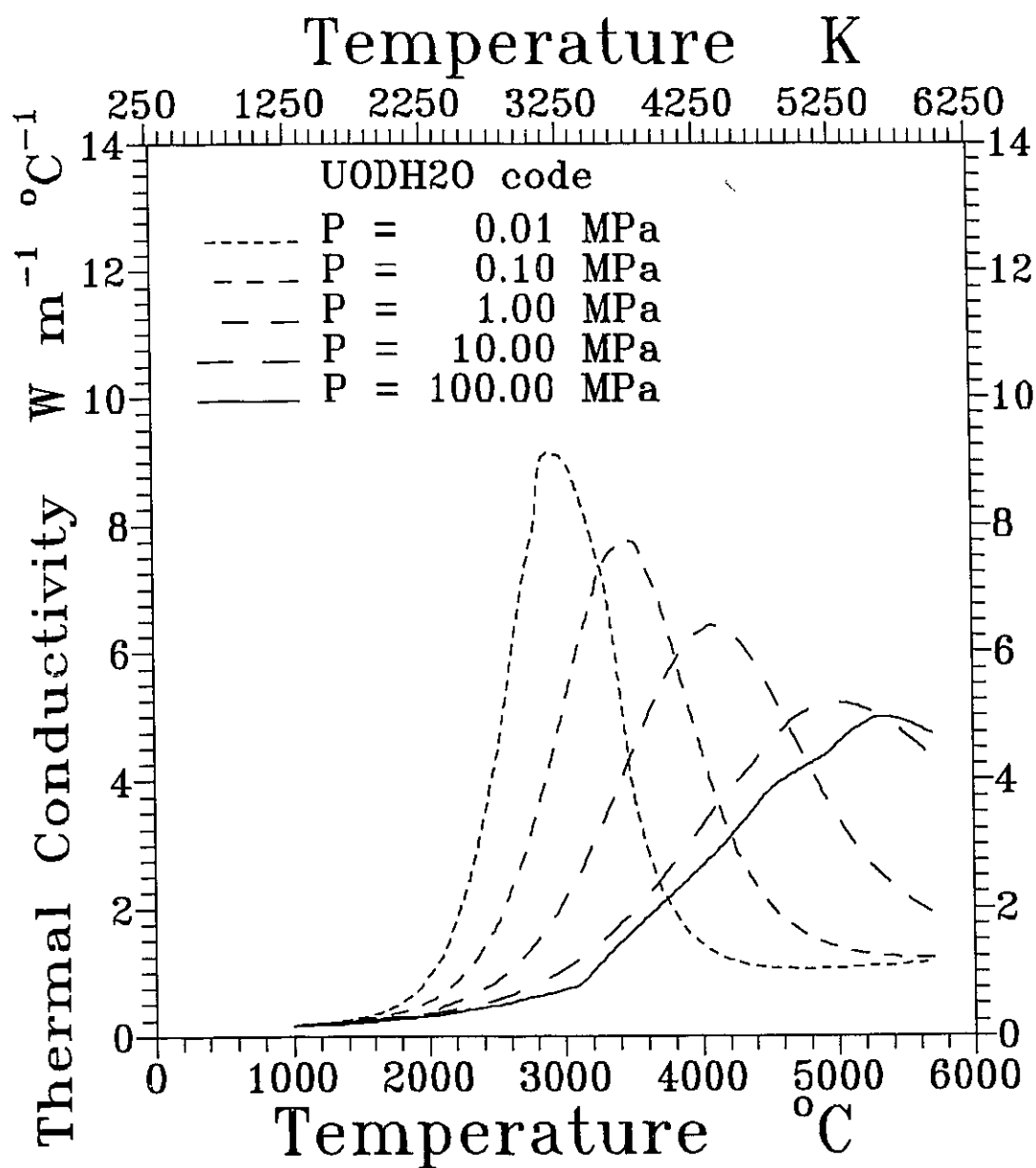


Figure 4.15: Thermal conductivity of dissociated steam as a function of temperature for a wide range of constant pressures, predicted by the UODH2O code.

4.5 Summary

In this chapter, the methods for predicting three groups of properties of dissociated steam were recommended. These three groups are:

- a) a method for predicting frozen properties (molar mass, enthalpy, heat capacity and thermal conductivity);
- b) a method for predicting mass diffusion (binary and multi-component mixture) coefficients of dissociated steam;
- c) a method for predicting effective thermodynamic (specific volume, entropy, enthalpy, heat capacity) and transport (viscosity and thermal conductivity) properties.

Each section included a description of the properties evaluated, then the properties with pressure and temperature dependence were illustrated in a number of charts.

Chapter 5

Heat Transfer for Pure Gases and Steam at Moderate Temperatures

5.1 General

Heat transfer for gases and steam at moderate temperatures ($<1000\text{K}$) is heat transfer to a single-phase, chemically-stable (non-reactive), pure (one component) fluid. For a gas flow with small Mach number ($\text{Ma} \ll 1$), the velocity of the fluid is much smaller than the local speed of sound, and the compressibility of the gas is negligible. One difference between heat transfer to liquids (incompressible fluid) and heat transfer to gases (fluid with negligible compressibility) is that properties of liquids, particularly viscosity, vary approximately inversely with temperature. The viscosity of liquids decreases rapidly with temperature increase, while the viscosity of gases increases with temperature. However, for minimal temperature differences between the heat transfer surface (tube wall) and the bulk of the convective fluid, the viscosity variance along the tube radius is not vital. Hence, same heat transfer correlations can apply to both liquids and gases.

Some heat transfer correlations are appropriate for any fluid, while some others are developed specifically for certain fluids. In section 5.2 the universal heat transfer correlations for the turbulent flow of pure fluids in tubes are presented. In section 5.3 heat transfer correlations developed specially for the turbulent flow of superheated steam in tubes are presented.

5.2 Heat Transfer Correlations for Pure Fluids in Smooth Tubes

The correlations listed in this section were found in the reference by Kakaç et al. (1987) and original papers. The correlations presented in this work are only a sample of the correlations available in the literature.

In Table 5.1 the heat transfer correlations for turbulent flow of fluids in smooth tubes, developed with properties evaluated at fluid bulk temperature, are presented. Table 5.2 gives the heat transfer correlations, for turbulent flow of gases with large temperature differences, in smooth tubes. Three of the correlations deserve special attention. They are: the classical empirical correlation by Dittus and Boelter¹⁸ (1930), the theory-based correlation by Petukhov et al. (1972) and the correlation with best agreement with experimental data by Gnielinski (1976). These three correlations will be addressed in more detail in Chapter 6.

¹⁸ The original correlation was expressed in imperial units but converted to dimensionless form and SI units. Sometimes, in the literature, this correlation is quoted with coefficient 0.023. Several correlations are found in the literature, i.e., Nusselt (1910), Dittus and Boelter (1930), Kraussold (1933), McAdams (1933), Colburn (1933), Drexel et al. (1945), Miheev (1952) and others, which have the same form but different numerical values for the coefficients, and may be the source of the difference.

Table 5.1 Heat Transfer Correlations for Turbulent Flow of Fluids in Smooth Tubes

Reference	Correlation	Range of application	Comments
Reynolds (1874)	$Nu_b = \left(\frac{f}{2} \right) Re_b Pr_b$	$Pr_b = 1$	
Nusselt (1910)	$Nu_b = 0.024 Re_b^{0.786} Pr_b^{0.45}$		
Prandtl (1910)	$Nu_b = \frac{\left(\frac{f}{2} \right) Re_b Pr_b}{1 + 5 \sqrt{\frac{f}{2} (Pr_b - 1)}}$	$5 \cdot 10^3 \leq Re_b \leq 5 \cdot 10^6$ $Pr_b \leq 10$	
Dittus and Boelter (1930)	$Nu_b = 0.024 Re_b^{0.8} Pr_b^{0.4}$	$2.5 \cdot 10^3 \leq Re_b \leq 1.24 \cdot 10^5$ $0.7 \leq Pr_b \leq 120$	For heating gases or liquids.
Petukhov and Kirillov (1958)	$Nu_b = \frac{\left(\frac{f}{2} \right) Re_b Pr_b}{1.07 + 12.7 \sqrt{\frac{f}{2} (Pr_b^{2/3} - 1)}} \left[\frac{Re_b}{8} \right]^{-2}$ $f = \left[3.64 \log \left(\frac{Re_b}{8} \right) \right]^{-2}$	$1 \cdot 10^4 \leq Re_b \leq 1 \cdot 10^6$ $0.7 \leq Pr_b \leq 200$	Developed for liquids. f by Filonenko (1954).

Table 5.1 Heat Transfer Correlations for Turbulent Flow of Fluids in Smooth Tubes

Reference	Correlation	Range of application	Comments
Petukhov and Popov (1963)	$Nu_b = \frac{\left(\frac{f}{2}\right) Re_b Pr_b}{k_1(f) + k_2(Pr_b)} \sqrt{\frac{f}{2} \left(Pr_b^{2/3} - 1\right)}$ $k_1(f) = 1 + 13.6 f \quad k_2(Pr) = 11.7 + \frac{1.8}{Pr^{1/3}}$ $f = \left[3.64 \log \left(\frac{Re_b}{8} \right) \right]^2$	$1 \cdot 10^4 \leq Re_b \leq 5 \cdot 10^6$ $0.5 \leq Pr_b \leq 2000$	f by Filonenko (1954).
Petukhov et al. (1972)	$Nu_b = \left(\frac{f}{2}\right) Re_b Pr_b C^{-1}$ $f = 0.0791 Re_b^{-0.25} \quad 4 \cdot 10^3 \leq Re_b < 1 \cdot 10^4$ $f = \left[3.64 \log \left(\frac{Re_b}{8} \right) \right]^2 \quad 1 \cdot 10^4 \leq Re_b \leq 5 \cdot 10^6$ $C = 1.07 + \frac{900}{Re_b} - \frac{0.63}{1+10 Pr_b} + 12.7 \sqrt{\frac{f}{2} (Pr_b^{2/3} - 1)}$	$4 \cdot 10^3 \leq Re_b \leq 5 \cdot 10^6$ $0.5 \leq Pr_b \leq 1 \cdot 10^6$	f by Blasius (1913) and by Filonenko (1954).

Table 5.1 Heat Transfer Correlations for Turbulent Flow of Fluids in Smooth Tubes

Reference	Correlation	Range of application	Comments
Gnielinski (1976)	$Nu_b = \frac{\left(\frac{f}{2}\right) (Re_b - 1000) Pr_b}{1 + 12.7 \sqrt{\frac{f}{2}} (Pr_b^{2/3} - 1) \left[1 + \left(\frac{L}{d}\right)^{-2/3}\right]}$ $f = 0.0791 Re_b^{-0.25} \quad 4 \cdot 10^3 \leq Re_b < 1 \cdot 10^4$ $f = \left[3.64 \log\left(\frac{Re_b}{8}\right)\right]^{-2} \quad 1 \cdot 10^4 \leq Re_b \leq 5 \cdot 10^6$	$2.3 \cdot 10^3 \leq Re_b \leq 1 \cdot 10^6$ $0.5 \leq Pr_b \leq 2000$	For gases and liquids, recommended by Kakaç et al.(1987). f by Blasius (1913) and Filonenko (1954).

Note:

*Correlations in this table are good for moderate temperature differences ($T_w - T_b$).

**If the equation for Fanning friction factor f is not specified, it may be evaluated from Techo et al. (1965).

$$f = \left[0.86859 \ln \left(\frac{Re}{1.964 \ln(Re) - 3.8215} \right) \right]^{-2} \quad 1 \cdot 10^4 \leq Re \leq 2.5 \cdot 10^8$$

***Equation incorporating length over diameter ratio (L/d) is for the local heat transfer at distance L from tube entrance.

Table 5.2 Heat Transfer Correlations for Turbulent Flow of Gases with Large Temperature Differences in Smooth Tubes

Reference	Correlation	Range of application	Comments
Colburn (1933)	$Nu_f = 0.023 Re_f^{0.8} Pr_f^{1/3}$	$1 \cdot 10^4 \leq Re_f \leq 1 \cdot 10^5$ $0.5 \leq Pr_f \leq 3$ $t_f = t_b + 0.5 (t_w - t_b)$	For liquids and for small temperature differences.
Sieder and Tate (1936)	$Nu_b = 0.023 Re_b^{0.8} Pr_b^{1/3} \left(\frac{\mu_b}{\mu_w} \right)^{0.14}$		Valid for many fluids for moderate temperature differences.
Miheev (1952) Kutateladze (1966)	$Nu_b = 0.021 Re_b^{0.8} Pr_b^{0.43} \left(\frac{T_w}{T_b} \right)^{-0.55}$		Original correlation is corrected by temperature ratio as recommended by Kutateladze.
Petukhov and Popov (1963)	$Nu_b = \frac{\left(\frac{f}{2} \right) Re_b Pr_b}{k_1(f) + k_2(Pr_b) \sqrt{\frac{f}{2} (Pr_b^{2/3} - 1)}} \left(\frac{T_w}{T_b} \right)^{-0.47}$ $k_1(f) = 1 + 13.6 f \quad k_2(Pr) = 11.7 + \frac{1.8}{Pr^{1/3}}$ $f = \left[3.64 \log \left(\frac{Re_b}{8} \right) \right]^{-1.2} \quad Re_w^* = \frac{G d}{\mu_w} \frac{\rho_w}{\rho_b}$	$1 \cdot 10^4 < Re_b < 5 \cdot 10^6$ $0.5 < Pr_b < 2000$ $1 < T_w/T_b < 3.7$ $14 \cdot 10^3 < Re_w^* < 1 \cdot 10^6$	f by Filonenko (1954).
Kutateladze (1966)	$Nu_b = 0.027 Re_b^{0.8} Pr_b^{0.4} \left(\frac{T_w}{T_b} \right)^{-0.55}$	$1 < T_w/T_b < 3.5$ $T_w, T_b (^{\circ}\text{C})$	Valid for gases.

Table 5.2 Heat Transfer Correlations for Turbulent Flow of Gases with Large Temperature Differences in Smooth Tubes

Reference	Correlation	Range of application	Comments
Petukhov et al. (1972)	$Nu_b = \left(\frac{f}{2} \right) Re_b Pr_b C^{-1} E_{vp}$ $f = 0.0791 Re_b^{-0.25} \quad 4 \cdot 10^3 \leq Re_b < 1 \cdot 10^4$ $f = \left[3.64 \log \left(\frac{Re_b}{8} \right) \right]^{-2} \quad 1 \cdot 10^4 \leq Re_b \leq 5 \cdot 10^6$ $C = 1.07 + \frac{900}{Re_b} - \frac{0.63}{1+10 Pr_b} + 12.7 \sqrt{\frac{f}{2}} (Pr_b^{2/3} - 1)$ $E_{vp} = \left(\frac{\rho_w}{\rho_b} \right)^{0.53} \left(\frac{Cp_w}{Cp_b} \right)^{1/4} \left(\frac{k_w}{k_b} \right)^{1/3} \left(\frac{\mu_w}{\mu_b} \right)^{-1.5 \log \left(\frac{T_w}{T_b} \right)}$	$Re_b > 7 \cdot 10^3$ $1 \leq T_w/T_b \leq 4$	f by Blasius (1913) and Filonenko (1954).
Gnielinski (1976)	$Nu_b = \frac{\left(\frac{f}{2} \right) (Re_b - 1000) Pr_b}{1 + 12.7 \sqrt{\frac{f}{2}} (Pr_b^{2/3} - 1)} \left[1 + \left(\frac{L}{d} \right)^{-0.45} \left(\frac{T_w}{T_b} \right) \right]$ $f = 0.0791 Re_b^{-0.25} \quad 4 \cdot 10^3 \leq Re_b < 1 \cdot 10^4$ $f = \left[3.64 \log \left(\frac{Re_b}{8} \right) \right]^{-2} \quad 1 \cdot 10^4 \leq Re_b \leq 5 \cdot 10^6$	$2.3 \cdot 10^3 \leq Re_b \leq 5 \cdot 10^6$ $0.5 \leq Pr_b \leq 2000$	f by Blasius (1913) and Filonenko (1954).

Note: *If the equation for Fanning friction factor f is not specified, it may be evaluated from Techo et al. (1965).

**Equation incorporating length over diameter ratio (L/d) is for the local heat transfer at distance L from tube entrance.

5.3 Heat Transfer Correlations for Superheated Steam in Smooth Tubes

Sources for the correlations listed in this section were found in references by Kakaç et al. (1987), Groeneveld (1982), Groeneveld et al. (1989) and the original papers. Some of the heat transfer correlations from the literature, for the flow of superheated steam (flow without liquid droplets entrained in the stream) in round tubes, are presented in Table 5.3. The mechanism of heat transfer depends to a large degree upon fluid properties and temperature, as well as on the velocity distribution in the thin boundary layer adjacent to the solid wall.

For a small temperature difference between the heat transfer surface and the bulk of the convective fluid, the variance in properties along the radius of tube is not significant. For such a case, correlations are developed with properties evaluated at steam bulk temperature, such as the first two correlations in Table 5.3. The correlation by Sutherland (1963) has a temperature-ratio correction term which may compensate for change in properties with temperature.

If the temperature difference is large, then change in properties along the tube radius is important. A reasonable approach is to evaluate the fluid properties at a reference temperature between the wall and bulk temperature. The choice of a reference temperature is arbitrary, however the average film temperature is often used. Three correlations in Table 5.3 are developed with properties evaluated at the average film temperature. The correlation by Hadallari and Banerjee (1969) is developed using experimental data by Heineman (1960), Sutherland (1963) and Bishop et al. (1964); consequently, it is recommended as the most accurate. These correlations will be addressed in more detail in Chapter 6.

5.4 Recommendation

The heat transfer coefficient to steam for turbulent flow in tubes may be computed by applying a correlation developed for any gas, or one specially for steam. The correlations developed specially for steam are, unfortunately, only applicable with confidence in a narrow range in which the correlation was developed (using experimental data). General correlations for all gases have a wider range of application, but they are not as accurate as the correlation constructed specifically for a given fluid. From the listed correlations, four were chosen: those of Dittus and Boelter (1930), Petukhov et al. (1972), Gnielinski (1976) and Hadallari and Banerjee (1969). They will be addressed in more detail in Chapter 6.

Table 5.3 Heat Transfer Correlations for Turbulent Flow of Superheated Steam in Smooth Tubes

Reference	Correlation	Range of application	Comments
Properties evaluated at bulk temperature t_b			
Sutherland (1963)	$Nu_b = 0.021 Re_b^{0.8} Pr_b^{0.6} \left(\frac{T_w}{T_b} \right)^{-0.575}$		T_w, T_b (K) Steam only.
Bishop et al. (1964)	$Nu_b = 0.00863 Re_b^{0.886} Pr_b^{0.39} \left(\frac{\rho_w}{\rho_b} \right)^{1.03} \left(1 + \frac{2.76}{L/d} \right)$	$30 < L/d < 350$	High pressure steam only.
Properties evaluated at film temperature $t_f = t_w - 0.5 (t_w - t_b)$			
Heineman (1960)	$Nu_f = 0.0157 Re_f^{0.84} Pr_f^{1/3} \left(\frac{L}{d} \right)^{-0.04}$ $Nu_f = 0.0133 Re_f^{0.84} Pr_f^{1/3}$	$2 \cdot 10^4 < Re_f < 3.7 \cdot 10^5$ $2 < P < 10 \text{ MPa}$ $3 < \left(\frac{L}{d} \right) < 36$ $\left(\frac{L}{d} \right) > 60$	Steam only.
Bishop et al. (1964)	$Nu_f = 0.0073 Re_f^{0.886} Pr_f^{0.61} \left(1 + \frac{2.76}{L/d} \right)$	$30 < L/d < 350$	High pressure steam only.

Table 5.3 Heat Transfer Correlations for Turbulent Flow of Superheated Steam in Smooth Tubes

Reference	Correlation	Range of application	Comments
Hadallal and Banerjee (1969)	(i) $Nu_f = 0.0101 Re_f^{0.8774} Pr_f^{0.6112} \left(\frac{L}{d}\right)^{-0.0328}$ (ii) $Nu_f = 0.008348 Re_f^{0.8774} Pr_f^{0.6112}$ (iii) $Nu_f = 0.0170 Re_f^{0.8216} Pr_f^{0.6250} \left(1 + \frac{0.9842}{\frac{L}{d}}\right)$	$6 \cdot 10^4 < Re_f < 5 \cdot 10^5$ $2 < P < 21.4 \text{ MPa}$ $295 < t_f < 580^\circ\text{C}$ $3 < L/d < 350$	Steam only. (ii) is Equation (i) for fully developed flow from Groeneveld et al. (1989).

Note: *Equations incorporating length over diameter ratio (L/d) is for the local heat transfer at distance L from tube entrance.

Chapter 6

Heat Transfer for Dissociated Steam at High Temperatures

6.1 Mechanism of Heat Transfer at High Temperatures

Heat transfer to a flow of dissociated steam at high temperatures is heat transfer to a mixture of chemically reacting gases. The difference between heat transfer to reacting gases and to non-reacting gases is that additional heat is transported as chemical enthalpy. The driving force for the transport of chemical enthalpy is the concentration gradient of the species (H_2O , H_2 , O_2 , HO , H and O) in the gaseous mixture. The number of dissociated molecules increases with temperature, while the concentration or fraction of steam (H_2O) decreases (see Figures 2.3 and 6.1). The temperature at the wall of a tube is higher than at the axis, therefore the steam concentration near the wall is lower. Hence, the steam concentration gradient causes a transfer of steam to the region adjacent to the wall. Steam at the higher temperature region (close to the wall) absorbs heat from the wall by dissociating into components and hence the concentration of dissociation products is higher. The concentration gradient of dissociation products (HO , H and O) causes a transfer of these products from the region adjacent to the wall to the region near the axis. The products of dissociation, brought by mass transfer from the high temperature region to lower temperature region, recombine and release the heat of dissociation. Thus, heat initially absorbed from the wall is released in the region proximate to the tubular axis, therefore the temperature of the fluid at the tubular axis increases. The temperature gradient in the high temperature gas mixture causes the concentration gradient and the transport of chemical enthalpy, which acts to decrease that same temperature gradient until an equilibrium state is reached.

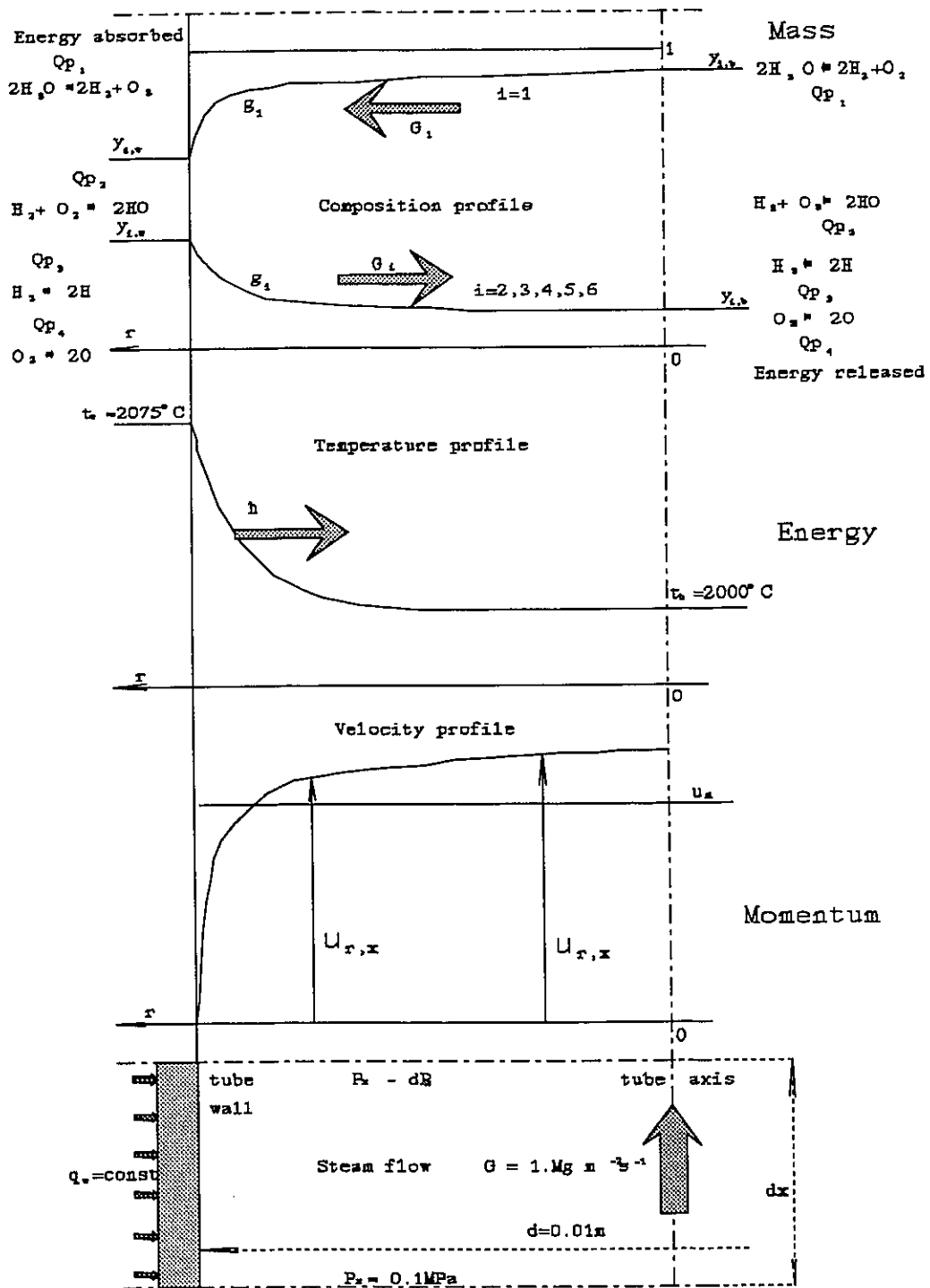


Figure 6.1: Heat Transfer mechanism for the turbulent flow of dissociated steam in a round tube.

The heat of dissociation is significantly larger than the heat of phase change. An example at atmospheric pressure $P = 0.101325\text{MPa}$ is shown as follows:

- heat of melting	= 333	kJ kg^{-1}	at	0.00°C (273.15K)
- heat of evaporation	= 2257	kJ kg^{-1}	at	100.00°C (373.15K)
- heat of sublimation	= 2834	kJ kg^{-1}	at	0.01°C (273.16K)
- heat of dissociation for reaction				
$2 \text{H}_2\text{O} \rightleftharpoons \text{H}_2 + 2 \text{HO}$	=15646	kJ kg^{-1}	at	126.85°C (400K)
	=16000	kJ kg^{-1}	at	1726.85°C (2000K)
- heat of dissociation for reaction				
$2 \text{H}_2\text{O} \rightleftharpoons 2 \text{H}_2 + \text{O}_2$	=13480	kJ kg^{-1}	at	126.85°C (400K)
	=13964	kJ kg^{-1}	at	1726.85°C (2000K)

From this example, it can be seen that the heat of dissociation is 6 to 7 times larger than the heat of evaporation at the same temperature and that the heat of dissociation increases with temperature. These phenomena suggest that using dissociating fluid as a heat transfer carrier is very effective. Unfortunately, the degree of steam dissociation is significant only at very high temperatures (above 1500°C).

Heat is transported from one region to another by mass diffusion and mass convection, as well as by heat conduction, heat convection and radiation. For a fluid flow, three transport phenomena exist: mass transport, momentum transport and energy transport.

In the theory of mass transfer, fluid flow and heat transfer, it was shown that mechanisms of molecular mass diffusion, molecular linear momentum transport, and molecular heat conduction, were analogous. Thus, Fick's law of diffusion

$$j_{i-i} \equiv -D_{i-i} \frac{\partial \rho_i}{\partial x} \quad (6.1)$$

Newton's law of viscosity

$$\tau \equiv -\mu \frac{\partial u}{\partial y} \quad (6.2)$$

and Fourier's law of heat conduction

$$q \equiv -k \frac{\partial T}{\partial x} \quad (6.3)$$

all have the same mathematical expression, i.e., the flux is proportional to the gradient of con-

centration, velocity or temperature. The coefficients of proportionality are the transport coefficients: mass diffusion coefficient, viscosity and thermal conductivity. The transport coefficients are properties of fluids at a given pressure and temperature. Combining transport coefficients, Schmidt, Prandtl and Lewis dimensionless numbers can be formed. Each of them is a ratio of the molecular diffusion rates for two transport phenomena.

$$Sc_{i-m} \equiv \frac{v}{D_{i-m}} = \frac{\mu}{\rho D_{i-m}} = Pr Le_i = \frac{\text{momentum diffusion rate}}{\text{mass diffusion rate}} \quad (6.4)$$

$$(6.5) Pr \equiv \frac{v}{a} = \frac{\mu Cp}{k} = \frac{Sc_{i-m}}{Le_i} = \frac{\text{momentum diffusion rate}}{\text{thermal diffusion rate}}$$

$$Le_i \equiv \frac{a}{D_{i-m}} = \frac{k}{Cp \rho D_{i-m}} = \frac{Sc_{i-m}}{Pr} = \frac{\text{thermal diffusion rate}}{\text{mass diffusion rate}} \quad (6.6)$$

It should be noted that some authors, like Cussler (1984) and Holman (1986), define the Lewis number according to Equation (6.6), yet in some older books, such as by Spalding (1963) and Eckert and Drake (1972), it was defined as the reciprocal value.

$$Le_i \equiv \frac{D_{i-m}}{a} = \frac{Cp \rho D_{i-m}}{k} = \frac{Pr}{Sc_{i-m}} = \frac{\text{mass diffusion rate}}{\text{thermal diffusion rate}} \quad (6.7)$$

Dimensionless Schmidt, Prandtl and Lewis numbers are properties of fluids. Since these numbers are rates of the molecular diffusion for two transport phenomena they apply in laminar flow. Employing the properties of dissociated steam presented in Chapter 3, these numbers are evaluated. In Figures 6.2 to 6.4, Schmidt, Prandtl and Lewis numbers are presented as a function of temperature at constant pressure. The Schmidt and Lewis numbers are characteristics of a single component i in a gas mixture formed by steam dissociation, but the Prandtl number is characteristics of the gas mixture itself.

In turbulent flow transport phenomena are disseminated additional to molecular diffusion by eddy diffusion. Analogy were found theoretically and experimentally for convective¹⁹ mass and heat transports such that the correlation for heat transfer can be used for mass transfer and vice versa. To be able to use semi-empirical correlations, the mass transfer coefficient of the species i is defined as

$$g_i \equiv \frac{G_i}{(C_{i,w} - C_{i,b})} \quad (6.8)$$

¹⁹ "Convection" from latin com "together" + valere "carry", transmitting by the actual movement of the fluid particles which carry some of the properties (mass, linear momentum or energy).

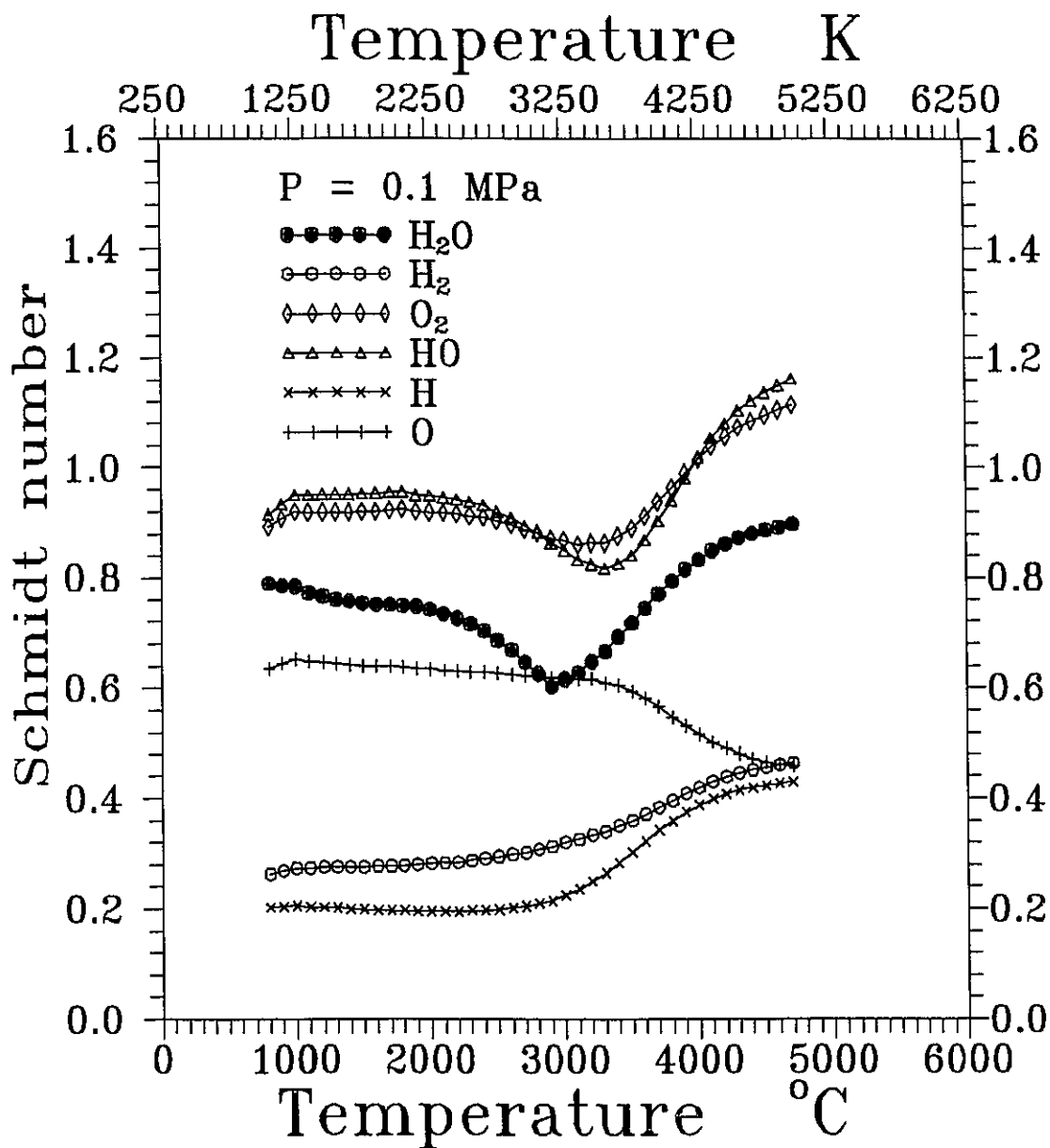


Figure 6.2: Schmidt number for the components of a gas mixture formed by steam dissociation as a function of temperature at constant pressure.

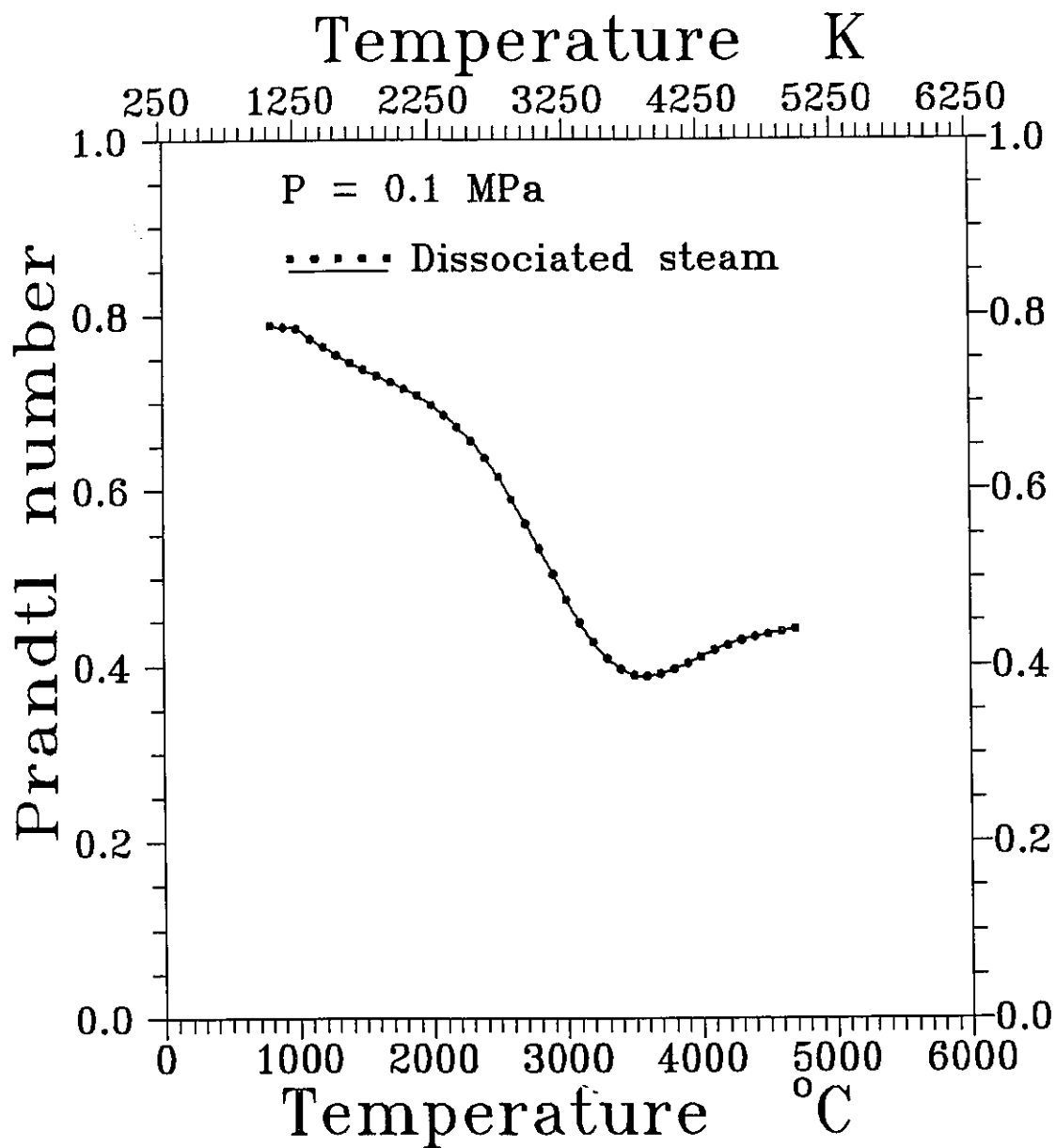


Figure 6.3: Prandtl number for a gas mixture formed by steam dissociation as a function of temperature at constant pressure.

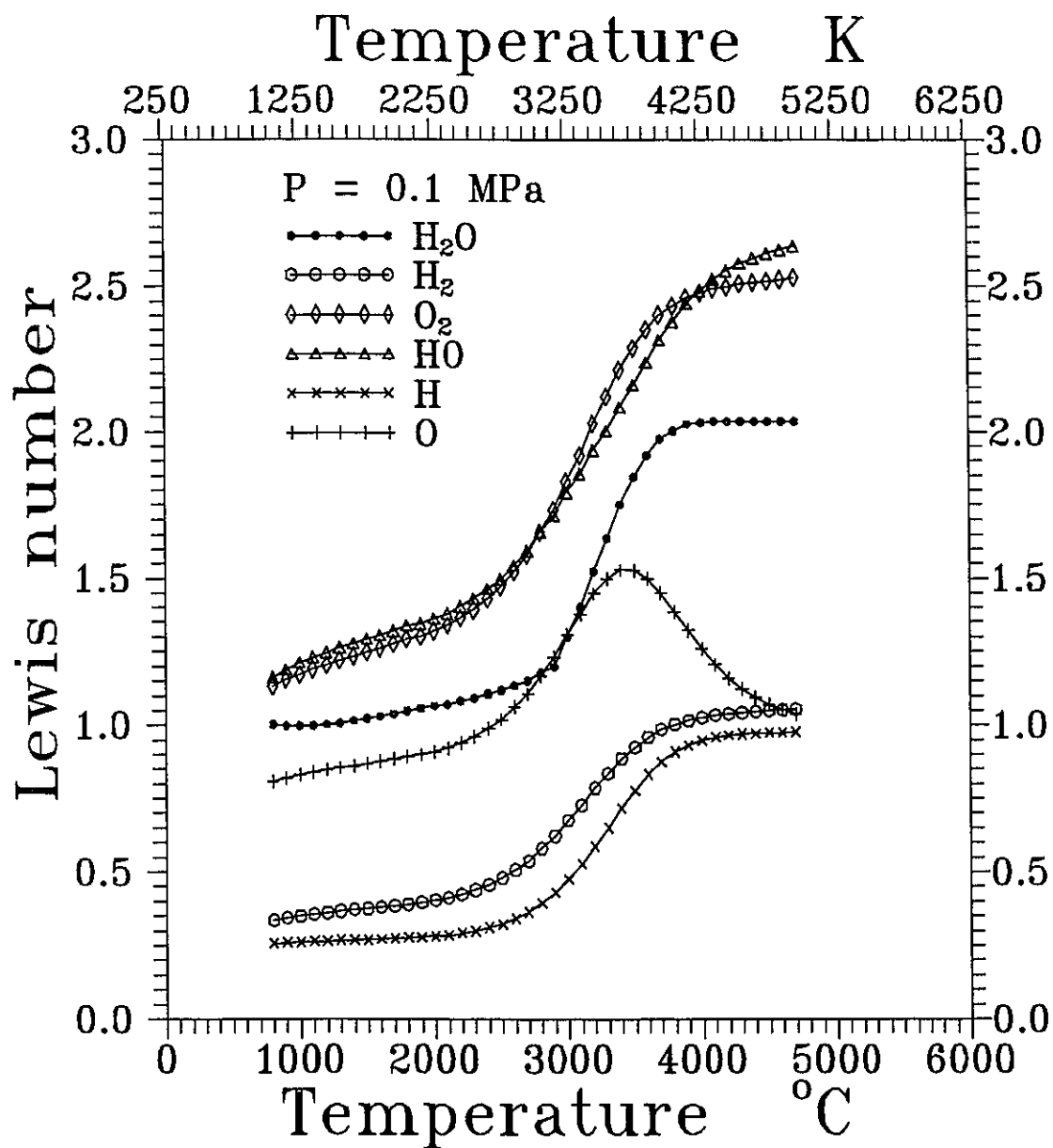


Figure 6.4: Lewis number for the components of a gas mixture formed by steam dissociation as a function of temperature at constant pressure.

The heat transfer coefficient is defined as

$$h_T \equiv \frac{q}{(T_w - T_b)} \quad (6.9)$$

Combining these two transfer coefficients with the properties of the fluid, the Sherwood, Reynolds and Nusselt dimensionless numbers can be formed:

$$Sh_i \equiv \frac{g_i d}{D_{i-m}} = \frac{\text{convective transfer of mass}}{\text{molecular transport of mass}} \quad (6.10)$$

$$Re \equiv \frac{G d}{\mu} = \frac{\text{convective transfer of momentum}}{\text{molecular transport of momentum}} \quad (6.11)$$

$$Nu \equiv \frac{h d}{k} = \frac{\text{convective transfer of heat}}{\text{molecular transport of heat}} \quad (6.12)$$

Sherwood, Reynolds and Nusselt numbers are functions of geometry, flow characteristics and fluid properties. In Figure 6.5, the Reynolds number for the adiabatic ($q_w = 0$) tubular flow of dissociated steam is presented as a function of temperature for a range of constant pressure. Since the Reynolds number declines as temperature increases, the transition from turbulent to laminar flow will occur at higher mass velocity at higher temperatures. The Sherwood and Nusselt numbers are presented in Chapter 7.

Theoretically, to solve the heat transfer problem in turbulent flow of dissociated steam in tubes requires the simultaneous solution of the equation for the conservation of mass, momentum and energy. An analytical solution of the heat transfer to a multi-component gas mixture of chemically reacting gases does not exist at this time, however, if it did, it would be very complex. Therefore, for engineering applications, solutions with semi-empirical in nature are quite acceptable. Some of the previous studies are presented in the following sections.

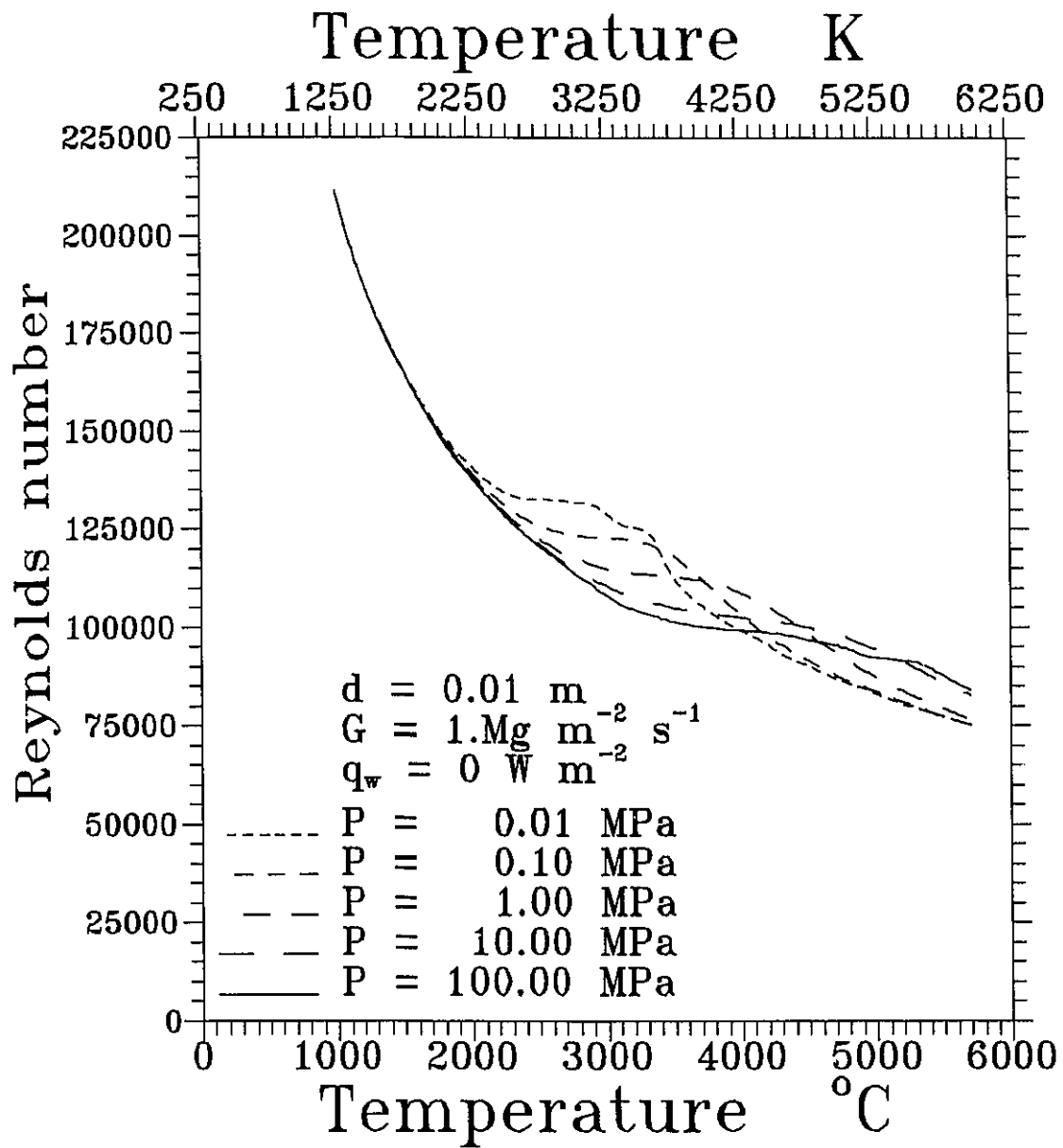


Figure 6.5: Reynolds number as a function of temperature for a range of constant pressure.

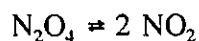
6.2 Previous studies

6.2.1 Heat transfer for dissociated gases

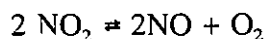
Only a few papers have dealt with heat transfer for dissociated gases. The general study of a flow with heat transfer to a chemically reacting fluid was dealt with in a number of papers by Callaghan and Mason (1964), Bromberg and Lipkis (1958), Hirschfelder (1957) and Altman and Wise (1956). A flow with heat transfer to a fluid with variable properties (due to temperature and/or chemical reactions) was analyzed by Petukhov and Popov (1963). While some works deal with specific fluids e.g. air, hydrogen (H_2) and nitrogen tetroxide (N_2O_4), there is no paper that examines heat transfer for dissociated steam.

Heat transfer in a flow along a flat plate of dissociated air at hypersonic flight speeds has been studied by Fay et al. (1957), Lees (1956), and recently by Borisov et al. (1986). Heat transfer for a turbulent flow of equilibrium dissociated hydrogen in a tube was analyzed theoretically by Petukhov and Popov (1964).

The heat transfer phenomena of reacting nitrogen tetroxide (N_2O_4) were the subject of study from 1965 on for a group of researchers from the Nuclear Energetics Institute of the Byelorussian SSR Academy of Sciences under the leadership of Nesterenko. In the West, heat transfer to N_2O_4 has been discussed by Furgason and Smith (1962), Irving and Smith (1961), Krieve and Mason (1961), Richardson et al. (1961), Schotte (1958), and Butler and Brokaw (1956). This gas dissociates in two stages at relatively low temperatures. The first stage (at atmospheric pressure from boiling point 22 to 150°C, or at pressure 98bar from 150 to 250°C) dissociation produces nitrogen dioxide (NO_2):



The second stage of dissociation (at atmospheric pressure from 150 to 900°C, or at 98 bar from 250 to 1450°C) is described by the chemical reaction:



Since this dissociation occurs at moderate temperatures where experiments are not very difficult to perform, many experiments have been performed with dissociating N_2O_4 .

From the quoted literature, two papers are closely applicable to the study of heat transfer to the flow of dissociated steam in tubes. These are several papers by Petukhov et al. and Nesterenko et al., and will be analyzed in the next section.

6.2.1.1 Petukhov et al.'s model

The papers by Petukhov and Popov (1963), Petukhov and Kirillov (1958), Petukhov (1970) and Petukhov et al. (1972) are derived from the same base, and different papers describe various improvements made on the basic model. Considering the influence of variable physical properties (due to temperature and/or chemical reactions), the authors derived an analytic expression for the Nusselt number of an incompressible turbulent fluid flow in tubes.

Assumptions and conditions under consideration are the following:

- 1 - Turbulent flow in a tube of an incompressible fluid with variable physical properties.
- 2 - Axially symmetric.
- 3 - Axial diffusions is negligible in comparison with in the radial direction.
- 4 - Negligible viscous dissipation.
- 5 - Low Mach number.
- 6 - Mass forces are insignificant compared to viscous and inertial forces.
- 7 - The flow is far from the tube inlet such that the mass velocity change along the tube axial direction x is small, i.e.,

$$\frac{\partial(\rho u_x)}{\partial x} \approx 0 \quad (6.13)$$

which imply that the radial component of the velocity is zero and pressure is constant over a cross section.

- 8 - Supplementary assumptions concerning the constant conditions over a cross section are

$$\frac{\partial H}{\partial x} = f_1(x) \quad \frac{\partial}{\partial x} (p + \rho u_x^2) = f_2(x) \quad (6.14)$$

- 9 - Effective properties are applied (all changes of fluid are included in properties).

The analytical expression for the Nusselt number for variable physical properties is

$$\frac{1}{Nu_w} = 2 \frac{Cp_w}{\langle Cp \rangle} \int_0^1 \frac{\left(\int_0^R \frac{\rho u_x}{\langle \rho u \rangle} R dR \right)^2}{\frac{k}{k_w} \frac{Cp_w}{Cp} \left(1 + \frac{\epsilon_q}{a} \right) R} dR \quad (6.15)$$

$$Nu_w = \frac{h d}{k_w} \quad (6.16)$$

$$\langle Cp \rangle = \frac{H_w - H_b}{T_w - T_b} = \frac{\int_{T_b}^{T_w} Cp \, dT}{T_w - T_b} \quad (6.17)$$

$$R = \frac{r}{r_w} \quad (6.18)$$

where:

Nu_w - Nusselt number evaluated at wall conditions at pipe cross section x ;

Cp_w - Heat capacity (effective properties) at the wall conditions (T_w) at cross section x ;

$\langle Cp \rangle$ - Mean integral heat capacity (effective properties) between fluid bulk temperature (T_b) and wall temperature (T_w);

$\rho u_x = G$ - Mass flow rate at local conditions at cross section x and radius r ;

$\langle \rho u \rangle = \langle G \rangle$ - Mean mass flow rate over pipe cross section;

k - Thermal conductivity (effective properties) at local conditions at cross section x and radius r ;

k_w - Thermal conductivity (effective properties) at wall conditions at section x ;

ϵ_q - Turbulent eddy thermal diffusivity;

a - Thermal diffusivity (effective properties) at local conditions at cross section x and radius r .

For constant physical properties (ρ , Cp and k), Equation (6.15) reduces to the Lyon integral

$$\frac{1}{Nu} = 2 \int_0^1 \frac{\left(\int_0^R \frac{u_x}{u} R \, dR \right)^2}{\left(1 + \frac{\epsilon_q}{a} \right) R} dR \quad (6.19)$$

Calculations were performed according to Equation (6.15), for constant physical properties, and the results are given by the interpolation formula

$$Nu_{CP} = Nu_b = \frac{\left(\frac{\xi}{8}\right) Re_b Pr_b}{k_1(\xi) + k_2(Pr_b) \sqrt{\frac{\xi}{8} (Pr_b^{2/3} - 1)}} \quad (6.20)$$

$$k_1(\xi) = 1 + 3.4 \xi \quad k_2(Pr) = 11.7 + \frac{1.8}{Pr^{1/3}}$$

$$10^4 < Re_b < 5 \cdot 10^6 \quad 0.5 < Pr_b < 2000$$

where ξ is the Darcy friction factor correlation by Filonenko (1954)

$$\xi = (1.82 \log Re_b - 1.64)^{-2} \quad 1 \cdot 10^4 < Re_b < 5 \cdot 10^6 \quad (6.21)$$

If $k_1(\xi)$ and $k_2(Pr_b)$ are considered to be constant and equal to $k_1 = 1.07$ and $k_2 = 12.7$, then Equation (6.20) becomes the form (quoted in many references) proposed by Petukhov and Kirillov (1958):

$$Nu_{CP} = Nu_b = \frac{\left(\frac{\xi}{8}\right) Re_b Pr_b}{1.07 + 12.7 \sqrt{\frac{\xi}{8} (Pr_b^{2/3} - 1)}} \quad (6.22)$$

$$10^4 < Re_b < 5 \cdot 10^6 \quad 0.5 < Pr_b < 2000$$

The more accurate expression for the constant-properties Nusselt number (k_l) has been obtained and presented by Petukhov et al. (1972)

$$Nu_{l,b,CP} = \frac{f}{2} Re_{l,b} Pr_{l,b} C^{-1}$$

$$f = \frac{\xi}{4} = \frac{0.0791}{Re_{l,b}^{0.25}} \quad 4 \cdot 10^3 \leq Re_{l,b} < 10^4 \quad f = \frac{\xi}{4} = \left[1.5808 \ln \left(\frac{Re_{l,b}}{8} \right) \right]^{-2} \quad 10^4 \leq Re_{l,b} \leq 5 \cdot 10^6$$

$$Re_{l,b} = \frac{G d}{\mu_{l,b}} \quad 4 \cdot 10^3 \leq Re_{l,b} \leq 5 \cdot 10^6 \quad Pr_{l,b} = \frac{Cp_{l,b} \mu_{l,b}}{k_{l,b}} \quad 0.5 \leq Pr_{l,b} \leq 10^6$$

$$C = 1.07 + \frac{900}{Re_{l,b}} - \frac{0.63}{1 + 10 Pr_{l,b}} + 12.7 \sqrt{\frac{f}{2} (Pr_{l,b}^{2/3} - 1)} \quad (6.23)$$

where f is the Fanning friction factor evaluated using correlations by Blasius (1913) and Filonenko (1954).

The constant properties model is valid under the following assumptions and conditions:

- The effective values of physical properties, heat capacity and thermal conductivity are used;
- The physical properties are evaluated at bulk temperature;
- The heat transfer coefficient is defined as in Equation (6.16);
- All the assumptions and conditions considered for the derivation of Equation (6.15);
- The fluid is in local chemical equilibrium (chemical reaction occurs instantaneously).

When comparing Equations (6.15) and (6.19) it is important to mention that the Nusselt number for variable physical properties is proportional to the following three ratios

$$\frac{Cp}{Cp_w} \quad \frac{\frac{k}{Cp}}{\frac{k_w}{Cp_w}} \quad \frac{\rho u}{\langle \rho u \rangle}$$

Since the heat capacity, thermal conductivity and density for gases vary with absolute temperature, the idea was to correlate temperature-dependent-property Nusselt number and Fanning friction factor, over constant-property Nusselt number and Fanning friction factor in gases, as the ratio of absolute wall temperature and bulk temperature:

$$\frac{Nu_{VP}}{Nu_{CP}} = \left(\frac{T_w}{T_b} \right)^n \quad \frac{f_{VP}}{f_{CP}} = \left(\frac{T_w}{T_b} \right)^m \quad (6.23)$$

The values of the exponents n and m were found empirically by comparing the analytical results with experimental data. The expressions for exponents n and m (for heated gases, air and hydrogen) from the paper by Petukhov and Popov (1963) are

$$n = -0.47 \quad m = -0.6 + \frac{3.3}{\sqrt{\eta_w}} \quad (6.24)$$

$$0.37 < \frac{T_w}{T_b} < 3.7 \quad 14 \cdot 10^3 < Re_w^* < 1 \cdot 10^6 \quad Re_w^* = Re_w \frac{\rho_w}{\rho_b}$$

$$\eta_w = Re_w^* \sqrt{\frac{\xi_w^*}{32}} \quad \xi_w^* = (1.82 \log Re_w^* - 1.64)^{-2}$$

Recommended expressions for the values of exponents for heated gases (air, hydrogen) by

Petukhov (1970) are

$$n = - \left[0.13 \ln \left(\frac{T_w}{T_b} \right) + 0.36 \right] \quad m = - 0.6 + 5.6 \left(Re_w^* \right)^{-0.38} \quad (6.25)$$

$$0.37 \leq \frac{T_w}{T_b} \leq 3.7 \quad 14 \cdot 10^3 \leq Re_w^* \leq 10^6$$

Finally, in the paper by Petukhov et al. (1972), the ratio of Nusselt numbers for variable and constant properties, with the assumption that dependence of properties on temperature is described by power functions, was compared with measured values (air, Ar, CO₂, N₂, NH₃) and recommended as

$$\frac{Nu_{VP}}{Nu_{CP}} = \left(\frac{\rho_w}{\rho_b} \right)^{0.53} \left(\frac{Cp_w}{Cp_b} \right)^{1/4} \left(\frac{k_w}{k_b} \right)^{1/3} \left(\frac{\mu_w}{\mu_b} \right)^{- \left[1.5 \log \left(\frac{T_w}{T_b} \right) \right]} \quad (6.26)$$

$$Re_b > 7 \cdot 10^3 \quad 1 \leq \frac{T_w}{T_b} \leq 4 \quad 0.006 < \frac{q_w}{G Cp_1 T_{b1}} < 0.007$$

where:

Cp₁ - heat capacity at a gas bulk temperature at the entrance;

T_{b1} - a gas bulk temperature at the entrance.

Applying Equations (6.26) and (6.23), predictions for heat transfer coefficients will be compared with the prediction method proposed in this work.

6.2.1.2 Nesterenko et al.'s model

The model presented by Nesterenko et al. (1967 a) and (1967 b) is a semi-empirical model, based on the mass and heat transfer analogy. The theoretical and experimental results obtained by study of heat transfer can be used in the application of mass transfer and vice versa. Hence, in this model, the same empirical correlation was used for the Sherwood and Nusselt numbers. The correlations proposed by M.A. Miheev and S.S. Kutateladze for forced convective turbulent flow in a tube were used:

$$Sh_{i,fr,b,eq} = 0.021 Re_b^{0.8} Sc_{i,fr,b,eq}^{0.43} \left(\frac{T_w}{T_b} \right)^{-0.55} \quad (6.27)$$

$$Nu_{fr,b} = 0.021 Re_b^{0.8} Pr_{fr,b}^{0.43} \left(\frac{T_w}{T_b} \right)^{-0.55} \quad (6.28)$$

Hence, the mass and heat transfer coefficients are

$$g_{l-m} = 0.021 \frac{D_{l-m}}{d} Re_b^{0.8} Sc_{l-m,b}^{0.43} \left(\frac{T_w}{T_b} \right)^{-0.55} \quad (6.29)$$

$$h_{fr} = 0.021 \frac{k_{fr,b}}{d} Re_b^{0.8} Pr_{fr,b}^{0.43} \left(\frac{T_w}{T_b} \right)^{-0.55} \quad (6.30)$$

The assumption is that heat transferred in chemically reacting gas flow with composition in equilibrium within each point of the flow is

$$q = q_{fr} + q_r \quad (6.31)$$

The second term is heat transferred in the gas mixture without chemical reaction, the so-called "frozen" gas mixture. The third term is the heat transferred due to the chemical reactions which occur in the gas mixture. Accordingly, the total or "effective" heat transfer coefficient can be written as a superposition of the "frozen" and reactive constituents:

$$h_{eff} = \frac{q}{T_w - T_b} = h_{fr} + h_r = h_{fr} + \sum_{j=1}^J \frac{Qp_j g_l (\rho_{l,w} - \rho_{l,b})}{a_{l,j} \tilde{M}_l (T_w - T_b)} \quad (6.32)$$

where:

h_{fr} - "frozen" heat transfer coefficient calculated by Equation (6.30) [=] W m⁻² K⁻¹;

j - chemical reaction in which product l appears only;

J - minimum number of chemical reactions such that one of the species l appears only in that chemical reaction j ;

Qp_j - heat effect of chemical reaction j [=] J;

g_l - mass transfer coefficient of l , Equation (6.29) [=] kg_l m⁻² s⁻¹ (kg_l m_m⁻³)⁻¹ = m s⁻¹;

$\rho_{l,w}, \rho_{l,b}$ - mass concentration (density) of the species l evaluated at the wall temperature (T_w) and at the bulk temperature (T_b) [=] kg_l m_m⁻³;

$\tilde{M}_l$ - molar mass of the species l [=] kg_l mol_l⁻¹;

$a_{l,j}$ - stoichiometric coefficient of the species l in chemical reaction j [=] mol_l;

T_w, T_b - wall and bulk fluid temperature [=] K.

The model is valid under the following assumptions and conditions:

- The frozen values for physical properties, heat capacity and thermal conductivity are used;
- The physical properties are evaluated at bulk temperature;
- The heat transfer coefficient is defined with temperature differences;
- Frozen Lewis number equals unity ($Le_{fr} = 1$);
- Flow is in local chemical equilibrium (chemical reactions occur instantaneously).

If the kinetics of a chemical reaction was considered (flow is in local non-equilibrium), Nesterenko et al. (1967 b) suggested using the Sherwood number of non-equilibrium flow as

$$Sh_{l,fr,b} = Sh_{l,fr,b,eq} Cr_l \quad (6.33)$$

$$Cr_l = \frac{J_l x}{G} = \frac{\text{mass velocity of component } l \text{ generated along } x}{\text{mass velocity of gas mixture}}$$

where:

Cr_l - Reaction number ($0 \leq Cr_l \leq 1$), a dimensionless criterion which characterizes the relation between the rate of appearance or disappearance of the species l along distance x , and the mass velocity of the mixture. When $Cr_l = 0$, there is a "frozen" state, i.e. no chemical reaction and when $Cr_l = 1$, the mixture is in chemical equilibrium;

J_l - rate of generation (appearance or disappearance) of the species l due to the kinetics of chemical reaction [=] $\text{kg m}^{-3} \text{s}^{-1}$, for N_2O_4 from papers by Nesterenko and Tverkovkin (1966 a) and (1966 b);

x - current axial coordinate [=] m;

G - mass velocity of gas mixture [=] $\text{kg m}^{-2} \text{s}^{-1}$.

Using the same approach, thermal calculations for an active zone of a nuclear reactor cooled with chemically reactive coolant N_2O_4 were performed. As reported by Nesterenko et al. (1968), the predicted values were in very good agreement with the experimental ones as presented in Figure 6.6.

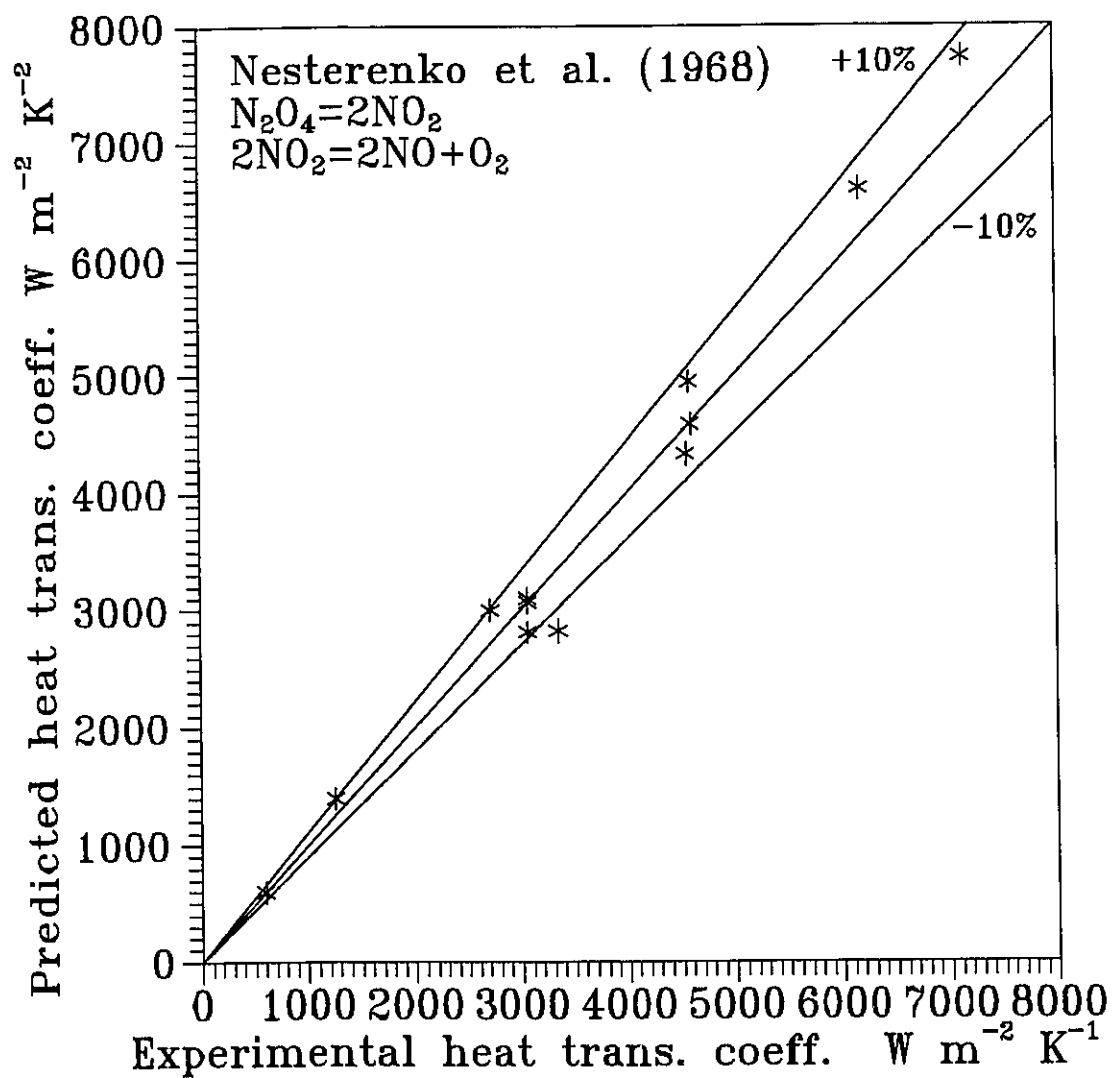


Figure 6.6: Comparison of experimental and predicted heat transfer coefficients, applying the model by Nesterenko et al. (1968), including the kinetics of chemical reaction.

6.3 Heat Transfer by Radiation for Dissociated Steam

Radiation heat transfer from the grey enclosure surface to the gas mixture volume is according Holman (1986)

$$q_{rad} = \epsilon_{eff} \sigma [a_{mix}(T_w) T_w^4 - \epsilon_{mix}(T_b) T_b^4] \quad (6.34)$$

$$\epsilon_{eff} = \frac{1 + \epsilon_w}{2} \quad \epsilon_w > 0.8 \quad (6.35)$$

$$\epsilon_{mix}(T_b) = \sum_{i=1}^6 \epsilon_i - \Delta\epsilon \quad (6.36)$$

$$a_{mix}(T_w) = \sum_{i=1}^6 a_i - \Delta a \quad (6.37)$$

where: ϵ_{eff} = effective emissivity of enclosure surface;

σ = Stefan-Boltzmann constant [=] $\text{W m}^{-2} \text{K}^{-4}$;

a_{mix} = gas mixture absorptance;

ϵ_{mix} = gas mixture emittance;

T_w = wall temperature [=] K;

T_b = bulk temperature [=] K;

a_i = gas absorptance;

ϵ_i = gas emittance.

Emissivity of water vapour $\epsilon_i(T_w)$ at high pressure conditions can be predicted using the method proposed by Cheng and Nguyen (1989).

Convective heat transfer is proportional to temperature difference - $(T_w - T_b)$, but radiative heat transfer is proportional to temperature difference to the fourth power - $(T_w^4 - T_b^4)$. Therefore, radiation heat transfer is very important in a high temperature environment such as the one involved in dissociation. The radiation exchange between a heat transfer surface and a gas layer depends on the character of the gas. While some gases absorb and emit radiation, others are essentially transparent. Atomic (H and O) and diatomic (H_2 , O_2 and HO) gases are transparent to radiation. Steam dissociation results in a six-component (H_2O , H_2 , O_2 , HO, H and O) gas mixture. Only water vapour (H_2O) is an absorbing/emitting component of the mixture. The emissivity of steam is a function of its partial pressure, gas layer thickness (mean beam length or characteristic dimension) and temperature.

$$\begin{aligned}\varepsilon(H_2O) &= f[p(H_2O), L, T] \quad L = d \\ p(H_2O) &= p_1 = y(H_2O) P = y_1 P\end{aligned}\tag{6.38}$$

The molar fraction of steam (y_1) decreases as a function of temperature (Figure 2.2), hence the partial pressure of steam (p_1) diminishes in the process of dissociation. Figure 6.7 demonstrates water vapour emissivity in a dissociating steam gas mixture for two mean beam lengths at constant total pressure from Holman (1986, Figure 8-35, pp.417), corrected for molar fraction. Eventually when steam becomes totally dissociated, it will become non-emissive because very little radiation occurs (products of dissociation - HO, H and O, are transparent to radiation). Convective heat transfer of steam have substantial increase at high temperature due to process of dissociation. As a consequence, at high temperature the radiative heat transfer of steam is of the smaller order of magnitude then convective heat transfer. The radiative heat transfer of steam at moderate temperature may be of the same order of magnitude then convective heat transfer, however, at high temperatures that is not the case. Thus, the radiative heat transfer of dissociated steam may be neglected at high temperatures. The inclusion of radiative heat transfer would render this work substantially more complex, hence, it is left for future consideration.

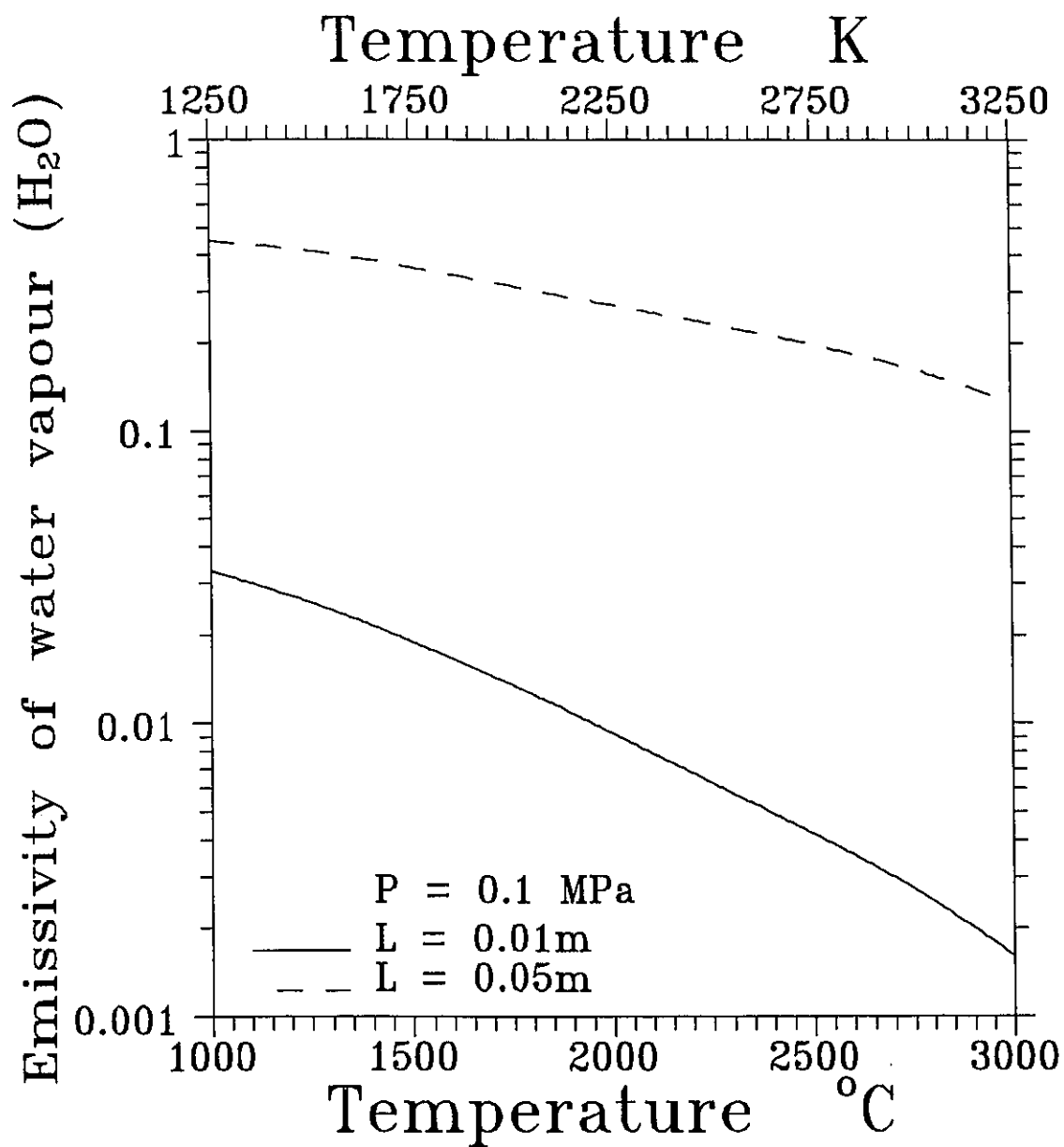


Figure 6.7: Water vapour (H_2O) emissivity at a constant total pressure of a dissociating steam gas mixture, for two mean beam lengths.

6.4 Effect of Dissociated Steam Compressibility on Heat Transfer

Heat transfer to water flow with constant heat flux in a tube may be divided into four regions:

- liquid-water flow;
- two-phase flow;
- superheated-steam flow;
- dissociated-steam flow.

The first and part of the second region can be considered as incompressible flow. However, for the remainder of the second region, and the third and fourth regions, compressibility is an important factor. Mach number is a measure of compressibility (density change) in a gas flow. The definition of Mach number is

$$Ma \equiv \frac{u}{a} \quad (6.39)$$

The Mach number is a function of pressure and temperature. Also, the mass velocity is defined as

$$G \equiv \frac{\dot{m}}{A} = \rho u = \frac{u}{v} \quad (6.40)$$

The flow velocity can be eliminated from the above two equations, and the Mach number can be written as

$$Ma \equiv \frac{G v}{a} \quad (6.41)$$

At constant pressure and temperature, the specific volume and local speed of sound are constant. Hence, the Mach number is proportional to mass velocity and vice versa:

$$G \equiv \frac{a}{v} Ma \quad (6.42)$$

From the gas dynamic analyses of Shapiro (1953) and Zucrow and Hoffman (1976) and (1977), it can be demonstrated that for gas flow with heat transfer (adiabatic flow) in a constant-area duct with heat addition the gas will reach the state of maximum entropy. The limiting state with maximum entropy is the state where the fluid velocity is equal to the local acoustic speed.

$$G = G_{\max} = G^* = \frac{a}{v} \quad \text{for } Ma = 1 \quad (6.43)$$

Such a flow is said to be operating with thermal choking. Addition of heat does not cause the gas at exit to alter the sonic condition beyond the choking condition but propagates a change in the upstream conditions. The mass velocity in the thermal choking condition ($Ma = 1$) is the maximal possible mass velocity (critical velocity). Consequently, upstream from the choking point (tube exit) since the mass flow rate ($\dot{m}$) is constant, velocity must adjust accordingly. Using data for sound velocity and the specific volume for dissociated steam tabulated by Vargaftik (1983), Figure 6.8 illustrates maximal mass velocity as a function of temperature at constant pressure. The maximal mass velocity is lower for lower pressure and declines as a function of temperature.

Comparing the typical range of the mass velocity required for cooling in industry ($0.1 \leq G \leq 7.5$ [=] $\text{Mg m}^{-2} \text{s}^{-1}$) with the maximal mass velocity from Figure 6.8, one notices that operation with maximum mass velocity ($7500 \text{kg m}^{-2} \text{s}^{-1}$) is possible only at higher pressures (10MPa). The prediction method for calculation of heat transfer to dissociated steam recommended in this work requires that the mass velocity at the tube exit conditions be lower than or at most equal to the critical value otherwise choking condition will occur.

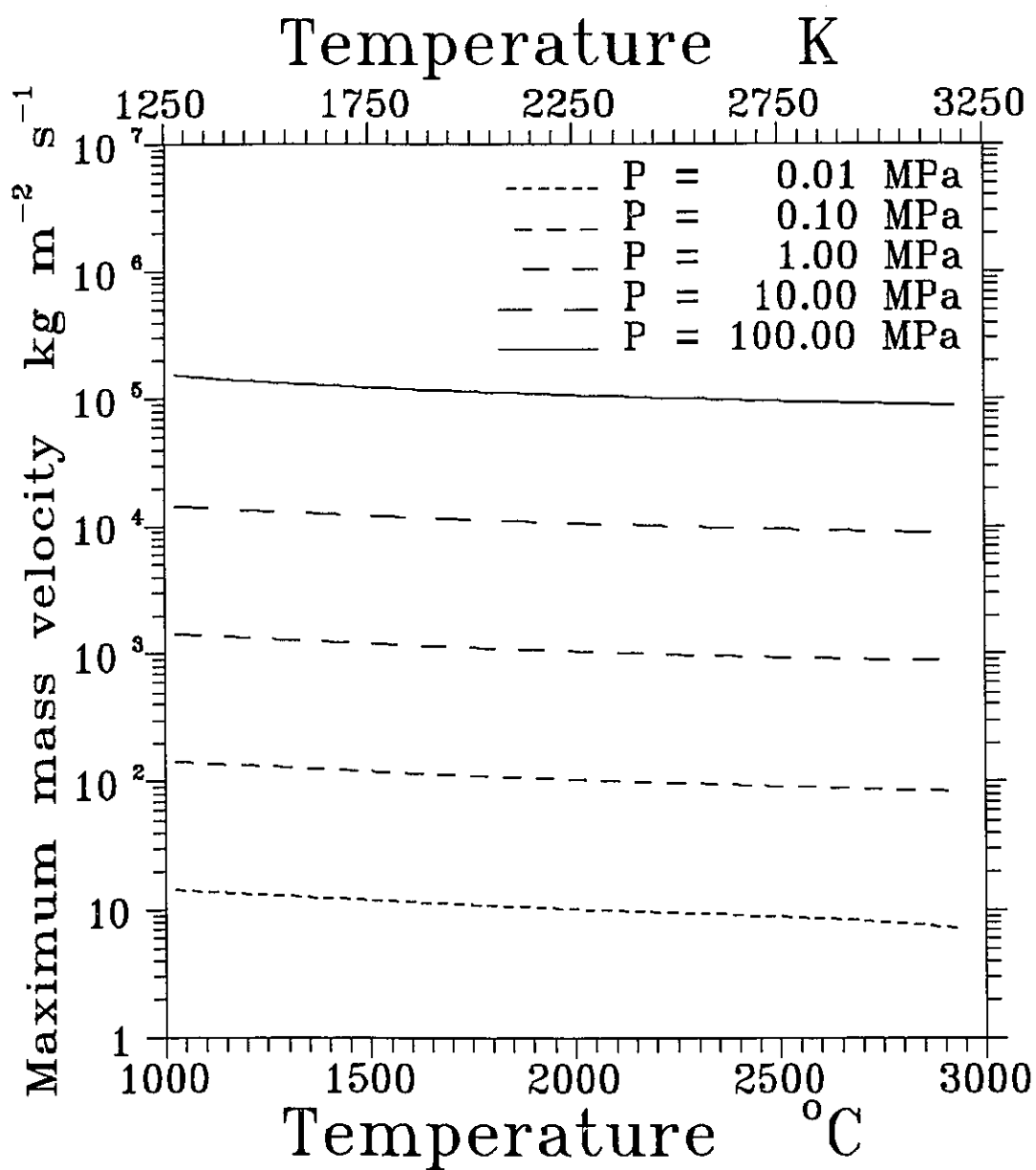


Figure 6.8: Maximal (critical) mass velocity as a function of temperature at constant pressure.

6.5 Summary

Studies of heat transfer to steam at high temperatures ($t > 1000^{\circ}\text{C}$) were not found in the literature, particularly for temperatures where dissociation occurs. An analytical solution of heat transfer for a laminar flow is very complex, and one for a turbulent flow even more so. Therefore, for engineering needs, solutions with semi-empirical relations are satisfactory. Unfortunately, even such solutions for heat transfer to dissociated steam at high temperatures are not available from the literature either. As a first approximation, the results obtained for other fluids treated in previous works may be used. The objective of this study is to apply, by analogy, the principles and experiences from previous works with N_2O_4 (a two or three-component gas mixture) to the heat transfer of dissociated steam (a six-component gas mixture).

Experimental data for heat transfer to steam found in the literature are for lower temperatures where dissociation does not occur. Therefore, it is the task of an experimenter to ratify the analytical results presented in this work.

Radiation and compressibility effects on heat transfer are analyzed briefly; however, due to complexity of these effects, this analysis is left for future consideration.

Chapter 7

Prediction Method of Heat Transfer for Dissociated Steam

7.1 Introduction

Based on the semi-empirical model by Nesterenko et al. (1967 a) for dissociated nitrogen tetroxide ($\text{N}_2\text{O}_4 \rightleftharpoons 2\text{NO}_2$, a two component gas mixture), a method was developed to determine the Nusselt number of a chemically reacting (dissociated) fluid flow. Derivation of the effective Nusselt number for a mixture of chemically reacting gases is presented in Appendix D. The method includes the effect of Lewis number (the former works assumed that Lewis number equals 1.0). The methods proposed in this work were applied to dissociated steam (a six-component gas mixture). The Gnielinski (1976) correlation is applied for evaluation of Nusselt number for a gas mixture without chemical reactions and Sherwood numbers for the components of steam dissociation. The Bhatti and Shah (1987) correlations are applied for evaluation of Fanning friction factors. The complete method for computation of the local heat transfer coefficient and of the wall temperature, for a turbulent tube flow of dissociated steam heated with constant heat flux at the wall, is presented in Appendix E. The High Temperature Steam Heat Transfer computer code (VASICA) was developed to predict heat transfer in a turbulent tube flow of steam. The listing of subroutines is presented in Appendix I. The Frozen Properties code listed in Appendix G is used for properties prediction. Predictions according to the proposed method are compared to the predictions of three typical correlations from the literature developed for low and moderate temperature conditions: Dittus and Boelter (1930), Petukhov et al. (1972) and Hadaller and Banerjee (1969). The look-up tables for heat transfer coefficients of high temperature dissociated steam in tube flow were generated for a typical range of values applicable in industry and are presented in Appendix M.

7.2 Prediction Method of Heat Transfer for Dissociated Steam

Steam at temperatures $<1500^{\circ}\text{C}$ is a pure one component gas. However, dissociated steam is a multi-component mixture of six chemically reacting gases. There are two different approaches for predictions of heat transfer for dissociated steam. First, dissociated steam could be treated as one homogenous fluid possessing the effective properties of a gas mixture. Practically, this means that properties of the mixture include all the effects of chemical reactions in this gas mixture. Second, dissociated steam can be treated as a gas mixture where the heat transfer of each component of the mixture is considered separately. The frozen properties of a gas mixture are applied; however, the effects of chemical reactions in the gas mixture on heat transfer are introduced with mass transfer. Although the first approach is easier to apply once the effective properties of gas mixture are determined, it has some negative aspects. Properties are usually evaluated with attached fixed conditions; these are the equilibrium state of gas mixture, constant pressure and temperature. The equilibrium state is a condition in which no change occurs in the system as long as its surroundings are not changed and represents the local maximal state for that system. Heat transfer to turbulent flow in a tube is a non-equilibrium transient process with an imbalance of pressure, composition, momentum and energy. If effective properties are applied with the heat transfer correlations (developed at low and moderate temperatures), the real phenomena of transitions in multi-component mixtures will be hidden. The improvement of such models can not be made because real phenomena are not shown. The second approach is more laborious, but describes the phenomena better and can be improved further.

Utilizing the first approach, any of the correlations for heat transfer from the literature listed in Chapter 5 can be applied simply using the effective properties for dissociated steam generated by the IAPS²⁰ and the UODH₂O property code.

Utilizing the second approach in this work, a new method was developed to predict heat transfer to dissociated steam. The method is based on the semi-empirical model by Nesterenko et al. (1967 a) for dissociated nitrogen tetroxide ($\text{N}_2\text{O}_4 \rightleftharpoons 2\text{NO}_2$, a two-component gas mixture).

²⁰ For temperatures $< 1000^{\circ}\text{C}$, properties are evaluated using the IAPS (International Association for the Properties of Steam) Property code listed by Haar et al. (1984) and subroutines developed for prediction of viscosity and thermal conductivity according to IAPS Formulations 1985 published by Sengers and Watson (1986).

Derivation of the effective Nusselt number for a mixture of chemically reacting gases is presented in Appendix D. It has the following form

$$Nu_{eff,b} = Nu_{fr,b} + \sum_{j=1}^4 \frac{Qp_j}{a_{l,j} \tilde{C}p_{fr,b}} \frac{Sh_{l,fr,b}}{Le_{l,fr,b}} \frac{(y_{l,w} - y_{l,b})}{(t_w - t_b)} \quad (7.1)$$

$j=1 \quad l=1$
 $j=2,3,4 \quad l=j+2=4,5,6$

The first right-hand term represents the Nusselt number of the mixture of chemically non-reacting gases (frozen state). The second term is the sum of the effects of the chemical reactions occurring in the gas mixture. It represents the contribution to heat transfer due to mass transfer of the species in the gas mixture and consists of three ratios. The first ratio is of the heat effect of each chemical reaction, to the heat capacity of a gas mixture without chemical reaction (frozen).

The second ratio (with the form of a Nusselt number), Equation (7.2²¹), is the ratio of heat transferred by mass convection of component l , to the thermal diffusion rate for the gas mixture. The term in parentheses is volumetric heat capacity of a gas mixture. The term in square brackets represents the heat transfer coefficient of component l (heat transferred by mass convection).

$$\frac{Sh_{l,fr,b}}{Le_{l,fr,b}} = \frac{[(Cp_{fr,b} \rho_{m,b}) g_l] d}{k_{fr,b}} = \frac{\text{transfer of heat by convection of mass}}{\text{thermal diffusion rate}} \quad (7.2)$$

Finally, the third ratio is a ratio of the composition gradient in radial direction, to the temperature gradient in radial direction. The composition of the dissociated steam may be determined using the Fraction code listed in Appendix F. Since the values of gradients are not known in advance, an iterative process of computation is required. The properties used are either the properties of pure gas components, or the frozen properties of a gas mixture generated by the Frozen Properties code listed in Appendix G.

The analogy between heat transfer and mass transfer permits the use of the same correlation for the Nusselt and Sherwood numbers. In the heat transfer correlation for the Nusselt number, the Sherwood number replaces the Nusselt number and the Schmidt number replaces the Prandtl number for mass transfer correlation.

²¹ The results in this work are obtained for the Sherwood number at equilibrium state, the Reaction number $Cr_1 = 1$.

The correlation by Gnielinski (1976) having the overall best accord with the experimental data, as recommended by Kakaç (1987), was used in this work.

$$Nu_{fr,b,VP} = \frac{\frac{f}{2} (Re_b - 1000) Pr_{fr,b}}{1 + 12.7 \left(\frac{f}{2}\right)^{0.5} (Pr_{fr,b}^{2/3} - 1) \left(\frac{T_b}{T_w}\right)^{0.45}} \quad (7.3)$$

$$2300 < Re_b < 1 \cdot 10^6 \quad 0.5 < Pr_b < 2000$$

This correlation is a modified version of the correlations by Petukhov et al. (1958), (1963) and (1972) and extends the lower limit of Reynolds numbers from 10^4 to 2300. The effect of variable properties for a large temperature difference is considered with the ratio of bulk and wall gas temperatures. The Fanning friction factor correlation for a smooth circular channel, correlations by Bhatti and Shah (1986), Equation (7.4), (explicit formula recommended by Kakaç et al. (1987) for practical computations), was used in this work.

$$f = A + B Re_b^C$$

$$\begin{array}{llll} Re_b < 2100 & A = 0 & B = 16. & C = -1. \\ 2100 \leq Re_b \leq 4000 & A = 0.54 \cdot 10^{-2} & B = 0.23 \cdot 10^{-7} & C = 1.5 \\ 4000 < Re_b < 1 \cdot 10^7 & A = 0.128 \cdot 10^{-2} & B = 0.1143 & C = -0.311 \end{array} \quad (7.4)$$

A set of computer subroutines, the High Temperature Steam Heat Transfer code (VASICA), was developed for predicting the wall temperature and local heat transfer coefficients for a turbulent tube flow of dissociated steam with constant wall heat flux. The listing of VASICA code is presented in Appendix I. The following few paragraphs will address the analysis of some VASICA code predictions.

The heat effect of chemical reactions is pressure and temperature dependent. Figure 7.1 presents heat effect (Qp_j/a_{ij}) of chemical reactions j per mol_l of component l (H_2O , HO , H and O) as a function of temperature at constant pressure. Four chemical reactions ($j = 1$ to 4) occurring in steam dissociation are chosen in such a way that the component l appears only in chemical reaction j . The second reaction (generating or degrading HO) definitely has a smaller heat effect than the others. As mentioned in Chapter 6, the heat effect of liquid water vaporization is in the vicinity of 40 kJ mol^{-1} ($\sim 2250 \text{ kJ kg}^{-1}$), which is much less than the heat absorbed by dissociating reactions. The heat capacity of a gas mixture without chemical reaction (frozen) is also pressure and temperature dependent and was presented in Figure 4.3.

The temperature dependence of Sherwood and Lewis numbers at constant pressure is presented in Figures 7.2 and 6.4 for all components of dissociated steam. Lewis numbers differ

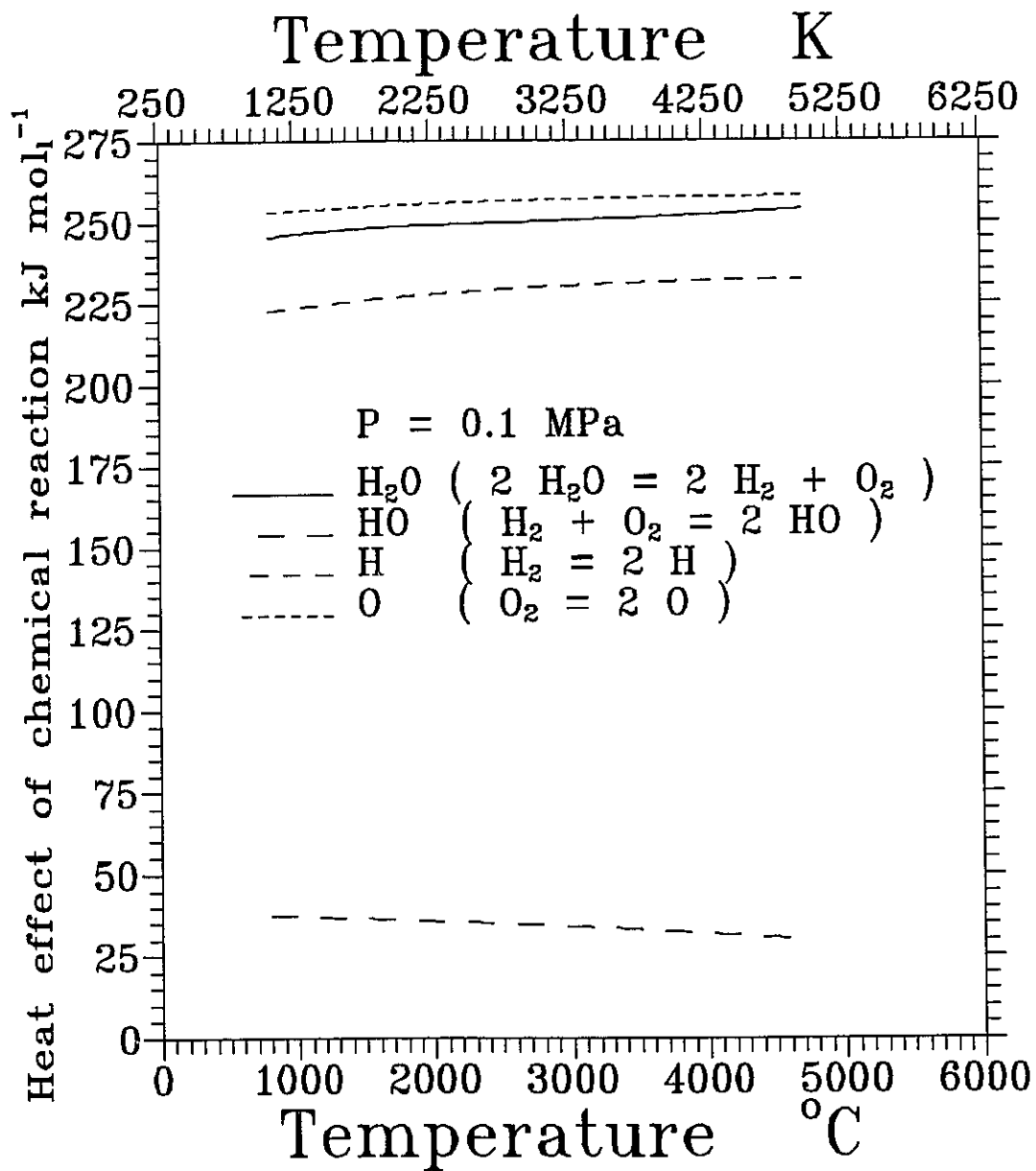


Figure 7.1: Heat effect of chemical reactions (during steam dissociation) as a function of temperature at constant pressure.

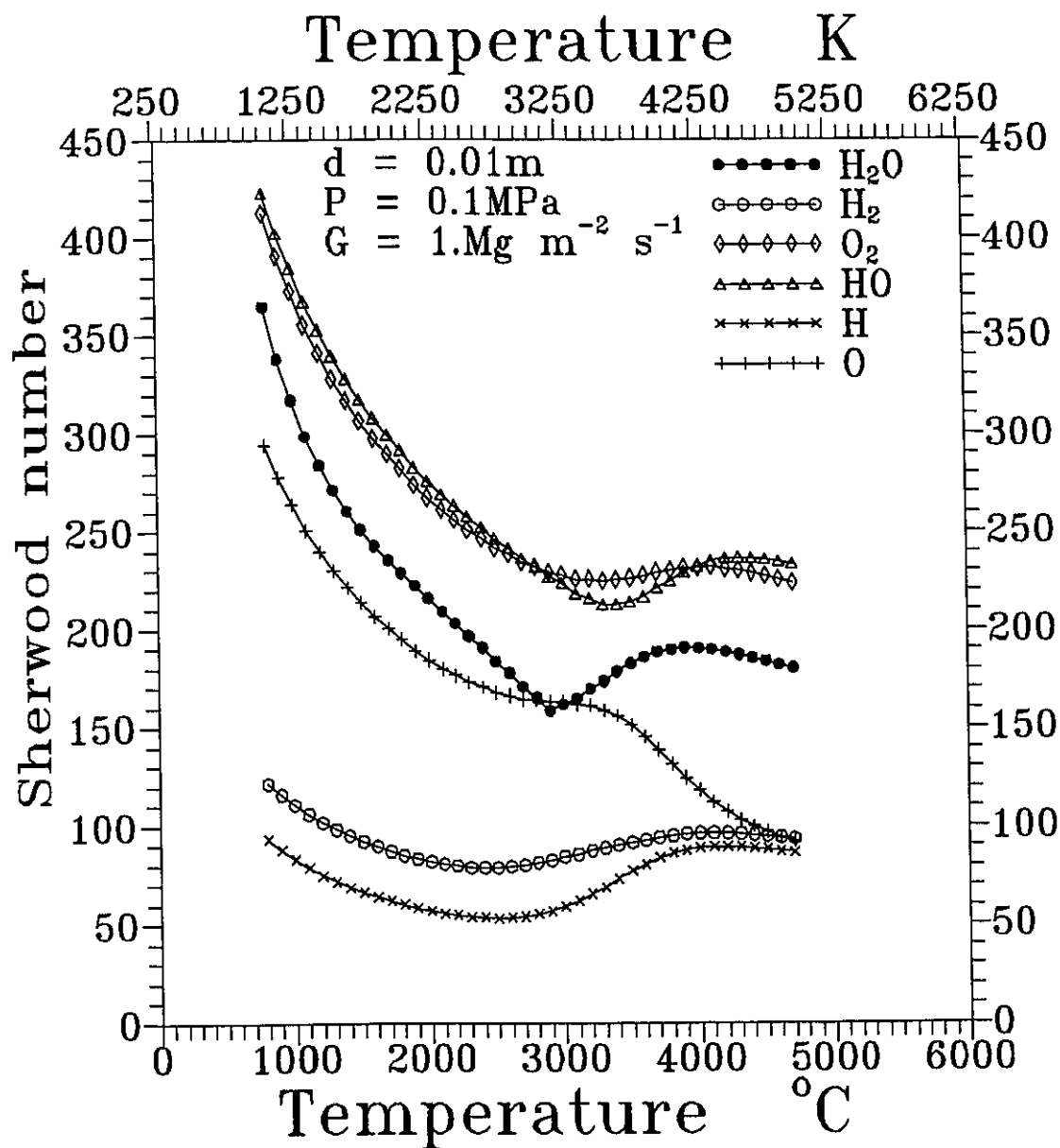


Figure 7.2: Sherwood number for components of steam dissociation as a function of temperature.

from the value 1.0, and therefore are justified to be included in the computation. The typical values of parameters applicable in industry ($P=0.1\text{MPa}$, $G=1000.\text{kg m}^{-2}\text{ s}^{-1}$, $Q_w=1.\text{MW}$, $d=0.01\text{m}$) are chosen as constants for example computations. Figure (7.3²²) illustrates the temperature dependence of the Nusselt number for each of five superposition terms in Equation (7.1). The first observation is that at temperatures less 3100°C , the chemical reaction generates hydroxyl (HO), hence some heat is absorbed ($\text{Nu}_{\text{HO}}>0$). At higher temperatures, hydroxyl deteriorates, hence a portion of heat is rejected ($\text{Nu}_{\text{HO}}<0$). Hydroxyl dissociates to atomic hydrogen and oxygen ($\text{HO} \rightleftharpoons \text{H} + \text{O}$). Consequently, hydroxyl has a negligible effect on heat transfer. The chemical reaction which degrades water vapour (steam) has the strongest effect on the Nusselt number. Its effect is almost twice that of the breakdown of hydrogen, and almost threefold more than that of the breakdown of oxygen.

Superposition of each of the five terms forms the effective Nusselt number for a dissociated steam mixture. Figure 7.4 shows the formation of effective Nusselt number and Figure 7.5 presents the effective heat transfer coefficient (sum of the five terms) as a function of temperature. The maximum heat transfer coefficient, which includes effects of all chemical reactions ($\sim 3300^\circ\text{C}$), is up to 11 times higher than the appropriate heat transfer coefficient without chemical reactions (frozen). Once the effective Nusselt number is determined, the temperature difference between the bulk and wall temperature may be evaluated²³:

$$T_w - T_b = \frac{(q_w - q_{rad}) d}{k_{fr,b} \text{Nu}_{eff,b,VP}} \quad (7.5)$$

Prediction of the temperature difference between wall and bulk temperature is presented in Figure 7.6. The process of dissociation commences at the curvature breaking point.

The look-up tables for heat transfer coefficients of high temperature dissociated steam in a tube flow were generated for a typical range of values applicable in industry. These tables are presented in Appendix M.

²² Deviation from a smooth curve at 1600°C is due to the calculation of compositions. Molar fractions of dissociation have very small values and hence there is a reduced accuracy for the subtraction results in Equation (7.1).

²³ Radiative heat transfer is not considered in this work; it is assumed that the values in parentheses are constant.

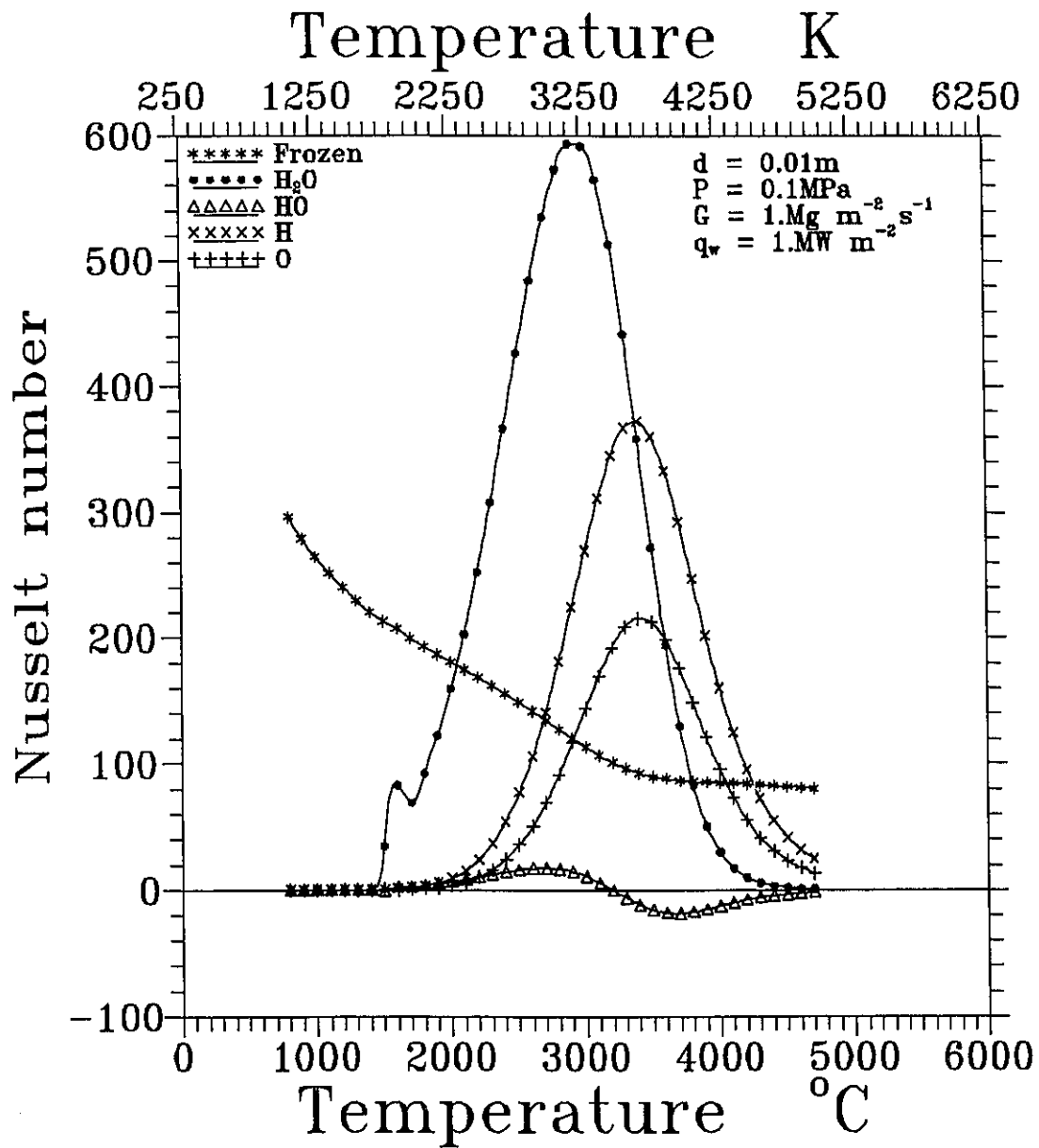


Figure 7.3: Change of Nusselt number as a function of temperature for each of the five terms that the proposed effective Nusselt number consists of.

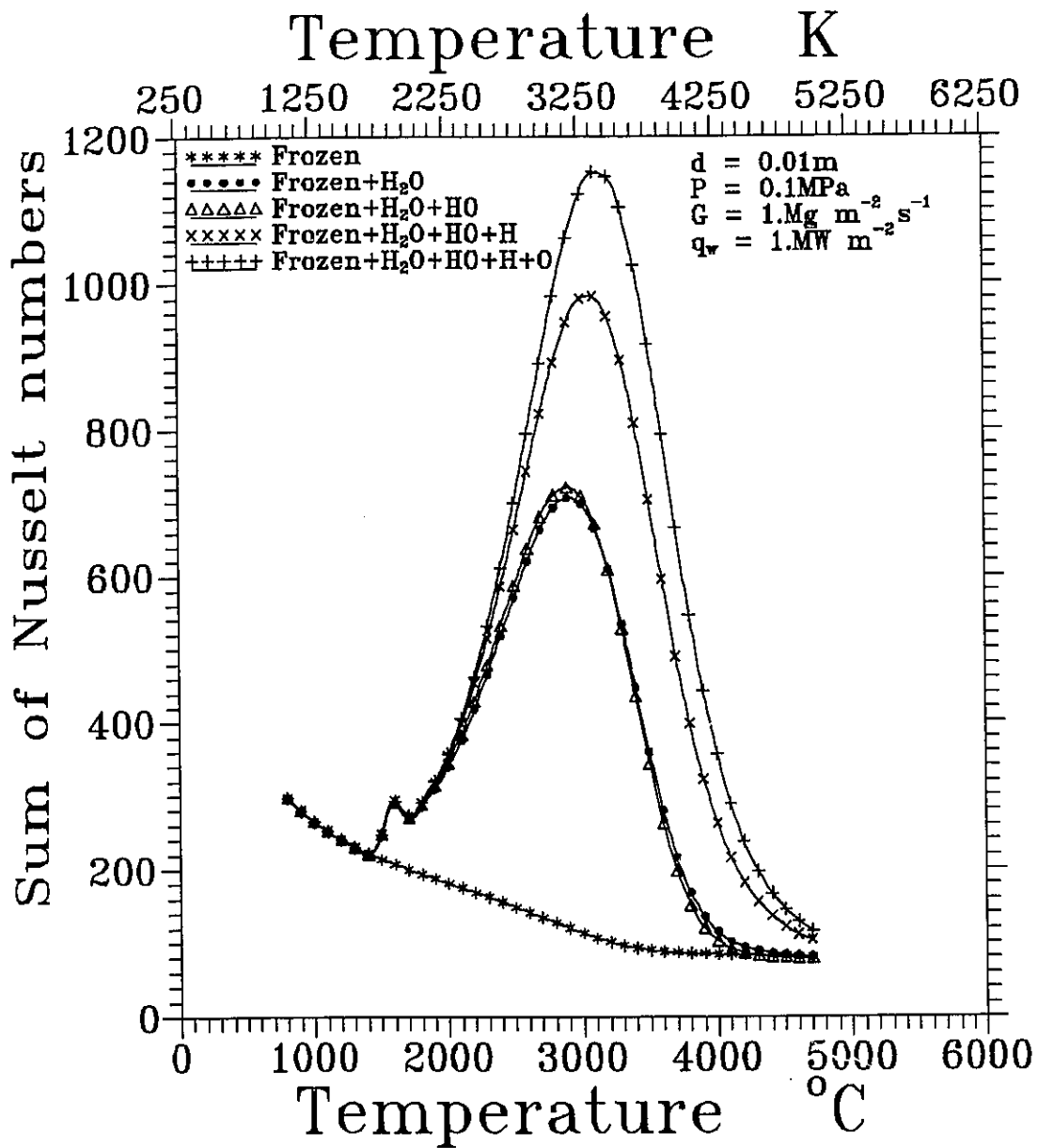


Figure 7.4: Formation of the effective Nusselt number (sum of the five terms) as a function of temperature.

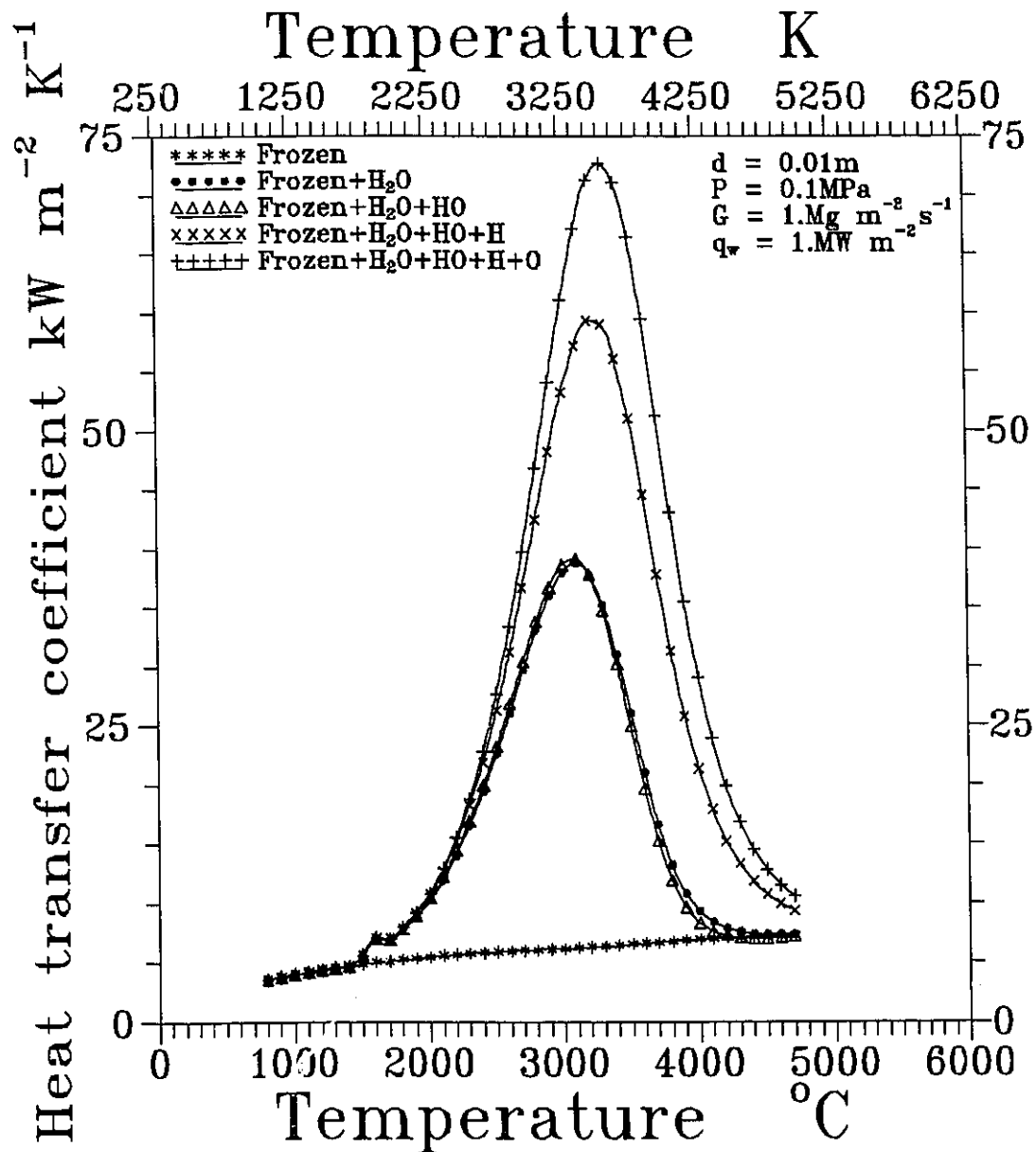


Figure 7.5: Formation of the effective heat transfer coefficients (sum of the five terms) as a function of temperature.

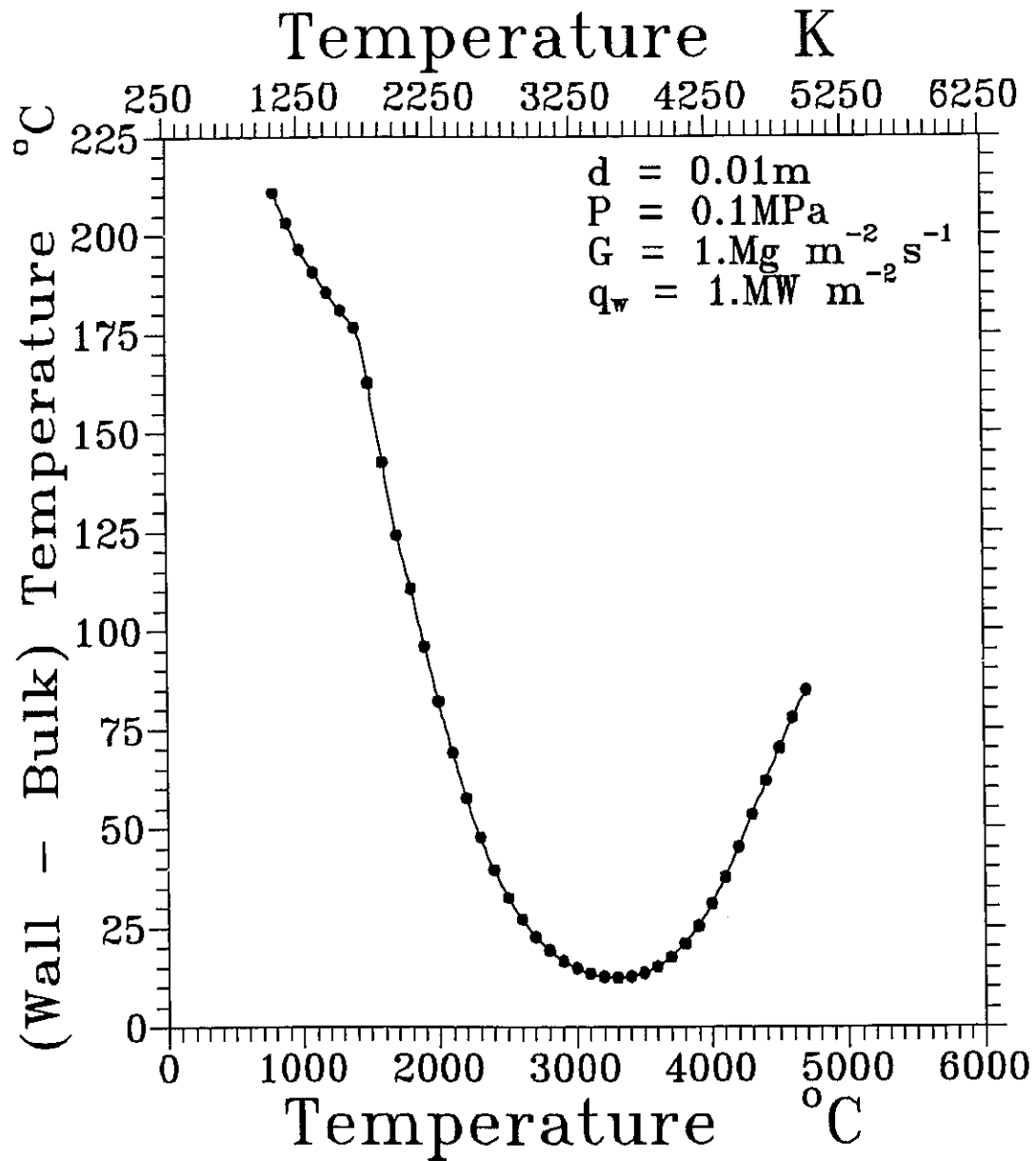


Figure 7.6: Difference between wall and bulk temperature during turbulent flow of dissociated steam in a tube as a function of bulk temperature at certain constant flow conditions.

7.3 Comparison of the Results

Comparison of the results predicted using the proposed model with measurements of steam heat transfer coefficients in turbulent flow at high temperature would bring legitimacy of the model. Unfortunately, the measurements of steam heat transfer coefficients are not available at high temperatures. The results predicted using the proposed model are compared with predictions using first approach. Three characteristic correlations are used for comparison. They are the Dittus and Boelter (1930), Petukhov et al. (1972) and Hadaller and Banerjee (1969) correlations. These correlations were derived for low and moderate temperature conditions. The first correlation is an empirical classical correlation by Dittus and Boelter (1930). It is one of the earliest developed correlations, and has a very simple form. It is consequently very popular. It was developed for heating a fluids.

$$Nu_{eff,b} = 0.024 \left(\frac{G d}{\mu_b} \right)^{0.8} \left(\frac{Cp_b \mu_b}{k_b} \right)^{0.4} \quad (7.6)$$

$$2.5 \cdot 10^3 < Re_b < 124 \cdot 10^3$$

$$0.7 < Pr_b < 120$$

Fluid properties are evaluated at bulk temperature, regardless of fact that properties are variable from bulk to wall temperature, especially for a large temperature difference.

The second correlation, by Petukhov et al. (1972), was derived from a theoretical base. In the paper by Petukhov and Popov (1963), a theoretical expression for the Nusselt number was derived. The theoretical calculations were performed in the range of Reynolds and Prandtl numbers, then these results were expressed by an interpolation equation. A more accurate expression for this interpolation equation has been obtained by Petukhov et al. (1972) and (1986). This equation was quoted by Kakaç et al. (1987) as the correlation which agrees with the most reliable experimental data.

$$Nu_{CP} = Nu_{eff,b} = \frac{f}{2} Re_b Pr_b C^{-1}$$

$$Re_b = \frac{G d}{\mu_b} \quad 4 \cdot 10^3 \leq Re_b \leq 5 \cdot 10^6 \quad Pr_b = \frac{Cp_b \mu_b}{k_b} \quad 0.5 \leq Pr_b \leq 1 \cdot 10^6 \quad (7.7)$$

$$C = 1.07 + \frac{900}{Re_b} - \frac{0.63}{1+10 Pr_b} + 12.7 \sqrt{\frac{f}{2}} (Pr_b^{2/3} - 1)$$

$$f = \frac{0.0791}{Re_b^{0.25}} \quad 4 \cdot 10^3 \leq Re_b < 1 \cdot 10^4$$

$$f = \left[3.64 \log \left(\frac{Re_b}{8} \right) \right]^{-2} \quad 1 \cdot 10^4 \leq Re_b \leq 5 \cdot 10^6$$
(7.8)

The Nusselt number in the above equation is evaluated for constant properties at bulk temperature. The effect of variable properties is accounted for by using a correction factor.

$$\frac{Nu_{vp}}{Nu_{cp}} = \left(\frac{\rho_w}{\rho_b} \right)^{0.53} \left(\frac{k_w}{k_b} \right)^{1/3} \left(\frac{Cp_w}{Cp_b} \right)^{1/4} \left(\frac{\mu_w}{\mu_b} \right)^{-1.5 \log_{10} \left(\frac{T_w}{T_b} \right)}$$

$$Re_b > 7 \cdot 10^3 \quad 1 \leq \frac{T_w}{T_b} \leq 4 \quad 0.006 < \frac{q_w}{\bar{\rho}_w Cp_{ent} T_{b,ent}} < 0.007$$
(7.9)

The last correlation, by Hadaller and Banerjee (1969), is a superheated-steam heat-transfer correlation developed with experimental data ($t_w < 685^\circ\text{C}$) from several sources for steam flow in a tube. The original equation has a thermal entrance correction factor but for the fully developed flow the equation quoted by Groeneveld et al. (1989) is in the following form:

$$Nu_f = 0.008348 Re_f^{0.8774} Pr_f^{0.6112}$$

$$60 \cdot 10^3 < Re_f < 600 \cdot 10^3$$
(7.10)

Properties are evaluated at the reference temperature - film temperature, an arithmetic average of fluid bulk and wall temperatures, to include the effect of variable properties.

$$t_f = t_w + c (t_b - t_w) \quad c = 0.5 < 1.0$$
(7.11)

A comparison of predictions from correlations in the literature using effective properties (IAPS and UODH2O code) and the new proposed method (Equation 7.1) is presented in Figure 7.7. The three correlations which used effective properties predicted higher heat transfer coefficients than the proposed method does. This was to be expected since the properties were evaluated at equilibrium state, which represents ideal diffusion and instantaneous chemical reactions, at constant pressure and temperature. The Dittus and Boelter (1930) correlation does not account for variable properties since it uses constant properties evaluated at bulk temperature. The Petukhov et al. (1972) correlation has a variable properties correction coefficient, yet the dependency of properties is described by power functions which may be of a different nature for dissociated gases. The evaluation of constant properties at film temperature for the Hadaller and Banerjee (1969) correlation may be more realistic, but the choice of constant c is arbitrary.

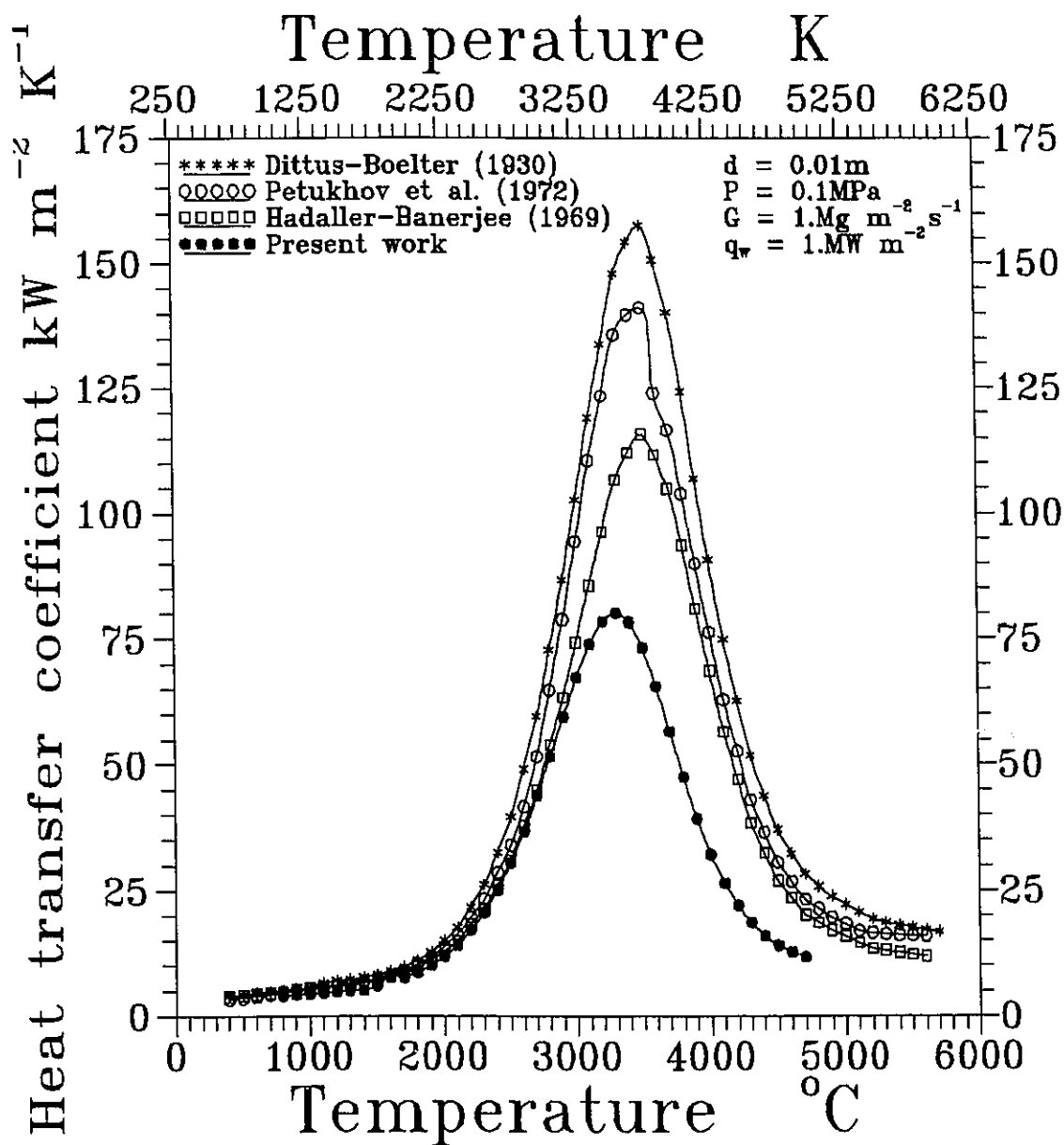


Figure 7.7: Comparison of predictions from three sources and the present work, for heat transfer coefficients in high temperature steam during turbulent tube flow.

It seems that the closer a fluid's temperature is to real temperatures, the smaller are the prediction results. The proposed method includes the effect of variable properties and furthermore, it considers the diffusion of species through the gas mixture. The results of the proposed method turn out to be lower than other predictions. The three correlations from the literature employ effective properties which are evaluated at equilibrium state - the local maximum possible state. However, heat transfer is a transient process leading to equilibrium. The proposed method employs properties evaluated as an ideal gas mixture, and the mass transfer contribution to heat transfer.

The results of predictions for temperature difference (between bulk and wall temperature) from the above sources and the new proposed method are shown in Figure 7.8²⁴. Within a bulk temperature range up to 3400°C, the predictions of temperature difference (between wall and bulk temperature) from all sources appear to be almost identical. However, though the values of predicted heat transfer coefficients (Figure 7.7) of some correlations are almost twice as large as the proposed method, the predictions of wall temperatures are within 3%, as shown in Figure 7.9.

²⁴ The curvature breaking points at temperature 1000°C are due to the change in properties evaluation from the IAPS code to the UODH2O code.

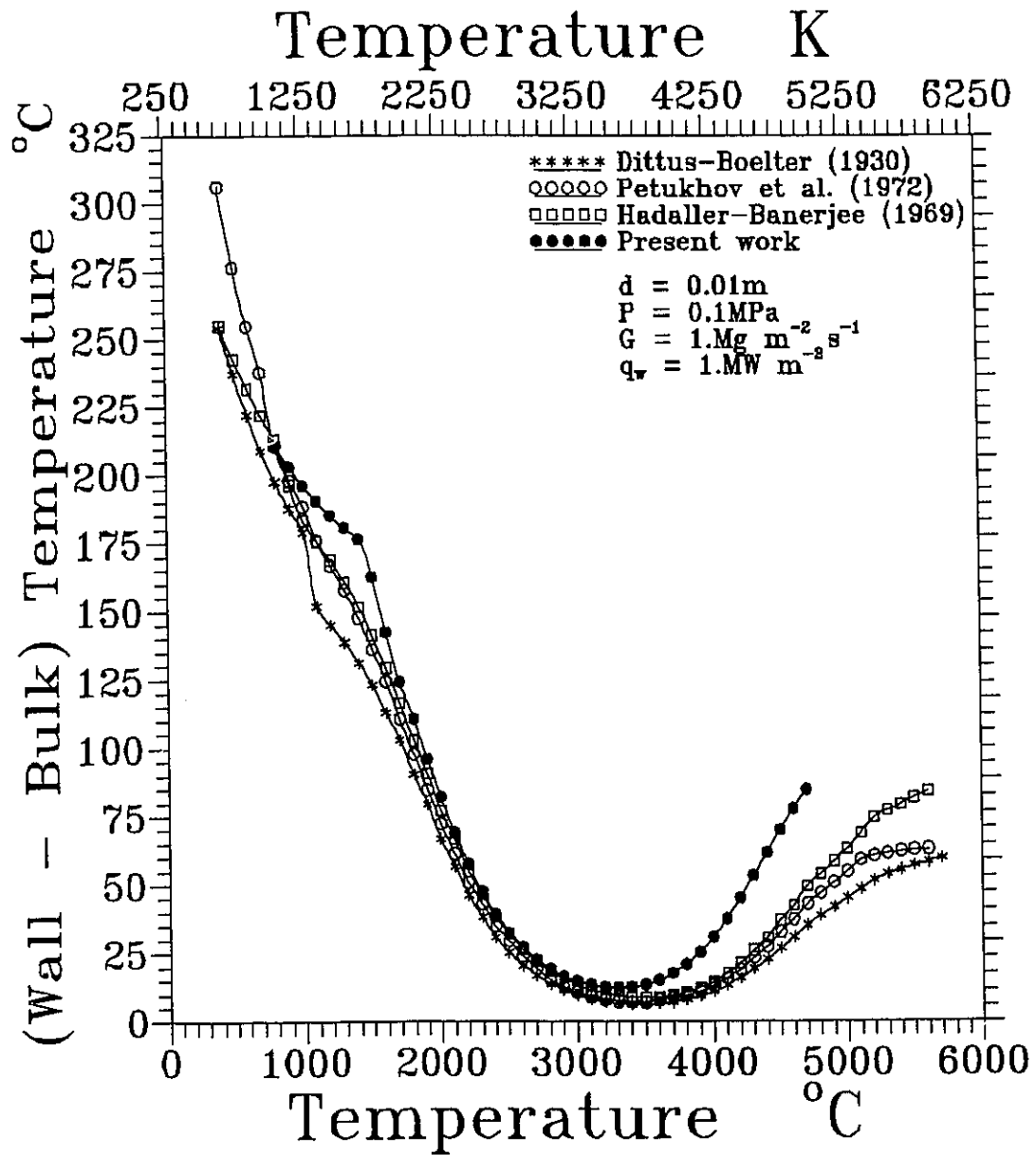


Figure 7.8: Difference between wall and bulk temperature during turbulent flow of dissociated steam in a tube as a function of bulk temperature at constant flow conditions.

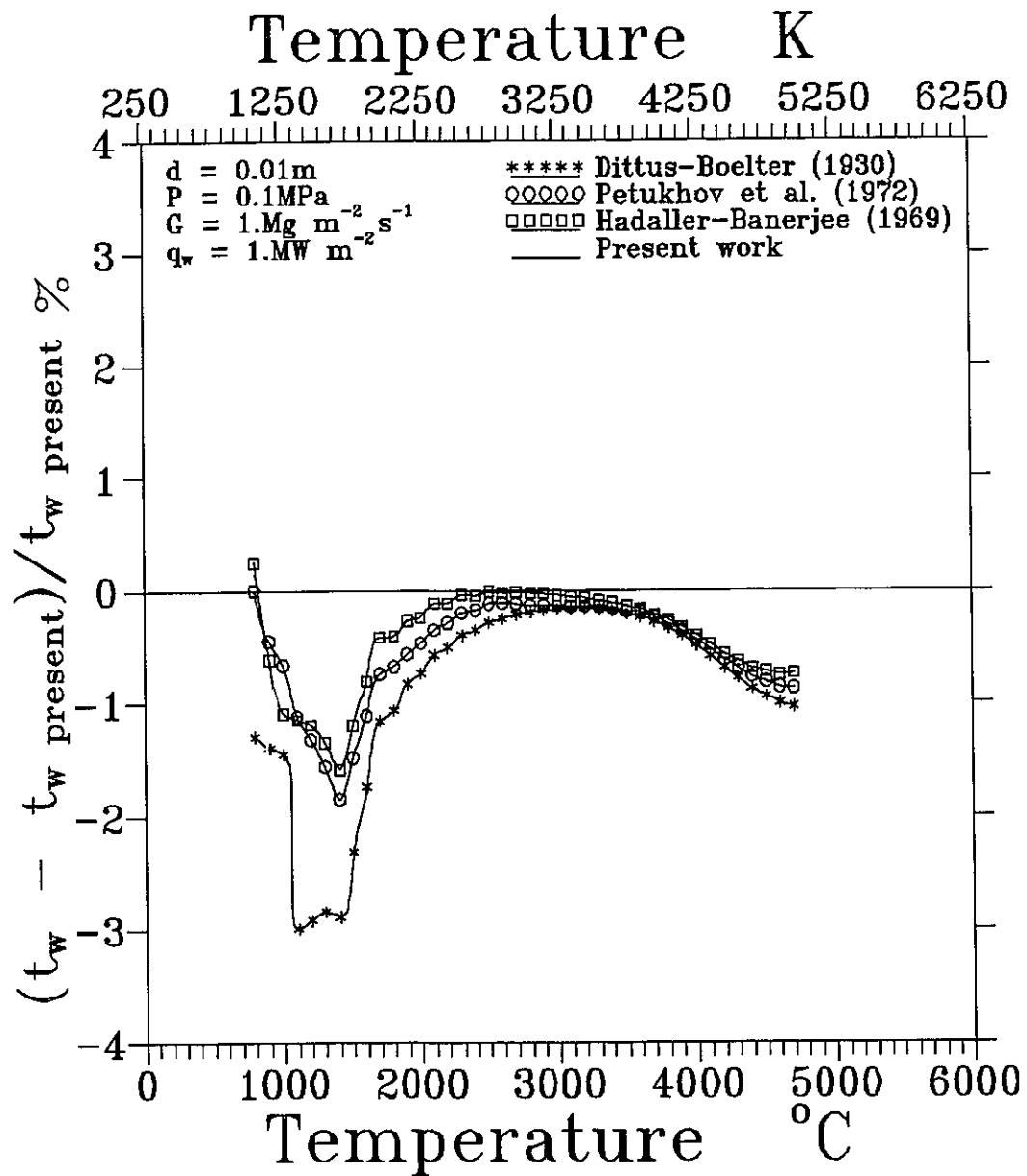


Figure 7.9: Comparison of the wall temperature predictions with predictions from the present work.

Chapter 8

Conclusion and Discussion

This work is divided into two sections. The first section is concerned with the properties of steam at high temperature. The second section is concerned with the phenomena of heat transfer for dissociated steam.

Properties of steam were, until now, calculated in industry using the ASME steam tables (valid up to 800°C). A number of computer codes have been developed to generate properties values at a desired pressure and temperature. In cases when the values of properties were needed for the temperature beyond the upper limit of steam tables, a general practice was to extrapolate properties to the higher temperature region. Predictions of heat transfer, required for the Loss-of-Coolant-Accident (LOCA) calculations in water-cooled nuclear reactors, require the knowledge of properties at very high temperatures (up to the tube melting point). As was shown in the calculation of heat transfer using values of properties obtained by extrapolation, ASME steam tables lead to the conclusion that heat transfer decreases at high temperature, and eventually becomes zero. Therefore, heat transfer calculations for the range over 1500°C must include consideration of steam dissociation, and this requires the consideration of the properties of multi-component chemically reactive mixtures.

First, a set of computer subroutines was developed - the Fraction code, for generating the composition (molar fractions) of a dissociating steam and gas mixture for a given pressure and temperature. Second, steam properties may be evaluated for an ideal gas mixture which includes no effects of chemical reactions - frozen state, or for a non-ideal solution at equilibrium state which includes maximal effects of chemical reactions - effective properties at equilibrium state. A set of computer subroutines was developed - the Frozen Properties code, for evaluating dissociated steam frozen properties for a given pressure and temperature. Finally, the recommended effective properties are the properties presented by Vargaftik (1983) using the

prediction method of Kesselman and Blank (1968 i). A computer code, UODH2O, was developed using a look-up table and interpolation technique to generate effective properties at a wide range of pressure and temperature. The computer codes, i.e. the Fraction code, the Frozen Properties code and the UODH2O code, are simple, accurate and easy to use with a mainframe or PC. They may be used alone or as subroutines of other programs. The results of sample computations, for a range of pressures and temperatures, using the codes, are presented in various tables and figures.

There are two different approaches in predicting of heat transfer for dissociated steam. First, dissociated steam can be treated as one homogeneous fluid using the effective properties of a gas mixture which include all effects of chemical reactions. Any of the correlations for heat transfer from the literature may be applied using effective properties. Second, dissociated steam can be treated as a gas mixture. The new proposed superposition method is based on the concept that total heat transfer is the sum of heat transferred to chemically-non-reacting gases and heat transferred due to chemical reactions in the gas mixture. The first term represents convective heat transfer of a gas mixture using frozen properties. The second term is the sum of the chemical reactions effects, and represents the contribution to heat transfer due to mass transfer of the species in the gas mixture. A computer code - the High Temperature Steam Heat Transfer code (VASICA), was developed for computing according to the new proposed method. The results of some sample computations, for a range of parameters applicable in industry, are presented as a look-up table and figures.

In current engineering practice, one is ready to assume that in a high temperature region convective heat transfer can be ignored relative to radiative heat transfer. Bearing in mind that atomic and diatomic gases are transparent for radiation, dissociating steam contains only molecular H_2O as an absorbing component. Emissivity of steam is a declining function of its partial pressure and temperature. The partial pressure of steam is reduced in the process of dissociation. Eventually, totally dissociated steam will become non-emissive, i.e. very little radiation occurs (products of dissociation are transparent to radiation in this temperature range). As a consequence, at high temperature the radiative heat transfer of steam is of the smaller order of magnitude than convective heat transfer. The radiative heat transfer of steam at moderate temperature may be of the same order of magnitude than convective heat transfer, however, at high temperatures that is not the case. Thus, the radiative heat transfer of dissociated steam may be neglected at high temperatures.

The liquid water flow at the tube entrance can transform into a sonic ($Ma = 1$) flow of a dissociated gas (steam) mixture at the tube exit. The critical mass velocity (maximum possible)

is lower for lower pressures and declines as a function of temperature. The prediction method recommended in this work for calculating heat transfer for dissociated steam requires that the mass velocity at the tube exit must be lower than or at most equal to the critical value.

Recommendations for further work to improve the prediction of heat transfer for dissociated steam are:

- to search for more accurate data for frozen thermal conductivity. Due to shortage of data, less accurate values of frozen thermal conductivity based on the predictions by Svehla (1964) were employed in this work.
- to consider the kinetics of chemical reactions with the introduction of the Reaction number ($0 \leq Cr_i \leq 1$). The results in this work are obtained for equilibrium state only, i.e. the Reaction number $Cr_i = 1$.
- to consider radiative heat transfer.

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Appendix A

Method for Calculating Molar Fraction of Dissociated Steam as a Mixture of Chemically Reacting Gases

The mole fraction of the species in the mixture at pressure P and temperature T can be generated using the principle for chemical equilibrium condition - the minimum of free energy.

$$(\Delta G)_{P,T} = 0 \quad (\text{A-1})$$

The definition of thermodynamic quantity of Gibbs free energy (or Gibbs function, G) can be found in classical textbooks of chemical thermodynamics as

$$\begin{aligned} G &= H - T S \\ \Delta G &= \Delta H - T \Delta S \end{aligned} \quad (\text{A-2})$$

Depending on the details of developing the above equation, three different methods were utilized, i.e. the element-potential method, the method of minimizing free energy and the equilibrium-constant method.

The element-potential method, introduced to the combustion community by Reynolds (1986), is not a new method; rather, it was neglected. The method was revived by Reynolds (1986), who developed the new interactive computer program STANJAN (named after STANford university and JANAF thermochemical tables). The program calculates the mole fractions of a mixture of arbitrarily chosen components without identifying the set of chemical reactions which may take place in the mixture. The STANJAN program as an interactive communication gives the option of forming the desired mixture from a list of the components which are contained in its data files. Should some of the components of a wanted mixture be missing, it is necessary to add data for that component from JANAF tables following instructions given by the program. Independence from the set of chemical reactions is the element-potential method's great

Appendix A

advantage over the equilibrium-constant method.

The concept of the method of minimizing free energy was developed in the last century by Gibbs. Based on the work by White et al. (1958) the mathematical procedures were developed by Zeleznik and Sanford (1968 a), and into a computer program by Sanford and McBride (1971). The method of determining the composition of the gas mixture in equilibrium consists in solving the system of n equations (one for each species of the mixture)

$$\ln p_i = [(-G^\circ)_i + \sum_{j=1}^m a_{ij} \lambda_j] \frac{1}{RT} \quad (\text{A-3})$$

$$p_i = y_i P \quad i = 1, \dots, n$$

where $(-G^\circ)_i$ is the free energy of species i at standard state $P = 0.1\text{MPa}$ and $T = 0\text{K}$; a_{ij} are the number of gram-atoms of the j^{th} element in the i^{th} species (stoichiometric coefficient) and λ_j are Lagrangian multipliers.

The equilibrium-constant method is based on the definition of pressure equilibrium constants

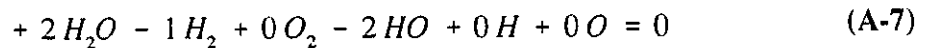
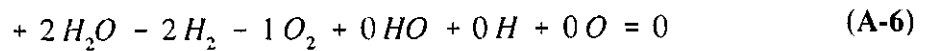
$$Kp_j(T) = \prod_{i=1}^n (p_i^{a_{ij}}) \quad (\text{A-4})$$

$$j=1, \dots, k$$

for each of the j chosen chemical reactions as shown in Equation (A-4). For a total number of species $n = 6$ (H_2O , H_2 , O_2 , HO , H and O) and two type of atoms (H , O) the minimum required number of independent chemical reactions which will describe the system is $k = 6 - 2 = 4$. It can be written in the balanced form as proposed by Brokaw (1960) as:

$$\sum_{j=1}^4 \sum_{i=1}^6 a_{ij} Y_i = 0 \quad (\text{A-5})$$

From a number of possible reactions between water vapour and its decomposition products, the following four most probable chemical reactions are chosen, according to Rybakov (1963). The choice is based on the highest heat of the reaction $([\Delta\tilde{H}]^\circ)_j$.



Appendix A

$$+ 0 H_2O + 1 H_2 + 0 O_2 + 0 HO - 2 H + 0 O = 0 \quad (\text{A-8})$$

$$+ 0 H_2O + 0 H_2 + 1 O_2 + 0 HO + 0 H - 2 O = 0 \quad (\text{A-9})$$

Then, the equilibrium constants can be written as

$$Kp_1 = \frac{y_1^2}{P^2 y_2^2 y_3} \quad (\text{A-10})$$

$$Kp_2 = \frac{y_1^2}{P^2 y_2 y_4^2} \quad (\text{A-11})$$

$$Kp_3 = \frac{y_2}{P y_5^2} \quad (\text{A-12})$$

$$Kp_4 = \frac{y_3}{P y_6^2} \quad (\text{A-13})$$

Dalton's law of partial pressure (one of the three following forms) gives an addition relation

$$P = \sum_{i=1}^6 p_i \quad , \quad p_i = y_i P \quad \text{and} \quad \sum_{i=1}^6 y_i = 1 \quad . \quad (\text{A-14})$$

Finally, from the law of conservation of mass, the initial condition, that the total number of hydrogen atoms is twice that of oxygen in non-dissociated water vapour, must also be obeyed in dissociated water vapour:

$$\frac{2y_1 + 2y_2 + y_4 + y_5}{y_1 + 2y_3 + y_4 + y_6} = 2 \quad (\text{A-15})$$

On the other hand, the pressure equilibrium constant, Kp_j , of a gas mixture for reaction, j , can be formed according to Straub and Maidhof (1987 a) by three different methods. Two possible thermodynamical approaches to calculate the equilibrium constant are suggested by Lutz (1955) and Schmidt (1960) and a third approach, from statistical thermodynamics, is by Ihara (1977).

Appendix A

In the first approach, Lutz (1955), the equilibrium constant can be calculated as

$$\ln Kp_j = \frac{1}{R} (a_{ij} \tilde{S}_i^o - \frac{J_i^*}{T}) \quad (\text{A-16})$$

where a_{ij} are the stoichiometric coefficients, $\tilde{S}_i^o$ are the temperature dependent part of the molar entropies and J_i^* are the reaction enthalpies of the components. In the second approach, Schmidt (1960), the equilibrium constant can be expressed as

$$\ln Kp_j = -\frac{1}{RT} [I_{oj} + v_i (G - J_{oj})] \quad (\text{A-17})$$

where I_{oj} and J_{oj} are the reaction enthalpy and the enthalpy at $T = 0\text{K}$.

Finally, from the statistical thermodynamic approach by Ihara (1977) and (1979), one can determine the equilibrium constant, using an approximation for the complete partition functions for the standard states at unit pressure. It can be shown that

$$\ln Kp_j = -\frac{\Delta E_{oj}}{RT} + \sum_{i=1}^4 a_{ij} \ln Qp_i \quad (\text{A-18})$$

where ΔE_{oj} is the zero point energy change calculated from the zero point energy of the species in the reaction j referring to their standard states and Q_{pi} is the total partition function of the species i . The zero point energy change for a chemical reaction is the enthalpy change for the chemical reaction j at standard state $T = 0\text{K}$, $P = 0.1\text{MPa}$ calculated with enthalpies of formation for products and reactants of that chemical reaction:

$$\Delta \tilde{E}_j^o = ([\Delta \tilde{H}]^o)_j = \sum_{i=1}^n a_{ij} ([\Delta_f \tilde{H}]^o)_i \quad (\text{A-19})$$

The values of $([\Delta_f \tilde{H}]^o)_i$ for the pure species, given in Table A-1, are the standard state enthalpies of formation at $T = 0\text{K}$ and $P = 0.1\text{MPa}$ found in the thermochemical table JANAF by Chase et al. (1985). In Equations (A-18) and (A-19), the chemical reaction balancing coefficients (a_{ij}) are from Equations (A-6) to (A-9), and are defined as positive for products and negative for reactants.

By convention, the JANAF tables are designed such that elements are in their most stable form; thus their formation enthalpies are equal to zero. The negative value of the formation enthalpy for water signifies that forming one mole of water requires less energy than hydrogen

Appendix A

and oxygen contained in their elemental state. Conversely, a positive value of formation enthalpy implies that forming these components requires more energy than their constituent elements hold in the elemental state.

Table A-1 The molar mass and the enthalpy of formation for components of water vapour dissociation at temperatures $T = 0\text{K}$ and $T = 298.15\text{K}$ (25°C), and pressure $P = 0.1\text{MPa}$, by Chase et al. (1985).

i	Symbol	$\tilde{M}_i$	$([\Delta_f \tilde{H}]^\circ)_i$	$([\Delta_f \tilde{H}]^\circ_{298.15})_i$
		$\text{kg}_i \text{ kmol}_i^{-1}$	kJ mol_i^{-1}	kJ mol_i^{-1}
1	H_2O	18.01528	-238.921	-241.826
2	H_2	2.01588	0.0	0.0
3	O_2	31.99880	0.0	0.0
4	HO	17.00734	38.390	38.987
5	H	1.00794	216.035	217.999
6	O	15.99940	246.790	249.173

Thus, the enthalpy changes at $T = 0\text{K}$ for the chosen chemical reactions are

$$([\Delta \tilde{H}]^\circ)_1 = -2 (-238.921) + 2 \cdot 0.0 + 1 \cdot 0.0 = +477.842 \text{ kJ mol}^{-1} \quad (\text{A- 20})$$

$$([\Delta \tilde{H}]^\circ)_2 = -2 (-238.921) + 1 \cdot 0.0 + 2 \cdot 38.390 = +554.622 \text{ kJ mol}^{-1} \quad (\text{A- 21})$$

$$([\Delta \tilde{H}]^\circ)_3 = -1 \cdot 0.0 + 2 \cdot 216.035 = +432.070 \text{ kJ mol}^{-1} \quad (\text{A- 22})$$

$$([\Delta \tilde{H}]^\circ)_4 = -1 \cdot 0.0 + 2 \cdot 246.790 = +493.580 \text{ kJ mol}^{-1} \quad (\text{A- 23})$$

Appendix A

The positive sign of the enthalpy change for the above the chemical reactions indicates an endothermic* process, a chemical reaction which is accompanied by the absorption of heat energy from the surroundings. Conversely, a chemical reaction where heat is evolved is said to be exothermic**. Considering the number of moles and the molar mass of the reactants, the enthalpy changes for chemical reactions per mass of the reactants are

$$([\Delta H]_o)_1 = \frac{([\Delta \tilde{H}]_o)_1}{2 \tilde{M}_1} = \frac{477.842}{2 \cdot 18.01528} = 13.262 \text{ MJ kg}^{-1} \quad (\text{A- 24})$$

$$([\Delta H]_o)_2 = \frac{([\Delta \tilde{H}]_o)_2}{2 \tilde{M}_1} = \frac{554.622}{2 \cdot 18.01528} = 15.393 \text{ MJ kg}^{-1} \quad (\text{A- 25})$$

$$([\Delta H]_o)_3 = \frac{([\Delta \tilde{H}]_o)_3}{\tilde{M}_2} = \frac{432.071}{2.01588} = 214.334 \text{ MJ kg}^{-1} \quad (\text{A- 26})$$

$$([\Delta H]_o)_4 = \frac{([\Delta \tilde{H}]_o)_4}{\tilde{M}_3} = \frac{493.579}{31.9988} = 15.424 \text{ MJ kg}^{-1} \quad (\text{A- 27})$$

The logarithms of the approximated total partition functions for the six components of dissociated water vapour given by Ihara (1977) are

$$\begin{aligned} \ln Q_{p_1} = & -\ln \left[1 - \exp \left(-\frac{5262}{T} \right) \right] - \ln \left[1 - \exp \left(-\frac{2294}{T} \right) \right] - \ln \left[1 - \exp \left(-\frac{5404}{T} \right) \right] \\ & + 4 \ln(T) - 4.1164 - \ln(P) \end{aligned} \quad (\text{A- 28})$$

* "endo", latin for in.

** "exo", latin for out.

Appendix A

$$\begin{aligned} \ln Q_{p_2} = & \ln \left[\frac{T}{682.6} + \frac{1}{24} + \frac{0.711}{T} + \frac{104}{T^2} + \left(\frac{T}{227.53} + 0.875 + \frac{87.458}{T} + \frac{6136.3}{T^2} \right) \exp\left(-\frac{171}{T}\right) \right] \\ & + \ln \left\{ \left[1 - \exp\left(-\frac{6338}{T}\right) \right]^{-1} + \left(\frac{360.65}{T} \right) \exp\left(-\frac{6338}{T}\right) \left[1 - \exp\left(-\frac{6338}{T}\right) \right]^{-3} \right\} \\ & + 2.5 \ln(T) - 2.6133 - \ln(P) \end{aligned} \quad (\text{A- 29})$$

$$\begin{aligned} \ln Q_{p_3} = & - \ln \left[1 - \exp\left(-\frac{2239}{T}\right) \right] + \ln \left[3 + 2 \exp\left(-\frac{11340}{T}\right) + \exp\left(-\frac{18878}{T}\right) \right] \\ & + 3.5 \ln(T) + 0.114 - \ln(P) \end{aligned} \quad (\text{A- 30})$$

$$\begin{aligned} \ln Q_{p_4} = & \ln \left(\frac{T}{26.638} + \frac{1}{3} + \frac{1.776}{T} \right) - \ln \left[1 - \exp\left(-\frac{5136}{T}\right) \right] + \ln \left[1 + \exp\left(-\frac{201}{T}\right) \right] \\ & + 2.5 \ln(T) + 1.2787 - \ln(P) \end{aligned} \quad (\text{A- 31})$$

$$\ln Q_{p_5} = 2.5 \ln(T) - 2.9604 - \ln(P) \quad (\text{A- 32})$$

$$\begin{aligned} \ln Q_{p_6} = & \ln \left[5 + 3 \exp\left(-\frac{228}{T}\right) + \exp\left(-\frac{326}{T}\right) + 5 \exp\left(-\frac{22830}{T}\right) \right] \\ & + 2.5 \ln(T) + 0.4939 - \ln(P) \end{aligned} \quad (\text{A- 33})$$

with temperature T (in K) and pressure P (in atmospheres).

Substituting values of the formation enthalpies for chemical reactions from Equations (A-20) to (A-23), the values of the universal gas constant and values of the partition functions,

Appendix A

Equation (A-18) becomes

$$\ln K_{p_1} = -\frac{57.471546}{T} - 2 \ln Q_{p_1} + 2 \ln Q_{p_2} + 1 \ln Q_{p_3} \quad (\text{A- 34})$$

$$\ln K_{p_2} = -\frac{66.706116}{T} - 2 \ln Q_{p_1} + 1 \ln Q_{p_2} + 2 \ln Q_{p_4} \quad (\text{A- 35})$$

$$\ln K_{p_3} = -\frac{51.966405}{T} - 1 \ln Q_{p_2} + 2 \ln Q_{p_5} \quad (\text{A- 36})$$

$$\ln K_{p_4} = -\frac{59.364404}{T} - 1 \ln Q_{p_3} + 2 \ln Q_{p_6} \quad (\text{A- 37})$$

Equations (A-34) to (A-37) are functions of temperature and pressure only. For given temperature and pressure values, the equilibrium constants for the chosen chemical reactions can be calculated. After substituting these values of the equilibrium constants for the left-hand side of Equations (A-10) to (A-13), and with Equations (A-14) and (A-15), we obtain a system of the six equations with the six unknowns, i.e. molar fractions (y_i , $i = 1, 6$) of the products at equilibrium state of water vapour dissociation. The molar fractions from these six equations can be obtained by solving this system of equations using one of the numerical methods (for example the Newton-Raphson method).

The set of computer subroutines known as the Fraction code has been developed for generating the mole fraction of the mixture. A listing of the subroutines is presented in Appendix F.

The composition of a gas mixture can be presented as a fraction (molar y_i or mass fraction ω_i) or a concentration (molar C_i or mass concentration ρ_i). Relationships between them are presented in Table A-2.

Appendix A

Table A-2 **Multiplying factors for conversion between molar fractions, mass fractions, molar concentrations and mass concentrations**

Conversion from $\rightarrow$ to $\downarrow$		Fraction		Concentration	
		y_i	ω_i	C_i	ρ_i
		$\text{mol}_i \text{ mol}_m^{-1}$	$\text{kg}_i \text{ kg}_m^{-1}$	$\text{mol}_i \text{ m}_m^{-3}$	$\text{kg}_i \text{ m}_m^{-3}$
y_i	$\text{mol}_i \text{ mol}_m^{-1}$	1	$\tilde{M}_m \tilde{M}_i^{-1}$	$\tilde{M}_m \rho_m^{-1}$	$\tilde{M}_m (\rho_m \tilde{M}_i)^{-1}$
ω_i	$\text{kg}_i \text{ kg}_m^{-1}$	$\tilde{M}_i \tilde{M}_m^{-1}$	1	$\tilde{M}_i \rho_m^{-1}$	ρ_m^{-1}
C_i	$\text{mol}_i \text{ m}_m^{-3}$	$\rho_m \tilde{M}_m^{-1}$	$\rho_m \tilde{M}_i^{-1}$	1	$\tilde{M}_i^{-1}$
ρ_i	$\text{kg}_i \text{ m}_m^{-3}$	$\rho_m \tilde{M}_i \tilde{M}_m^{-1}$	ρ_m	$\tilde{M}_i$	1

Appendix B

Method for Calculating Steam Properties as a Mixture of Chemically Non-Reacting Gases (Frozen)

Molar mass

Molecular mass of the n component mixture is

$$\tilde{M}_m = \sum_{i=1}^n y_i \tilde{M}_i \quad (\text{B-1})$$

where

$\tilde{M}_m$ - molecular mass of the mixture [=] $\text{kg}_m \text{ kmol}_m^{-1}$

n - number of components in the mixture

y_i - molar fraction of component i [=] $\text{kmol}_i \text{ kmol}_m^{-1}$

$\tilde{M}_i$ - molecular mass of the component i [=] $\text{kg}_i \text{ kmol}_i^{-1}$

Enthalpy

Enthalpy of the frozen gas mixture is

$$\tilde{H}_{fr} = \sum_{i=1}^n y_i \tilde{H}_i + k_H \quad (\text{B-2})$$

where:

$\tilde{H}_i$ - enthalpy of component i [=] J kmol_i^{-1} ;

Appendix B

k_H - constant for assigning the value of enthalpy reading at the reference point*
[=] J kmol⁻¹.

The enthalpy of the pure components are

$$\tilde{H}_i = (\Delta_f \tilde{H}_{298.15}^o)_i + (\tilde{H}_T^o - \tilde{H}_{298.15}^o)_i \quad (\text{B-3})$$

The first term $(\Delta_f \tilde{H}_{298.15}^o)_i$ is the enthalpy of formation of the component i at standard pressure 0.1MPa and standard temperature 298.15K (25°C), see Table A-1 in Appendix A. The second term $(\tilde{H}_T^o - \tilde{H}_{298.15}^o)_i$ is the enthalpy change from standard temperature up to the gas temperature T [=] K. For numerous chemical compounds, enthalpy of formation and enthalpy change are tabulated in the JANAF tables.

Heat capacity

Frozen mixture heat capacity (heat capacity of the mixture of non-reacting gases) can be expressed as

$$\tilde{C}p_{fr} = \sum_{i=1}^n y_i \tilde{C}p_i \quad (\text{B-4})$$

where $\tilde{C}p_i$ - molar heat capacity of the component i [=] J mol⁻¹

The heat capacity at constant pressure for components is tabulated in JANAF tables by Chase et al. (1985) for standard pressure 0.1MPa in a temperature range from 0K to 6000K.

Thermal conductivity

Values for thermal conductivity of the frozen six components in the gas (H₂O, H₂, O₂, HO, H and O) mixture are generated by Svehla (1964) in the temperature range from 326.85 to 4726.85°C (600 to 5000K) and pressure range from 101Pa to 101MPa (0.001 to 1000atm). For any required temperature and pressure in this range, thermal conductivity can be predicted by using a look-up table and interpolation technique. According to discussion in Chapter 3 predictions of thermal conductivity by Svehla (1964) are not accurate. Since, this are the only available data in literature for frozen thermal conductivity, they are adapted in this work. The

* In this work the zero value of enthalpy is assign at the triple point of water (t=0.01°C, P=611.73Pa).

Appendix B

estimated inaccuracy of the predictions is in order of -10%.

A set of computer subroutines known as the Frozen Properties code has been developed for generating dissociated water vapour frozen properties. The listing of subroutines is presented in Appendix G. A table of the frozen dissociated water vapour properties generated using subroutines is presented in Appendix K.

Appendix C

Method for Calculating Steam Properties as a Mixture of Chemically Reacting Gases (Effective)

The method for predicting effective properties involves the use of a look-up table and interpolation technique. The look-up table has been constructed using primarily entries directly from the table by Vargaftik (1983) and papers by Kesselman et al. (1968 h) and Kesselman and Blank (1968 i). Parameters required for evaluation properties according to Kesselman's methods as described in Chapter 3 are listed in Tables C-1 and C-2. Additional entries in the properties look-up table were added to expand the parametric range of the table.

The interpolation technique for prediction properties (A) for given conditions (pressure (P) and temperature (T)) has two steps. First, select the values of properties ($A_{11}, A_{12}, A_{21}, A_{22}$ as illustrated in Figure C.1) from the look-up table which have the closest values to the given conditions.

$$A = A(P, T) \quad A_{11} = A(P_1, T_1) \quad A_{12} = A(P_1, T_2) \quad A_{21} = A(P_2, T_1) \quad A_{22} = A(P_2, T_2)$$

$$P_1 \leq P \leq P_2 \quad T_1 \leq T \leq T_2$$

Second, interpolate properties, $A(P, T)$, for the given conditions. Three possible scenarios may occur: two, one or none of the two given conditions, pressure (P) and temperature (T), may be equal to an entry in the look-up table (P_1, P_2, T_1, T_2). The interpolation formulas depend on which of the scenarios happened.

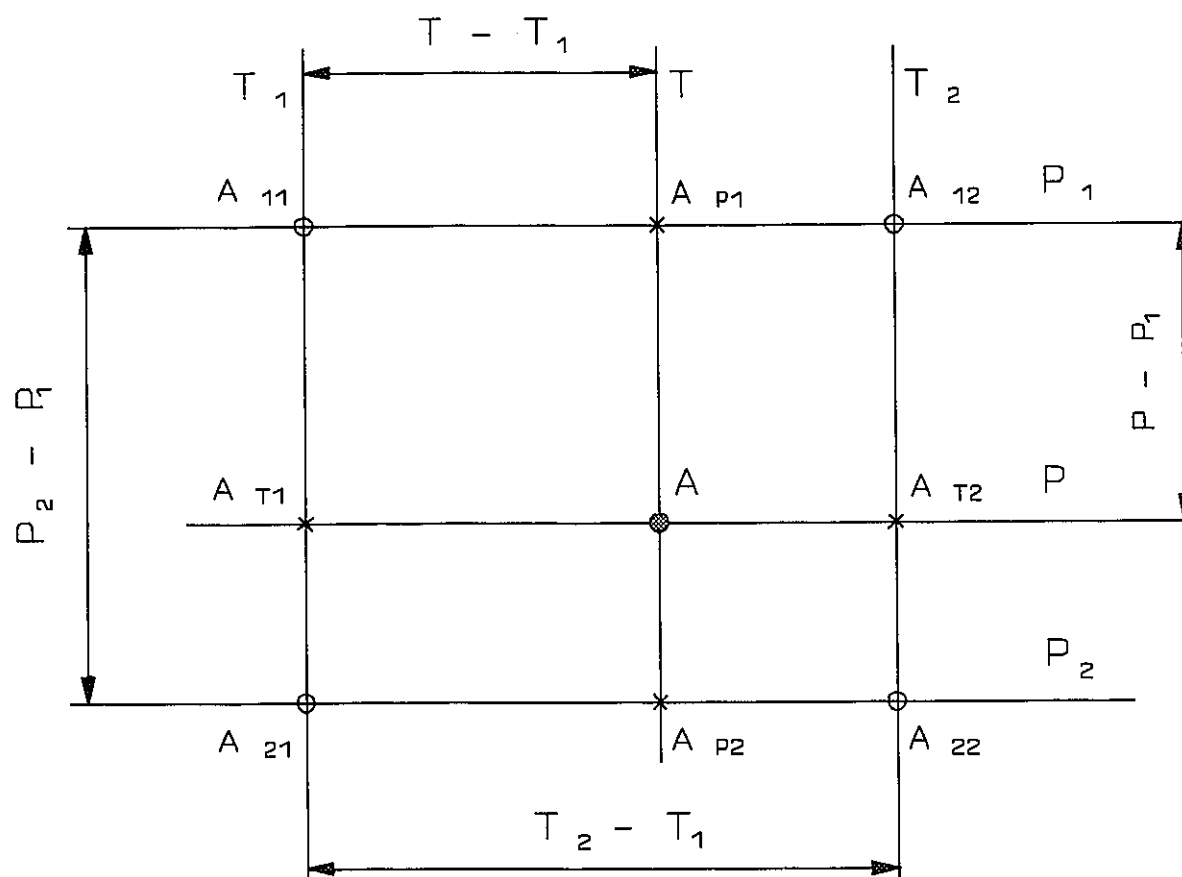


Figure C.1 Illustration of properties interpolation technique.

Appendix C

If two given conditions are equal to two entries in the look-up table, then the properties are the same as in the look-up table:

$$A = A(P, T)$$

$$\begin{array}{lll} P = P_1 & T = T_1 & A = A(P_1, T_1) = A_{11} \\ P = P_1 & T = T_2 & A = A(P_1, T_2) = A_{12} \\ P = P_2 & T = T_1 & A = A(P_2, T_1) = A_{21} \\ P = P_2 & T = T_2 & A = A(P_2, T_2) = A_{22} \end{array}$$

If one of the conditions is equal to an entry, the interpolation formulas are:

$$P=P_1 \quad A = A(P, T) = A(P_1, T) = A_{11} + (A_{12} - A_{11}) \frac{T - T_1}{T_2 - T_1}$$

$$T=T_1 \quad A = A(P, T) = A(P, T_1) = A_{11} + (A_{21} - A_{11}) \frac{P - P_1}{P_2 - P_1}$$

If none of the conditions is equal to an entry, then the interpolation formula is:

$$\begin{aligned} A = A(P, T) = A_{11} + (A_{12} - A_{11}) \frac{T - T_1}{T_2 - T_1} + (A_{21} - A_{11}) \frac{P - P_1}{P_2 - P_1} + \\ + [(A_{11} - A_{12}) - (A_{21} - A_{22})] \frac{T - T_1}{T_2 - T_1} \frac{P - P_1}{P_2 - P_1} \end{aligned}$$

The set of computer subroutines known as the UODH2O code has been developed for generating values of the effective thermodynamic and transport properties of dissociated steam. The code is valid in a pressure range from 0.01 to 100.00MPa, and in a temperature range from 1000 to 5726.85°C. A listing of the subroutines is presented in Appendix H.

Appendix C

Table C-1 Intermolecular force parameters, $\epsilon(T)/k$ and $\sigma(T)$, for Lennard-Jones potential function, in temperature range 1000-3400K, for components of water vapour dissociation by Kesselman and Blank (1968 i).

	H ₂ O-H ₂ O		H ₂ -H ₂		O ₂ -O ₂		HO-HO		H-H		O-O	
T	ϵ/k	σ	ϵ/k	σ	ϵ/k	σ	ϵ/k	σ	ϵ/k	σ	ϵ/k	σ
K	K	nm	K	nm	K	nm	K	nm	K	nm	K	nm
1000	523.5	.2876	34.1	.2938	117.4	.3462	100.0	.4050	350.0	.2370	118.3	.2910
1200	481.1	.2860	34.1	.2936	117.5	.3462	112.0	.4031	390.0	.2333	118.3	.2892
1400	458.0	.2845	34.1	.2935	117.5	.3462	124.0	.4012	430.0	.2297	118.3	.2874
1600	453.6	.2834	34.1	.2934	117.5	.3462	132.0	.3993	470.0	.2261	118.3	.2856
1800	456.0	.2824	34.1	.2934	117.5	.3461	140.0	.3974	507.0	.2225	118.3	.2838
2000	461.0	.2815	34.1	.2933	117.5	.3461	147.5	.3954	547.8	.2189	118.3	.2820
2200	467.4	.2807	34.1	.2933	117.5	.3461	156.0	.3933	588.9	.2161	118.3	.2807
2400	473.2	.2800	34.1	.2933	117.5	.3461	162.5	.3914	627.8	.2133	118.3	.2795
2600	478.2	.2794	34.1	.2932	117.5	.3460	166.7	.3900	665.6	.2107	118.2	.2784
2800	482.2	.2788	34.1	.2932	117.5	.3460	172.8	.3873	701.7	.2085	118.1	.2774
3000	485.5	.2782	34.1	.2932	117.4	.3460	177.0	.3857	736.7	.2063	118.0	.2765
3400	489.9	.2772	34.1	.2932	117.4	.3460	184.4	.3832	803.4	.2029	117.7	.2748

Appendix C

Table C-2 Virial coefficients for components of water vapour dissociation in temperature range 1000-3400K by Kesselman and Blank (1968 i).

	H ₂ O-H ₂ O		H ₂ -H ₂		O ₂ -O ₂		HO-HO		H-H		O-O	
T	B	C	B	C	B	C	B	C	B	C	B	C
K	cm ³ mol ⁻¹	cm ⁶ mol ⁻²	cm ³ mol ⁻¹	cm ⁶ mol ⁻²	cm ³ mol ⁻¹	cm ⁶ mol ⁻²	cm ³ mol ⁻¹	cm ⁶ mol ⁻²	cm ³ mol ⁻¹	cm ⁶ mol ⁻²	cm ³ mol ⁻¹	cm ⁶ mol ⁻²
1000	-21.16	407.9	16.86	226.0	22.47	805.4	40.71	0.0	0.06	0.0	14.90	0.0
1200	-9.29	331.7	16.70	213.0	24.41	783.4	40.43	0.0	0.08	0.0	14.84	0.0
1400	-2.82	295.7	16.51	202.0	25.63	762.4	40.16	0.0	0.10	0.0	14.78	0.0
1600	0.72	276.4	16.30	192.0	26.40	742.4	39.89	0.0	0.30	0.0	14.72	0.0
1800	3.02	263.9	16.11	184.0	26.89	722.9	39.62	0.0	0.50	0.0	14.67	0.0
2000	4.68	254.9	15.90	177.0	27.21	704.7	39.35	0.0	0.67	0.0	14.62	0.0
2200	5.93	247.5	15.72	171.0	27.41	687.5	39.01	0.0	0.87	0.0	14.57	0.0
2400	6.93	241.5	15.54	165.0	27.52	671.4	38.67	0.0	1.04	0.0	14.48	0.0
2600	7.78	235.9	15.36	160.0	27.58	656.3	38.34	0.0	1.18	0.0	14.34	0.0
2800	8.49	231.0	15.20	156.0	27.60	642.3	38.01	0.0	1.30	0.0	14.21	0.0
3000	9.08	226.6	15.05	152.0	27.59	629.2	37.65	0.0	1.41	0.0	14.07	0.0
3400	10.03	218.3	14.76	144.0	27.53	605.5	37.06	0.0	1.60	0.0	13.80	0.0

Appendix D

Derivation of the Effective Nusselt Number for a Mixture of Chemically Reacting Gases

Heat transfer from the pipe wall to the mixture of chemically-reacting gases is driven by two mechanisms: heat transfer to the mixture of chemically-non-reacting gases and the heat transfer due to chemical reactions which occur in the gas mixture. The first and simplest approach is to assume that total heat transfer could be described as a sum of the two separate mechanisms. This superposition concept is used to describe heat transfer in a two-phase flow. The superposition model, employed in a well-known correlation by Chen (1966), assumes that the total heat flux is the sum of the nucleate boiling component and the convective evaporation component. The interaction between the two components were regarded through the suppression factor (S). In this work interaction were not considered ($S = 1$).

Total heat flux transferred from the pipe wall to the mixture of reacting gases is the sum of the chemically-non-reacting gases component (frozen state) and the component due to chemical reactions in the gas mixture (reacting state).

$$q_{con} = q_{eff} = q_{fr} + q_r \quad (D-1)$$

In the classical theory of convective heat transfer, the first term on the right-hand side of equation (D-1) is known as Newton's law of cooling

$$q_{fr} = h_{fr} (t_w - t_b) \quad (D-2)$$

The second term on the right-hand side may be defined as heat transferred by transporting radially the mass of each of the species i in the mixture of n components. Total enthalpy is a thermodynamic property which is a measure of amount of energy per unit mass at constant pressure. Heat transported by mass transfer then is a summation, for all components of the mixture, of each component enthalpy multiplied by the mass flux of that component in the radial

Appendix D

direction.

$$q_r = \sum_{i=1}^n \tilde{H}_i \tilde{j}_i [=] (J \text{ mol}_i^{-1}) (\text{mol}_i \text{ m}^{-2} \text{ s}^{-1}) [=] J \text{ m}^{-2} \text{ s}^{-1} \quad (\text{D-3})$$

where:

q_r - heat transferred due to mass transfer (heat transferred due to chemical reaction)

$[=] J \text{ m}^{-2} \text{ s}^{-1}$;

$\tilde{H}_i$ - molar enthalpy of the species i $[=] J \text{ mol}_i^{-1}$;

$\tilde{j}_i$ - mass flux of the species i transferred by mass transfer $[=] \text{mol}_i \text{ m}^{-2} \text{ s}^{-1}$;

i - species of multi-component mixture;

n - total number of components in the mixture.

The mass flux of the species i is

$$\tilde{j}_i = \frac{\rho_{m,b}}{\tilde{M}_m} g_i (y_{i,w} - y_{i,b}) \quad (\text{D-4})$$

with

$$\rho_{m,b} = \sum_{i=1}^n \rho_i [=] \text{kg}_m \text{ m}_m^{-3} \quad (\text{D-5})$$

$$\tilde{M}_m = \sum_{i=1}^n y_i \tilde{M}_i [=] \text{kg}_m \text{ mol}_m^{-1} \quad (\text{D-6})$$

where:

$\rho_{m,b}$ - density of mixture $[=] \text{kg}_m \text{ m}_m^{-3}$;

$\tilde{M}_m$ - molar mass of mixture $[=] \text{kg}_m \text{ mol}_m^{-1}$;

g_i - mass transfer coefficient for species i $[=] \text{mol}_i \text{ m}^{-2} \text{ s}^{-1} (\text{mol}_i \text{ m}_m^{-3})^{-1} = \text{m s}^{-1}$

or $[=] \text{kg}_i \text{ m}^{-2} \text{ s}^{-1} (\text{kg}_i \text{ m}_m^{-3})^{-1} = \text{m s}^{-1}$;

$y_{i,w}, y_{i,b}$ - mole fraction of the species i at temperature of the wall and fluid bulk temperature $[=] \text{mol}_i \text{ mol}_m^{-1}$.

In the gas mixture with n chemically active components, it is possible to have Yn chemical reactions. If components of the mixture are formed by e chemical elements, then the minimum number of chemical reactions required to describe the system is $k = n - e$. From all Yn reactions, it is also feasible to isolate Yk chemical reactions such that one species of n appears

Appendix D

only in one chemical reaction. Let us symbolize that species with l . Since component l materializes in only one reaction, one is able to conclude that this component is neutral, reactant (dissipated in the reaction) or a product (generated in the reaction) of the overall chemical process. If the stoichiometric coefficient of component i in chemical reaction j is a_{ij} [=] mol_{ij} , then the molar mass flux of component i or l due to chemical reaction j is

$$\frac{\tilde{j}_i}{a_{ij}} \text{ [=] } \frac{\text{mol}_i \text{ m}^{-2} \text{ s}^{-1}}{\text{mol}_{ij}} \quad \frac{\tilde{j}_l}{a_{lj}} \text{ [=] } \frac{\text{mol}_l \text{ m}^{-2} \text{ s}^{-1}}{\text{mol}_{lj}} \quad (\text{D-7})$$

The component l appears only in chemical reaction j , thus generation or destruction of all other components i in that chemical reaction must be proportional to the mass flux of component l . Therefore, total mass flux of the component i is the weighted sum of the mass fluxes of components l in all chemical reactions k .

$$\tilde{j}_i = \sum_{j=1}^k \frac{a_{ij}}{a_{lj}} \tilde{j}_l \quad (\text{D-8})$$

Thus, it is possible to write Equation (D-3) as

$$q_r = \sum_{i=1}^n \tilde{H}_i \sum_{j=1}^k \frac{a_{ij}}{a_{lj}} \tilde{j}_l \quad (\text{D-9})$$

On the other hand, in the above equation the enthalpy of chemical reaction j is

$$Qp_j = \sum_{i=1}^n a_{ij} \tilde{H}_i \text{ [=] } \text{mol}_{ij} J \text{ mol}_i^{-1} \text{ [=] } J \quad (\text{D-10})$$

Substituting Equations (D-4) and (D-10) into (D-9), heat flux due to chemical reactions becomes

$$q_{r,h} = \sum_{j=1}^k \frac{Qp_j}{a_{lj}} \frac{\rho_{m,h}}{\tilde{M}_m} g_l (y_{l,w} - y_{l,h}) \quad (\text{D-11})$$

Appendix D

Dividing Equation (D-1) with the difference between wall and bulk temperature ($t_w - t_b$), it is possible to define the effective heat transfer coefficient and the heat transfer coefficient of a chemically non-reactive gas mixture (frozen):

$$h_{eff,b} \equiv \frac{q_{eff}}{(t_w - t_b)} \quad (D-12)$$

$$h_{fr,b} \equiv \frac{q_{fr}}{(t_w - t_b)} \quad (D-13)$$

The heat transfer coefficient due to the effect of chemical reactions (reactive) is as follows :

$$h_{r,b} = \sum_{j=1}^k \frac{Qp_j \rho_{m,b} g_l (y_{l,w} - y_{l,b})}{a_{lj} \tilde{M}_m (t_w - t_b)} \quad (D-14)$$

$j=1,2,3,\dots,x \quad l=1,2,3,\dots,k \quad k < x$

The effective heat transfer coefficient is a superposition of frozen and reactive components.

$$h_{eff,b} = h_{fr,b} + \sum_{j=1}^k \frac{Qp_j \rho_{m,b} g_l (y_{l,w} - y_{l,b})}{a_{lj} \tilde{M}_m (t_w - t_b)} \quad (D-15)$$

$j=1,2,3,\dots,x \quad l=1,2,3,\dots,k \quad k < x$

If the above equation is multiplied by ($d / k_{fr,b}$), the left-hand side of the equation becomes the effective Nusselt number, defined as

$$Nu_{eff,b} \equiv h_{eff,b} \frac{d}{k_{fr,b}} \quad (D-16)$$

The first term on the right-hand side becomes the Nusselt number of the mixture without chemical reaction (frozen properties), defined as

$$Nu_{fr,b} \equiv h_{fr,b} \frac{d}{k_{fr,b}} \quad (D-17)$$

Using the definition of Sherwood number as

$$Sh_{fr,b} \equiv \frac{g_l d}{D_{l-m}} \quad (D-18)$$

Appendix D

and Lewis number as

$$Le_{l-m,fr,b} = \frac{k_{fr,b}}{\rho_{m,b} Cp_{fr,b} D_{l-m}} \quad (D-19)$$

then the group of terms from Equation (D-15) can be expressed as

$$\rho_{m,b} g_l \frac{d}{k_{fr,b}} = \frac{Sh_{l,fr,b}}{Cp_{fr,b} Le_{l,fr,b}} \quad (D-20)$$

Equation (D-15) can be rewritten in the dimensionless form as

$$Nu_{eff,b} = Nu_{fr,b} + \sum_{j=1}^k \frac{Qp_j}{a_{lj} \dot{M}_m Cp_{fr,b} Le_{l,fr,b}} \frac{Sh_{l,fr,b} (y_{l,w} - y_{l,b})}{(t_w - t_b)} \quad (D-21)$$

$j=1,2,3,\dots,k \quad l=1,2,3,\dots,k$

Non-equilibrium flow requires that kinetics of the chemical reactions be considered. The Sherwood number for non-equilibrium flow proposed by Nesterenko et al. (1967 b) is

$$Sh_{l,fr,b} = Sh_{l,fr,b,eq} Cr_l \quad (D-22)$$

$$Cr_l \equiv \frac{J_l x}{G} = \frac{\text{mass velocity of component } l \text{ generated along } x}{\text{mass velocity of gas mixture}}$$

where:

Cr_l - Reaction number ($0 \leq Cr_l \leq 1$), a dimensionless criterion which characterizes the relation between the rate of appearance or disappearance of the species l along distance x , and the mass velocity of the mixture. When $Cr_l = 0$, there is a "frozen" state, i.e. no chemical reaction and when $Cr_l = 1$, the mixture is in chemical equilibrium*;

J_l - rate of generation (appearance or disappearance) of the species l due to the kinetics of chemical reaction [=] $\text{kg m}^{-3} \text{s}^{-1}$;

x - current axial coordinate [=] m;

G - mass velocity [=] $\text{kg m}^{-2} \text{s}^{-1}$.

The Reaction number has the same physical meaning as the Boiling number (Bo) used in two-

* The results in this work are obtained for equilibrium state, Reaction number $Cr_l = 1$.

Appendix D

phase flow. It represents a ratio of the mass velocity of the component generated by the heat transfer process to the mass velocity of the fluid mixture.

$$Bo \equiv \frac{q}{G H_{lv}} = \frac{\frac{q}{H_v - H_l}}{G} = \frac{\text{mass velocity of generated vapour}}{\text{mass velocity of liquid-vapour mixture}} \quad (\text{D-23})$$

Considering that $\tilde{C}p_{fr,b} = \tilde{M}_m Cp_{fr,b}$, Equation (D-21) results in the final form

$$Nu_{eff,b} = Nu_{fr,b} + \sum_{j=1}^k \frac{Qp_j}{a_{lj} \tilde{C}p_{fr,b}} \frac{Sh_{lfr,b}}{Le_{lfr,b}} \frac{(y_{l,w} - y_{l,b})}{(t_w - t_b)} \quad (\text{D-24})$$

$j=1,2,3,\dots,k \quad l=1,2,3,\dots,k$

The second term of Equation (D-24) represents the Nusselt number of the mixture of chemically non-reacting gases (frozen state). The third term is the sum of the effects of all chemical reactions which occur in the gas mixture. It represents the contribution to heat transfer due to mass transfer of the species in gas mixture. It consists of three ratios. The first ratio is of the heat effect of each chemical reaction to the heat capacity of the gas mixture without chemical reaction (frozen). The second ratio is

$$\frac{Sh_{lfr,b}}{Le_{lfr,b}} = \frac{Cp_{fr,b} \rho_{m,b} g_l d}{k_{fr,b}} = \frac{\text{transfer of heat due to mass transfer}}{\text{thermal diffusion rate}} \quad (\text{D-25})$$

and the third ratio is a ratio of gradient of composition to gradient of temperature.

The composition of the gas mixture can be evaluated in four different ways, as was shown in Table A-2; therefore, Equation (D-24) may be written in the following four forms:

$$Nu_{eff,b} = Nu_{fr,b} + \sum_{j=1}^k \frac{Qp_j}{a_{lj} \tilde{C}p_{fr,b}} \frac{Sh_{lfr,b}}{Le_{lfr,b}} \frac{(y_{l,w} - y_{l,b})}{(t_w - t_b)} \quad (\text{D-26})$$

$j=1,2,3,\dots,k \quad l=1,2,3,\dots,k$

$$Nu_{eff,b} = Nu_{fr,b} + \sum_{j=1}^k \frac{Qp_j}{a_{lj} \tilde{M}_l Cp_{fr,b}} \frac{Sh_{lfr,b}}{Le_{lfr,b}} \frac{(\omega_{l,w} - \omega_{l,b})}{(t_w - t_b)} \quad (\text{D-27})$$

$j=1,2,3,\dots,k \quad l=1,2,3,\dots,k$

Appendix D

$$Nu_{eff,b} = Nu_{fr,b} + \sum_{j=1}^k \frac{Qp_j}{a_{lj} \rho_{m,b} Cp_{fr,b}} \frac{Sh_{lfr,b}}{Le_{lfr,b}} \frac{(C_{l,w} - C_{l,b})}{(t_w - t_b)} \quad (D-28)$$

$$j=1,2,3,\dots,k \quad l=1,2,3,\dots,k$$

$$Nu_{eff,b} = Nu_{fr,b} + \sum_{j=1}^k \frac{Qp_j}{a_{lj} \tilde{M}_l \rho_{m,b} Cp_{fr,b}} \frac{Sh_{lfr,b}}{Le_{lfr,b}} \frac{(\rho_{l,w} - \rho_{l,b})}{(t_w - t_b)}$$

$$j=1,2,3,\dots,k \quad l=1,2,3,\dots,k$$

Appendix E

Method for Calculating the Local Heat Transfer Coefficient and the Wall Temperature for a Turbulent Pipe Flow of Dissociated Steam with Constant Heat Flux at the Wall

For mass velocity G of water vapour turbulent flow, at pressure P and entrance bulk temperature t_b , in a pipe of diameter d , with Zn oxidized surface emissivity ϵ_w , heated with constant heat flux at the wall q_w , calculate

A) local heat transfer coefficient - h [=] $\text{W m}^{-2} \text{K}^{-1}$

B) local wall temperature of the pipe - t_w [=] $^{\circ}\text{C}$

Given data are:

$$\begin{array}{ll} G = 1000 \text{ kg m}^{-2} \text{ s}^{-1} & d = 0.01 \text{ m} \\ T_b = 2300 \text{ K} & P = 0.1 \text{ MPa} \\ q_w = 1 \text{ MW m}^{-2} & \epsilon_w = 0.6 \end{array}$$

A) The local heat transfer coefficient - h [=] $\text{W m}^{-2} \text{K}^{-1}$

Heat flux transferred from the pipe wall can be divided into heat flux transferred by convection and heat flux transferred by radiation.

Appendix E

$$q_w = q_{con} + q_{rad} \quad [=] \text{ W} \quad (\text{E-1})$$

The second term in the above equation q_{con} is the heat flux transferred by convection. From Newton's law of cooling the convective heat flux can be written as

$$q_{con} = h_{eq} (T_w - T_b) \quad [=] \text{ W} \quad (\text{E-2})$$

where:

h_{eq} - convective heat transfer coefficient at equilibrium.

The third term in Equation (E-1), q_{rad} , is the heat flux transferred by radiation; it may be calculated as

$$q_{rad} = \epsilon_{eff} \sigma [a_{mix}(T_w) T_w^4 - e_{mix}(T_b) T_b^4] \quad [=] \text{ W} \quad (\text{E-3})$$

The local heat transfer coefficient for the mixture of chemically reacting gases in equilibrium can be calculated from the effective Nusselt number derived at Appendix D

$$Nu_{eff,b} = Nu_{fr,b} + \sum_{j=1}^4 \frac{Qp_j}{a_{l,j} \bar{C}p_{fr,b}} \frac{Sh_{l,fr,b}}{Le_{l,fr,b}} \frac{(y_{l,w} - y_{l,b})}{(t_w - t_b)} \quad (\text{E-4})$$

$j=1 \quad l=1$
 $j=2,3,4 \quad l=j+2=4,5,6$

The Nusselt number for non-reacting gases or "frozen" for variable physical properties is the Gnelinski (1972) correlation, valid in the following (turbulent flow) range:

$$Re_b = 2300 - 5 \cdot 10^6 \quad Pr_{fr,b} = 0.5 - 2000$$

$$Nu_{fr,b,VP} = \frac{\frac{f}{2} (Re_b - 1000) Pr_{fr,b}}{1 + 12.7 \left(\frac{f}{2}\right)^{0.5} (Pr_{fr,b}^{2/3} - 1)} \left(\frac{T_b}{T_w}\right)^{0.45} \quad (\text{E-5})$$

For laminar flow it is

$$Nu_{fr,b} = 4.364 \quad (\text{E-6})$$

The Reynolds number and Prandtl number in the above equations are defined as

$$Pr_{fr,b} = \frac{\mu_b Cp_{fr,b}}{k_{fr,b}} \quad Re_b = \frac{G d}{\mu_b} \quad (\text{E-7})$$

Appendix E

The Fanning friction factor correlation for a smooth circular duct can be calculated using correlations by Bhatti and Shah (1987). This explicit formula is recommended by Kakaç et al. (1987):

$$f = A + B Re_h^C$$

$$\begin{array}{llll} Re_h < 2100 & A = 0 & B = 16. & C = -1. \\ 2100 \leq Re_h \leq 4000 & A = 0.54 \cdot 10^{-2} & B = 0.23 \cdot 10^{-7} & C = 1.5 \\ 4000 < Re_h < 1 \cdot 10^7 & A = 0.128 \cdot 10^{-2} & B = 0.1143 & C = -0.311 \end{array} \quad (\text{E-8})$$

The last term of Equation (E-4), consisting of the sum of four terms, is the mass transfer contribution to heat transfer. The first member of the seven member term is the heat effect of the chemical reaction j defined in Appendix D as

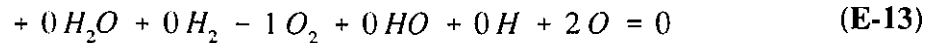
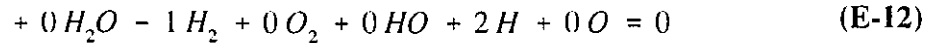
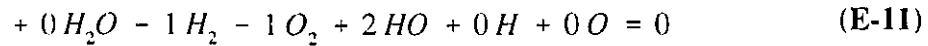
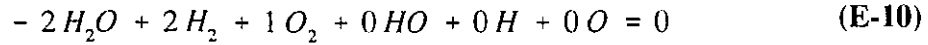
$$Qp_j = \sum_{i=1}^6 a_{ij} \tilde{H}_i [=] J \quad (\text{E-9})$$

where:

a_{ij} - coefficient of the component i in the chemical reaction j ;

$\tilde{H}_i$ - enthalpy of the pure component i .

The following four chemical reactions are chosen:



Enthalpy of the pure components is defined in Appendix B as

$$\tilde{H}_i = (\Delta_f \tilde{H}_{298.15}^o)_i + (\tilde{H}_T^o - \tilde{H}_{298.15}^o)_i [=] J \text{ mol}_i^{-1} \quad (\text{E-14})$$

An analogy exists between heat and mass transfer such that the correlation for the Nusselt number can be used to calculate the Sherwood number by replacing the Prandtl number with the Schmidt number.

Appendix E

Using the Gnielinski (1972) correlation, the Sherwood number for turbulent flow is

$$Sh_{l,fr,b,VP,eq} = \frac{\frac{f}{2} (Re_b - 1000) Sc_{l,fr,b}}{1 + 12.7 \left(\frac{f}{2}\right)^{0.5} (Sc_{l,fr,b}^{2/3} - 1)} \left(\frac{T_b}{T_w}\right)^{0.45} \quad (E-15)$$

For laminar flow it is

$$Sh_{l,fr,b} = 4.364 \quad (E-16)$$

Non-equilibrium flow requires that the kinetics of the chemical reactions be considered. The Sherwood number for non-equilibrium proposed by Nesterenko et al. (1967 b) is

$$Sh_{l,fr,b} = Sh_{l,fr,b,VP,eq} Cr_l \quad (E-17)$$

$$Cr_l = \left(\frac{J_l x}{G} \right) = \frac{\text{mass velocity of component } l \text{ generated along } x}{\text{mass velocity of gas mixture}}$$

where:

Cr_l - Reaction number ($0 \leq Cr_l \leq 1$), a dimensionless criterion which characterizes the relation between the rate of appearance or disappearance of the species l along distance x , and the mass velocity of the mixture. When $Cr_l = 0$, there is a "frozen" state, i.e. no chemical reaction and when $Cr_l = 1$, the mixture is in chemical equilibrium*;

J_l - rate of generation (appearance or disappearance) of the species l due to the kinetics of chemical reaction [=] $\text{kg m}^{-3} \text{s}^{-1}$;

x - current axial coordinate [=] m;

G - mass velocity [=] $\text{kg m}^{-2} \text{s}^{-1}$.

In addition, the Schmidt number is defined as

$$Sc_{l-m,fr,b} \equiv \frac{\mu_b}{\rho_{m,b} D_{l-m}} \quad (E-18)$$

* The results in this work are obtained for equilibrium state, Reaction number $Cr_l = 1$.

Appendix E

The diffusion coefficient of component l through the mixture of gases (Blanc's law) is

$$D_{l-m} = \frac{1 - y_l}{\sum_{i=1}^n \frac{y_i}{D_{l-i}}} [=] m^2 s^{-1} \quad (E-19)$$

The diffusion coefficient D_{l-i} is a binary diffusion coefficient of component l through component i in the binary mixture of gases. From the text by Reid et al. (1987) or Hirschfelder et al. (1967), the diffusion coefficient may be calculated using the following formula:

$$D_{l-i} = \frac{0.1882899 \cdot 10^{-9} T^{1.5}}{\bar{M}_{li}^{0.5} \sigma_{li}^2 \Omega_{Dli} P} [=] m^2 s^{-1} \quad (E-20)$$

where:

T - absolute temperature [=] K;

$1/\bar{M}_{li} = (1/\bar{M}_l) + (1/\bar{M}_i)$ - reduced mass of the system [=] kmol kg⁻¹;

$\bar{M}_l, \bar{M}_i$ - molecular mass of the species l and i [=] kg kmol⁻¹;

σ_{li} - characteristic length, [=] nm;

Ω_{Dli} - diffusion collision integral, [=] dimensionless;

P - pressure, [=] MPa.

The characteristic lengths are calculated from parameters of individual species using the combination rule

$$\sigma_{li} = \frac{\sigma_l + \sigma_i}{2} \quad (E-21)$$

The collision integral is tabulated for the Lennard-Jones potential function by Hirschfelder et al. (1967) or it may be calculated very accurately using the following approximation relation by Neufield et al. (1972):

$$\Omega_{Dli} = \frac{1.06036}{(T^*)^{0.15610}} + \frac{0.19300}{\exp(0.47635 T^*)} + \frac{1.03587}{\exp(1.52996 T^*)} + \frac{1.76474}{\exp(3.89411 T^*)} \quad (E-22)$$

$$T^* = \frac{T}{\left(\frac{\epsilon_{li}}{k} \right)} \quad (E-23)$$

Appendix E

$$\left(\frac{\varepsilon_{li}}{k} \right) = \sqrt{\left(\frac{\varepsilon_l}{k} \right) \left(\frac{\varepsilon_i}{k} \right)} \quad [=] \text{ K} \quad (\text{E-24})$$

The values of temperature-dependent parameters $\varepsilon_i(T)/k$ and $\sigma_i(T)$ for individual species are presented in Table C-1.

Coefficients a_{ij} , which can be obtained from Equations (E-10) to (E-13), are

$$a_{11} = -2 \quad [=] \text{ mol}_1 \quad a_{42} = 2 \quad [=] \text{ mol}_4 \quad a_{53} = 2 \quad [=] \text{ mol}_5 \quad a_{64} = 2 \quad [=] \text{ mol}_6$$

Frozen heat capacity (heat capacity of the mixture of non-reacting gases) is defined (for details see Appendix B) as

$$\tilde{C}p_{fr,b} = \sum_{i=1}^n y_{i,b} \tilde{C}p_{i,b} \quad [=] \text{ J mol}_m^{-1} \text{ } ^\circ\text{C}^{-1} \quad (\text{E-25})$$

The frozen Lewis number of component l diffusing through the mixture m of gases is

$$Le_{l-m,fr,b} = \frac{k_{l,b}}{\rho_{m,b} \tilde{C}p_{fr,b} D_{l-m}} \quad (\text{E-26})$$

Finally, from the definition of effective Nusselt number, the local heat transfer coefficient can be calculated as

$$h_{eff} = \frac{N_{eff,b} k_{fr,b}}{d} \quad [=] \text{ W m}^{-2} \text{ } ^\circ\text{C}^{-1} \quad (\text{E-27})$$

Calculation of the local heat transfer coefficient according to Equation (E-27) requires the knowledge of the wall and fluid bulk temperatures. If wall temperature is not known, it must be calculated by iteration (as described in part B).

Appendix E

B) The local wall temperature of the pipe - $t_w [=]$ °C

From Equations (E-1) and (E-2) and the definition of Nusselt number, the wall temperature can be written as

$$t_w = t_b + \frac{(q_w - q_{rad}) d}{k_{fr,b} N_{eff,b}} [=] \text{ } ^\circ\text{C} \quad (\text{E-28})$$

If the wall temperature is to be calculated, the first step is the estimation of the Nusselt number or the heat transfer coefficient calculated from Equation (E-4). In the second step, the wall temperature is calculated from Equation (E-28)**. The third step compares the values of the calculated wall temperature with the estimated value. Then the above mentioned calculations are repeated with a new value for the wall temperature. This procedure is repeated until the difference between the estimated and calculated wall temperature is sufficiently small.

A set of computer subroutines known as the High Temperature Steam Heat Transfer code (VASICA) has been developed for calculation of the local heat transfer coefficient and pipe wall temperature. A listing of the subroutines is presented in Appendix I.

** In this work the heat transferred by radiation is not considered.

Appendix F

Programming Specifications for the Mole Fraction Calculation of Dissociated Steam

This chapter includes all subroutines of the Fraction code, written in FORTRAN77 computer language, for the prediction of the composition of dissociated steam, using the method described in Appendix A. For determination of the mole fraction of the dissociated components, a main program needs to call the subroutine FRACTION(PMPA,TC), with entering parameters absolute pressure PMPA(MPa), and absolute temperature TC("C) in the range from 25°C (298.15K) to 5726.85°C (6000K). Accompanying subroutines are PARFAN, NEWTON, functions Y6 and F. The results of calculations will be stored in COMMON BLOCK /FRACT/ as Y.

Appendix F

```

SUBROUTINE FRACTION(PMPA,TC)
***** SUBROUTINE IDENTIFICATION *****
*
*   This is the FRACTION code for composition prediction of
*   Dissociated High Temperature Steam.
*
*   Code has total 154 lines.
*
*   Code generates Mole Fractions of Components in the mixture
*   of reacting gases formed by Dissociated Steam.
*
*   Written by ALEKSANDAR VASIC'      Revised  March /1990
*   Ottawa University
*
*****
*
***** VARIABLE IDENTIFICATION *****
*
*   PMPA  = Input Pressure (MPa = MN/m**2)
*   TC    = Input Temperature (degC)
*   Y(1)  = H2O mole fraction (mol1/molm)
*   Y(2)  = H2  mole fraction (mol2/molm)
*   Y(3)  = O2  mole fraction (mol3/molm)
*   Y(4)  = HO  mole fraction (mol4/molm)
*   Y(5)  = H   mole fraction (mol5/molm)
*   Y(6)  = O   mole fraction (mol6/molm)
*
*****
*
IMPLICIT REAL*8 (A-H,O-Z)
REAL*8 PMPA,P,TC,TK,Q(6),Y(6)
I      ,ELN(4),E(4),GUESS,EP,DEL,Y5,Y6,SUM
COMMON /PARTI/ Q
COMMON /EQCON/ E,P
COMMON /FRACT/ Y
EXTERNAL Y6
DATA EP,DEL/ .1D-14, .1D-14/
*   Conversion MPa to atm
P=PMPA*.9869232667D1
TK=TC+.27315D3

```

Appendix F

```

IF (TC.LT.1650.) THEN
    Y(1)= .1D1
    DO 5 I=2,6
        Y(I)=0.0D0
5    CONTINUE
    RETURN
END IF
CALL PARFAN(TK)
C    WRITE(14,55) TK,(Q(I),I=1,6)
55  FORMAT(T2,1F9.2,6F10.5)
    ELN(1)=(-.5937444953D5/TK)+Q(4)+Q(5)-Q(1)
    ELN(2)=(-.510073396D5/TK)-Q(4)+Q(5)+Q(6)
    ELN(3)=( .519618653D5/TK)-.2D1*Q(5)+Q(2)
    ELN(4)=( .593675100D5/TK)+Q(3)-.2D1*Q(6)
C    WRITE(15,56) TK,(ELN(I),I=1,4)
56  FORMAT(T2,1F9.2,4F10.5)
    DO 6 I=1,4
        E(I)=DEXP(ELN(I))
6    CONTINUE
    IF ((E(1).LT..1D-24).OR.(E(2).LT..1D-23)) THEN
        Y(1)= .1D1
        DO 7 I=2,6
            Y(I)=0.0D0
7        CONTINUE
        RETURN
    END IF
    GUESS=.1D0
    CALL NEWTON(GUESS,EP,DEL,Y5)
    Y(5)=Y5
    Y(6)=Y6(Y5)
    IF ((Y(5).LT..1D- 9).OR.(Y(6).LT..1D- 9)) THEN
        Y(1)= .1D1
        DO 8 I=2,6
            Y(I)=0.0D0
8        CONTINUE
        RETURN
    END IF
    SUM=P*E(3)*(Y(5)**.2D1)
    Y(2)=SUM
    Y(3)=P*E(4)*(Y(6)**.2D1)

```

Appendix F

```

Y(4)=Y(5)+.2D1*Y(2)-.2D1*(Y(6)+.2D1*Y(3))
DO 9 I=3,6
    SUM=SUM+Y(I)
9 CONTINUE
Y(1)=.1D1-SUM
RETURN
END

      SUBROUTINE PARFAN(TK)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 TK,Q(6)
      COMMON /PARTI/ Q
      Q(1)=.4D1*DLOG(TK)-.41164D1-DLOG(.1D1-DEXP(-.526172D4/TK))-
1      DLOG(.1D1-DEXP(-.229428D4/TK))-DLOG(.1D1-DEXP(-.540379D4/TK))
      Q(2)=.25D1*DLOG(TK)-.26133D1+DLOG((TK/.6826D3)+(.1D1/.24D2)+
1      .711041D0/TK+ (.10400508D3/(TK**.2D1)))+(TK/.2275333D3)+.875D0
2      +(.87458125D2/TK)+(.613629974D4/(TK**.2D1)))*EXP(-.17065D3/TK
3      ))+DLOG((.1D1/(.1D1-DEXP(-.6338295D4/TK)))+( .36064898D3/TK)*
4      DEXP(-.6338295D4/TK)*(.1D1-DEXP(-.6338295D4/TK))**(-.3D1))
      Q(3)=.35D1*DLOG(TK)+.114D0-DLOG(.1D1-DEXP(-.2238905D4/TK))+
1      DLOG(.3D1+.2D1*DEXP(-.1133996D5/TK)+DEXP(-.1887834D5/TK))
      Q(4)=.25D1*DLOG(TK)+.12786535D1+DLOG((TK/.26638D2)+(.1D1/.3D1)+
1      (.17759D1/TK))-DLOG(.1D1-DEXP(-.513589D4/TK))+
2      DLOG(.1D1+DEXP(-.201D3/TK))
      Q(5)=.25D1*DLOG(TK)-.29604D1
      Q(6)=.25D1*DLOG(TK)+.4939D0+DLOG(.5D1+.3D1*DEXP(-.22805D3/TK)+
1      DEXP(-.32589D3/TK)+.5D1*DEXP(-.2283027D5/TK))
      RETURN
      END

      FUNCTION Y6(X5)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 X5,Y6,E(4),P
      COMMON /EQCON/ E,P
      Y6=(.2D1*E(1)*E(2)-.5D1*E(1)*E(2)*X5/.2D1-.3D1*P*E(1)*E(2)*E(3)*
1      X5**2)/( .2D1*P**2*X5**2+.3D1*P*E(1)*X5/.2D1+E(1)*E(2))
      RETURN
      END

```

Appendix F

```

      FUNCTION F(X5,X6)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 X5,X6,F,E(4),P
      COMMON /EQCON/ E,P
      F=.3D1*P*E(1)*E(2)*E(4)*X6**2+(P**2*X5**2+.3D1*P*E(1)*
1    X5/.2D1+.2D1*E(1)*E(2))*X6+E(1)*E(2)*(X5-.2D1)/.2D1
      RETURN
      END

      SUBROUTINE NEWTON(Y5OLD,EPS,DELTA,Y0)
      IMPLICIT REAL*8 (A-H,O-Z)
      INTEGER I
      REAL*8 Y5OLD,Y5NEW,D,DY,Y6,F,FA,EPS,DELTA,Y0
      EXTERNAL Y6,F
      DO 9 I=1,500
        Y6OLD=Y6(Y5OLD)
        FA=F(Y5OLD,Y6OLD)
        IF (FA.NE.0.0D0) THEN
          D=Y5OLD*.1D-6
          X1=Y5OLD+D
          Y1=Y6(X1)
          F1=F(X1,Y1)
          Y5NEW=Y5OLD- D/((F1/FA)-.1D1)
        ELSE
          PRINT*, 'Dividing by zero - f(yold)=0'
          Y0=Y5NEW
          RETURN
        END IF
        DY=Y5OLD-Y5NEW
        IF (((ABS(DY)).LT.EPS).OR.(ABS(FA).LT.DELTA)) THEN
          Y0=Y5NEW
          RETURN
        END IF
        Y5OLD=Y5NEW
      9 CONTINUE
      RETURN
*
***** END OF BLOCK DATA *
***** THIS IS THE END OF SUBROUTINES RELATED TO FRACTION CODE *****
      END

```

Appendix F

```

                                PROGRAM COMPOSIT
***** PROGRAM IDENTIFICATION *****
*
*      This is a sample program which will serve as an
*      example how to use subroutines for calculating
*      Mole Fractions of Components in the mixture of
*      reacting gases formed by Dissociated Steam.
*
*      Written by ALEKSANDAR VASIC'      Revised March /1992
*      Ottawa University
*
*****
***** TYPE DECLARATION AND INITIALIZATION ***** BLOCK 0000 *
*
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Y(6)
      COMMON /FRACT/ Y
*
***** COMPUTATION AND PRINTING ***** BLOCK 0100 *
*
      OPEN (UNIT=1,FILE='YH2O.DAT')
      PMPA = 0.010D0
      DO 99 I = 1,5
        WRITE(1,1) PMPA
1      FORMAT (/T20.4HP = ,1F6.3,3HMPa,/)
        DO 9 TC = 400.D0,6000.D0,100.D0
          CALL FRACTION(PMPA,TC)
          WRITE(1,2) TB,(Y(J),J=1,6)
2      FORMAT(T2,1F5.0,6F11.6)
9      CONTINUE
        PMPA = PMPA*10.D0
99 CONTINUE
*
***** TERMINATION BLOCK ***** BLOCK 0800 *
*
      CLOSE (1)
*
***** END OF MAIN PROGRAM *****
      END

```

Appendix G

Programming Specifications for the Frozen Properties of Dissociated Steam for Pressure from 0.000101325 to 101.325MPa and Temperature from 726.85 to 4726.85°C

This chapter includes subroutines, written in FORTRAN77 computer language, of the Frozen Properties code for the prediction of frozen properties of high temperature steam. A main program is needed to call first subroutine FRACTION(PMPA,TC) from the Fraction code listed in Appendix F, using the method described in Appendix A, for determination of the mole fraction of dissociated components. The next step is to call subroutine FROZPROP(PMPA,TC), with entering parameters absolute pressure PMPA(MPa) in the range from 0.000101 to 101MPa, and temperature TC(°C) in the range from 726.85°C to 4726.15°C. Accompanying subroutines are: JANAF, MOLARMAS, FRENTA, FRCOND, SEARCH, WORKAK; and functions are: INSERT, INTE2P, INTE2T, INTER4; and blocks are: DATAJAN and DATAKT. The subroutine SEARCH and the functions INTE2P, INTE2T, INTER4 are also portions of the UODH2O code; hence, they are listed in Appendix H. The results of calculations will be stored in COMMON BLOCK /FRPRO/ as MMIX, MM, CPFM, HFM and KFM.

Appendix G

```

SUBROUTINE FROZPROP(PMPA,TC)
*****
SUBROUTINE IDENTIFICATION
*****
*
*   This is FROZEN Property code for High Temperature Steam
*
*   Code has total 580 lines.
*
*   Code generates Thermodynamic and Transport Properties
*   of High Temperature Dissociated Steam
*   for Pressures from 0.000101325 to 101.325 MPa
*   at Temperatures from 726.85 to 4726.85 degC.
*
*   Written by ALEKSANDAR VASIC*      Revised March /1990
*   Ottawa University
*
*****
*
  IMPLICIT REAL*8 (A-H,O-Z)
  REAL*8 PMPA,TC,MMIX,MM(6),HFM,CPFM,KFM,Y(6),DH(6),CPI(6),FH(6)
  COMMON /FRACT/ Y
  COMMON /JANENT/ DH,CPI
  COMMON /FRPRO/ MMIX,MM,HFM,CPFM,KFM
  CALL JANAF(TC)
  CALL MOLARMAS(MMIX,MM)
  CALL FRENTA(FH)
  HFM=(0.0D0)
  CPMF=(0.0D0)
  DO 9 I=1,6
    HFM=HFM+(Y(I)*FH(I))
    CPMF=CPMF+(Y(I)*CPI(I))
9  CONTINUE
  CALL FRCOND(PMPA,TC,KFM)
  RETURN
  END

```

Appendix G

```
      SUBROUTINE JANAF(TC)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 JT(61),DELH(6,61),CPS(6,61),DH(6),CPI(6),INSERT
      LOGICAL EQUAL
      COMMON /JANTAB/ JT,DELH,CPS
      COMMON /JANENT/ DH,CPI
      TK=TC+.27315D3
      CALL SEARCH(JT,TK,61,J,EQUAL)
      DO 9 I=1,6
        IF (EQUAL.EQV..TRUE.) THEN
          DH(I)=DELH(I,J)
          CPI(I)=CPS(I,J)
        ELSE
          D1=TK-JT(J)
          D2=JT(J+1)-TK
          Y1=DELH(I,J)
          Y2=DELH(I,J+1)
          F1=INSERT(Y1,Y2,D1,D2)
          DH(I)=F1*.1D4
          Y1=CPS(I,J)
          Y2=CPS(I,J+1)
          F2=INSERT(Y1,Y2,D1,D2)
          CPI(I)=F2
        END IF
      9 CONTINUE
      RETURN
      END

      REAL*8 FUNCTION INSERT(Y1,Y2,D1,D2)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 Y1,Y2,D1,D2
      INSERT=((Y1*D2)+(Y2*D1))/(D1+D2)
      RETURN
      END
```


Appendix G

```

BLOCK DATAJAN
INTEGER I
REAL*8 JT(61),DELH(6,61),CPS(6,61)
COMMON /JANTAB/ JT,DELH,CPS
*   Temperature K
    DATA (JT(I),I=1,61) /
*   .298150D+03, .300000D+03, .350000D+03, .400000D+03, .450000D+03
*   .500000D+03, .600000D+03, .700000D+03, .800000D+03, .900000D+03
*   .100000D+04, .110000D+04, .120000D+04, .130000D+04, .140000D+04
*   .150000D+04, .160000D+04, .170000D+04, .180000D+04, .190000D+04
*   .200000D+04, .210000D+04, .220000D+04, .230000D+04, .240000D+04
*   .250000D+04, .260000D+04, .270000D+04, .280000D+04, .290000D+04
*   .300000D+04, .310000D+04, .320000D+04, .330000D+04, .340000D+04
*   .350000D+04, .360000D+04, .370000D+04, .380000D+04, .390000D+04
*   .400000D+04, .410000D+04, .420000D+04, .430000D+04, .440000D+04
*   .450000D+04, .460000D+04, .470000D+04, .480000D+04, .490000D+04
*   .500000D+04, .510000D+04, .520000D+04, .530000D+04, .540000D+04
*   .550000D+04, .560000D+04, .570000D+04, .580000D+04, .590000D+04
*   .600000D+04/
*
*   JANAF Thermochemical Tables by Chase et al. (1985)
*   Enthalpy change kJ/mol   (Zero value at t=25degC)
*
*   Steam H2O
*
    DATA (DELH(I,I),I=1,61) /
*   .000000D+00, .062000D+00, .175700D+01, .345200D+01, .518850D+01
*   .692500D+01, .105010D+02, .141920D+02, .180020D+02, .219380D+02
*   .260000D+02, .301910D+02, .345060D+02, .389420D+02, .434930D+02
*   .481510D+02, .529080D+02, .577580D+02, .626930D+02, .677060D+02
*   .727900D+02, .779410D+02, .831530D+02, .884210D+02, .937410D+02
*   .991080D+02, .104520D+03, .109973D+03, .115464D+03, .120990D+03
*   .126549D+03, .132139D+03, .137757D+03, .143403D+03, .149073D+03
*   .154768D+03, .160485D+03, .166222D+03, .171980D+03, .177757D+03
*   .183522D+03, .189363D+03, .195191D+03, .201034D+03, .206982D+03
*   .212764D+03, .218650D+03, .224548D+03, .230458D+03, .236380D+03
*   .242313D+03, .248258D+03, .254215D+03, .260184D+03, .266164D+03
*   .272157D+03, .278161D+03, .284177D+03, .290204D+03, .296244D+03
*   .302295D+03/
*

```

Appendix G

* Hydrogen H2

*

DATA (DELH(2,I),I=1,61) /

```
* .000000D+00, .530000D-01, .150200D+01, .295900D+01, .442000D+01
*, .588200D+01, .881100D+01, .117490D+02, .147020D+02, .176760D+02
*, .206800D+02, .237190D+02, .267970D+02, .299180D+02, .330820D+02
*, .362900D+02, .395410D+02, .428350D+02, .461690D+02, .495410D+02
*, .529510D+02, .563970D+02, .598760D+02, .633870D+02, .669280D+02
*, .704980D+02, .740960D+02, .777200D+02, .813690D+02, .850430D+02
*, .887400D+02, .924600D+02, .962020D+02, .999660D+02, .103750D+03
*, .107555D+03, .111380D+03, .115224D+03, .119089D+03, .122972D+03
*, .126874D+03, .130795D+03, .134734D+03, .138692D+03, .142667D+03
*, .146660D+03, .150670D+03, .154698D+03, .158741D+03, .162801D+03
*, .166876D+03, .170967D+03, .175071D+03, .179190D+03, .183322D+03
*, .187465D+03, .191621D+03, .195787D+03, .199963D+03, .204148D+03
*, .208341D+03/
```

*

* Oxygen O2

*

DATA (DELH(3,I),I=1,61) /

```
* .000000D+00, .540000D-01, .153100D+01, .302500D+01, .454300D+01
*, .608400D+01, .924400D+01, .124990D+02, .158350D+02, .192410D+02
*, .227030D+02, .262120D+02, .297610D+02, .333440D+02, .369570D+02
*, .405990D+02, .442660D+02, .479580D+02, .516730D+02, .554130D+02
*, .591750D+02, .629610D+02, .667690D+02, .706000D+02, .744530D+02
*, .783280D+02, .822240D+02, .861410D+02, .900790D+02, .940360D+02
*, .980130D+02, .102009D+03, .106023D+03, .110054D+03, .114102D+03
*, .118165D+03, .122245D+03, .126339D+03, .130447D+03, .134569D+03
*, .138705D+03, .142854D+03, .147015D+03, .151188D+03, .155374D+03
*, .159572D+03, .163783D+03, .168005D+03, .172240D+03, .176488D+03
*, .180749D+03, .185023D+03, .189311D+03, .193614D+03, .197933D+03
*, .202267D+03, .206618D+03, .210987D+03, .215375D+03, .219782D+03
*, .224210D+03/
```

*

* Hydroxyl HO

*

DATA (DELH(4,I),I=1,61) /

```
* .000000D+00, .550000D-01, .154900D+01, .303500D+01, .451500D+01
*, .599200D+01, .894300D+01, .119020D+02, .148800D+02, .178880D+02
*, .209350D+02, .240240D+02, .271600D+02, .303420D+02, .335690D+02
```

Appendix G

```
* ,.368390D+02, .401510D+02, .435020D+02, .468890D+02, .503100D+02
* ,.537620D+02, .572430D+02, .607520D+02, .642850D+02, .678410D+02
* ,.714190D+02, .750170D+02, .786330D+02, .822670D+02, .859180D+02
* ,.895840D+02, .932650D+02, .969600D+02, .100667D+03, .104387D+03
* ,.108119D+03, .111863D+03, .115617D+03, .119381D+03, .123155D+03
* ,.126939D+03, .130732D+03, .134534D+03, .138345D+03, .142164D+03
* ,.145991D+03, .149827D+03, .153670D+03, .157521D+03, .161380D+03
* ,.165246D+03, .169120D+03, .173001D+03, .176889D+03, .180784D+03
* ,.184687D+03, .188597D+03, .192514D+03, .196438D+03, .200369D+03
* ,.204308D+03/
```

*

* Hydrogen H

*

DATA (DELH(5,I),I=1,61) /

```
* ,.000000D+00, .380000D+01, .107800D+01, .211700D+01, .315600D+01
* ,.419600D+01, .627400D+01, .835300D+01, .104310D+02, .125100D+02
* ,.145890D+02, .166670D+02, .187460D+02, .208240D+02, .229030D+02
* ,.249820D+02, .270600D+02, .291390D+02, .312170D+02, .332960D+02
* ,.353750D+02, .374530D+02, .395320D+02, .416100D+02, .436890D+02
* ,.457680D+02, .478460D+02, .499250D+02, .520040D+02, .540820D+02
* ,.561610D+02, .582390D+02, .603180D+02, .623970D+02, .644750D+02
* ,.665540D+02, .686320D+02, .707110D+02, .727900D+02, .748680D+02
* ,.769470D+02, .790250D+02, .811040D+02, .831830D+02, .852610D+02
* ,.873400D+02, .894180D+02, .914970D+02, .935760D+02, .956540D+02
* ,.977330D+02, .998110D+02, .101890D+03, .103969D+03, .106047D+03
* ,.108126D+03, .110204D+03, .112283D+03, .114362D+03, .116440D+03
* ,.118519D+03/
```

*

* Oxygen O

*

DATA (DELH(6,I),I=1,61) /

```
* ,.000000D+00, .410000D+01, .112900D+01, .220700D+01, .327800D+01
* ,.434300D+01, .646200D+01, .857000D+01, .106710D+02, .127670D+02
* ,.148600D+02, .169500D+02, .190390D+02, .211260D+02, .232120D+02
* ,.252960D+02, .273810D+02, .294640D+02, .315470D+02, .336300D+02
* ,.357130D+02, .377960D+02, .398780D+02, .419620D+02, .440450D+02
* ,.461300D+02, .482160D+02, .503030D+02, .523910D+02, .544810D+02
* ,.565740D+02, .586690D+02, .607670D+02, .628670D+02, .649710D+02
* ,.670790D+02, .691900D+02, .713050D+02, .734240D+02, .755470D+02
* ,.776750D+02, .798080D+02, .819450D+02, .840870D+02, .862340D+02
```

Appendix G

* .883860D+02, .905430D+02, .927050D+02, .948720D+02, .970450D+02
 * .992220D+02, .101405D+03, .103592D+03, .105784D+03, .107982D+03
 * .110184D+03, .112391D+03, .114602D+03, .116818D+03, .119039D+03
 * .121264D+03/

*

* Heat Capacity J/mol K

*

* Steam H2O

*

DATA (CPS(1,I),I=1,61) /

* .335900D+02, .335960D+02, .339290D+02, .342620D+02, .347440D+02
 * .352260D+02, .363250D+02, .374950D+02, .387210D+02, .399870D+02
 * .412680D+02, .425360D+02, .437680D+02, .449450D+02, .460540D+02
 * .470900D+02, .480500D+02, .489350D+02, .497490D+02, .504960D+02
 * .511800D+02, .518230D+02, .524080D+02, .529470D+02, .534440D+02
 * .539040D+02, .543290D+02, .547230D+02, .550890D+02, .554300D+02
 * .557480D+02, .560440D+02, .563230D+02, .565830D+02, .568280D+02
 * .570580D+02, .572760D+02, .574800D+02, .576750D+02, .578590D+02
 * .580330D+02, .581990D+02, .583570D+02, .585070D+02, .586500D+02
 * .587870D+02, .589180D+02, .590440D+02, .591640D+02, .592750D+02
 * .593900D+02, .595090D+02, .596280D+02, .597460D+02, .598640D+02
 * .599820D+02, .601000D+02, .602180D+02, .603350D+02, .604530D+02
 * .605710D+02/

*

* Hydrogen H2

*

DATA (CPS(2,I),I=1,61) /

* .288360D+02, .288490D+02, .290810D+02, .291810D+02, .292290D+02
 * .292600D+02, .293270D+02, .294410D+02, .296240D+02, .298810D+02
 * .302050D+02, .305810D+02, .309920D+02, .314230D+02, .318610D+02
 * .322980D+02, .327250D+02, .331390D+02, .335370D+02, .339170D+02
 * .342800D+02, .346240D+02, .349520D+02, .352630D+02, .355590D+02
 * .358420D+02, .361110D+02, .363700D+02, .366180D+02, .368560D+02
 * .370870D+02, .373110D+02, .375280D+02, .377400D+02, .379460D+02
 * .381490D+02, .383480D+02, .385440D+02, .387380D+02, .389280D+02
 * .391160D+02, .393010D+02, .394840D+02, .396650D+02, .398420D+02
 * .400170D+02, .401880D+02, .403550D+02, .405180D+02, .406760D+02
 * .408290D+02, .409760D+02, .411170D+02, .412520D+02, .413790D+02
 * .414980D+02, .416090D+02, .417120D+02, .418060D+02, .418900D+02
 * .419650D+02/

Appendix G

*

* Oxygen O2

*

DATA (CPS(3,I),I=1,61) /

* .293760D+02, .293850D+02, .296940D+02, .301060D+02, .305840D+02
*, .310910D+02, .320900D+02, .329810D+02, .337330D+02, .343550D+02
*, .348700D+02, .353000D+02, .356670D+02, .359880D+02, .362770D+02
*, .365440D+02, .367960D+02, .370400D+02, .372770D+02, .375100D+02
*, .377410D+02, .379690D+02, .381950D+02, .384190D+02, .386390D+02
*, .388560D+02, .390680D+02, .392760D+02, .394780D+02, .396740D+02
*, .398640D+02, .400480D+02, .402250D+02, .403950D+02, .405590D+02
*, .407160D+02, .408680D+02, .410130D+02, .411540D+02, .412890D+02
*, .414210D+02, .415490D+02, .416740D+02, .417980D+02, .419200D+02
*, .420420D+02, .421640D+02, .422870D+02, .424130D+02, .425420D+02
*, .426750D+02, .428130D+02, .429560D+02, .431050D+02, .432620D+02
*, .434260D+02, .435990D+02, .437810D+02, .439730D+02, .441750D+02
*, .443870D+02/

*

* Hydroxyl HO

*

DATA (CPS(4,I),I=1,61) /

* .299860D+02, .299770D+02, .297800D+02, .296500D+02, .295670D+02
*, .295210D+02, .295270D+02, .296630D+02, .299170D+02, .302640D+02
*, .306760D+02, .311240D+02, .315860D+02, .320460D+02, .324920D+02
*, .329170D+02, .333190D+02, .336940D+02, .340440D+02, .343690D+02
*, .346700D+02, .349500D+02, .352090D+02, .354490D+02, .356730D+02
*, .358810D+02, .360750D+02, .362560D+02, .364260D+02, .365860D+02
*, .367360D+02, .368780D+02, .370130D+02, .371400D+02, .372610D+02
*, .373760D+02, .374860D+02, .375920D+02, .376930D+02, .377910D+02
*, .378850D+02, .379760D+02, .380640D+02, .381500D+02, .382330D+02
*, .383150D+02, .383940D+02, .384720D+02, .385490D+02, .386250D+02
*, .386990D+02, .387730D+02, .388460D+02, .389190D+02, .389910D+02
*, .390620D+02, .391340D+02, .392060D+02, .392780D+02, .393500D+02
*, .394230D+02/

*

* Hydrogen H

*

DATA (CPS(5,I),I=1,61) /61*.207860D+02/

*

* Oxygen O

Appendix G

*

DATA (CPS(6,I),I=1,61) /

```
* .219110D+02, .219010D+02, .216570D+02, .214820D+02, .213540D+02
*, .212570D+02, .211240D+02, .210400D+02, .209840D+02, .209440D+02
*, .209150D+02, .208930D+02, .208770D+02, .208640D+02, .208530D+02
*, .208450D+02, .208380D+02, .208330D+02, .208300D+02, .208270D+02
*, .208260D+02, .208270D+02, .208300D+02, .208350D+02, .208410D+02
*, .208510D+02, .208620D+02, .208770D+02, .208940D+02, .209140D+02
*, .209370D+02, .209630D+02, .209910D+02, .210220D+02, .210560D+02
*, .210920D+02, .211300D+02, .211700D+02, .212130D+02, .212570D+02
*, .213020D+02, .213490D+02, .213970D+02, .214450D+02, .214950D+02
*, .215450D+02, .215960D+02, .216470D+02, .216970D+02, .217480D+02
*, .217990D+02, .218490D+02, .218990D+02, .219490D+02, .219970D+02
*, .220450D+02, .220930D+02, .221390D+02, .221840D+02, .222290D+02
*, .222730D+02/
```

*

***** END OF BLOCK DATA *

END

SUBROUTINE MOLARMAS(MMIX,MM)

IMPLICIT REAL*8 (A-H,O-Z)

REAL*8 M(6),MM(6),MMIX,Y(6)

COMMON /FRACT/ Y

DATA M /.1801528D2, .201588D1, .319988D2, .1700734D2, .100794D1

1, .1599940D2/

MMIX=0.0D0

DO 9 I=1,6

MMIX=MMIX+(Y(I)*M(I)*.1D-2)

MM(I)=M(I)*.1D-2

9 CONTINUE

RETURN

END

Appendix G

```
      SUBROUTINE FRENTA(FH)
      IMPLICIT REAL*8 (A-H,O-Z)
      INTEGER I
      REAL*8 DH(6),CPI(6),FH25C(6),FH(6)
      COMMON /JANENT/ DH,CPI
*   Enthalpys of formation at t=25degC and P=0.1MPa from Chase (1985) *
      DATA FH25C/-.241826D6, .000000D0, .000000D0, .389870D5, .217999D6
      1      , .249173D6/
      DO 9 I=1,6
          FH(I)=FH25C(I)+DH(I)
9   CONTINUE
      RETURN
      END

      SUBROUTINE FRCOND(PMPA,TC,KFM)
      INTEGER I,J,L
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 PMPA,TC,TK,KF,KFM
      REAL*8 PKF(13),TKF(45),AKFM(13,45),AP(2),AT(2),AKF(2,2)
      LOGICAL EQUAP,EQUAT
      COMMON /FRKON/ PKF,TKF,AKFM
      COMMON /WAREAK/ AKF
      PATM = PMPA*.986813D+01
      CALL SEARCH(PKF,PATM,13,I,EQUAP)
      TK=TC+.27315D3
      CALL SEARCH(TKF,TK,45,J,EQUAT)
      CALL WORKAK(I,J,EQUAP,EQUAT)
      IF (.NOT.(EQUAP.EQV..TRUE.).AND..NOT.(EQUAT.EQV..TRUE.)) THEN
          DO 8 L=1,2
              AP(L)=PKF(I-1+L)
              AT(L)=TKF(J-1+L)
8   CONTINUE
      ELSE IF(EQUAT.EQV..TRUE.) THEN
          AT(1)=TKF(J)
          DO 9 L=1,2
              AP(L)=PKF(I-1+L)
9   CONTINUE
      ELSE
          AP(1)=PKF(I)
          DO 10 L=1,2
              AT(L)=TKF(J-1+L)
```

Appendix G

```
10  CONTINUE
    END IF
    IF (EQUAP.EQV..TRUE.) THEN
        IF (EQUAT.EQV..TRUE.) THEN
            KFM= AKFM(I,J) * .418680D+03
            RETURN
        ELSE
            CALL INTE2P(TK,AT,AKF,KF)
            KFM = KF * .418680D+03
            RETURN
        END IF
    ELSE
        PRK=(PATM*AP(2)-AP(1)*AP(2))/(PATM*AP(2)-AP(1)*PATM)
        IF (EQUAT.EQV..TRUE.) THEN
            CALL INTE2T(PRK,AKF,KF)
            KFM = KF * .418680D+03
            RETURN
        END IF
        CALL INTER4 (PRK,TK,AT,AKF,KF)
        KFM = KF * .418680D+03
    END IF
    RETURN
*
```

***** END OF SUBPROGRAM *

END

Appendix G

```

      SUBROUTINE WORKAK(IT,JT,EQUAPT,EQUATT)
      ***** SUBROUTINE IDENTIFICATION *****
      *
      *   This subroutine identifies given pressure and temperature that
      *   may be equal to any of the pressures and temperatures for
      *   thermodynamic properties data stored in BLOCK DATA DATAKF.
      *   Should they not equal it identify values of properties
      *   from BLOCK DATAKF for first large and first smaller pressure
      *   and temperature then given pressure and temperature.
      *
      *****
      *
      INTEGER IT,JT,II,JJ,IL,JL
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 PKF(13),TKF(45),AKFM(13,45),AKF(2,2)
      LOGICAL EQUAPT,EQUATT
      COMMON /FRKON/ PKF,TKF,AKFM
      COMMON/WAREAK/ AKF
      IF (EQUAPT,EQV..TRUE.) THEN
        IL=1
      ELSE
        IL=2
      END IF
      IF (EQUATT,EQV..TRUE.) THEN
        JL=1
      ELSE
        JL=2
      END IF
      DO 99 II=1,IL
        DO 9 JJ=1,JL
          AKF(II,JJ)=AKFM(IT,JT)
          JT=JT+1
        9 CONTINUE
        JT=JT-JL
        IT=IT+1
      99 CONTINUE
      IT=IT-IL
      RETURN
      ***** END OF SUBPROGRAM *****
      END

```

Appendix G

BLOCK DATAKF

INTEGER I

REAL*8 PKF(13),TKF(45),AKFM(13,45)

COMMON /FRKON/ PKF,TKF,AKFM

*

*

* Pressure (atm) table

*

DATA (PKF(I),I=1,13) / .100000D-02, .300000D-02, .100000D-01
*, .300000D-01, .100000D+00, .300000D+00, .100000D+01, .300000D+01
*, .100000D+02, .300000D+02, .100000D+03, .300000D+03, .100000D+04/

*

*

* Temperature (K) table

*

DATA (TKF(I),I=1,45) /
* .600000D+03, .700000D+03, .800000D+03, .900000D+03
*, .100000D+04, .110000D+04, .120000D+04, .130000D+04, .140000D+04
*, .150000D+04, .160000D+04, .170000D+04, .180000D+04, .190000D+04
*, .200000D+04, .210000D+04, .220000D+04, .230000D+04, .240000D+04
*, .250000D+04, .260000D+04, .270000D+04, .280000D+04, .290000D+04
*, .300000D+04, .310000D+04, .320000D+04, .330000D+04, .340000D+04
*, .350000D+04, .360000D+04, .370000D+04, .380000D+04, .390000D+04
*, .400000D+04, .410000D+04, .420000D+04, .430000D+04, .440000D+04
*, .450000D+04, .460000D+04, .470000D+04, .480000D+04, .490000D+04
*, .500000D+04/

*

*

* Frozen Thermal Conductivity of the mixture

* by Svehla (1964) (cal/cm³ K)

*

DATA (AKFM(I,J),I=1,45) /
* .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .406000D-03
*, .442000D-03, .480000D-03, .518000D-03, .560000D-03, .605000D-03
*, .657000D-03, .721000D-03, .800000D-03, .901000D-03, .102500D-03
*, .115900D-02, .127200D-02, .133900D-02, .137200D-02, .139600D-02

Appendix G

```
* ,.142300D-02, .145500D-02, .148900D-02, .152500D-02, .156200D-02
* ,.159900D-02, .163700D-02, .167500D-02, .171200D-02, .175000D-02
* ,.178700D-02, .182500D-02, .186300D-02, .190000D-02, .193700D-02
* ,.197500D-02, .201200D-02, .204900D-02, .208500D-02, .212200D-02
* ,.215900D-02/
DATA (AKFM(2,I),I=1,45) /
*      .131000D-03, .161000D-03, .193000D-03, .226000D-03
* ,.261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
* ,.442000D-03, .479000D-03, .517000D-03, .556000D-03, .598000D-03
* ,.644000D-03, .697000D-03, .761000D-03, .839000D-03, .935000D-03
* ,.105100D-02, .117800D-02, .129300D-02, .137400D-03, .141900D-03
* ,.144700D-02, .147200D-02, .150100D-02, .153300D-02, .156700D-02
* ,.160300D-02, .163900D-02, .167600D-02, .171300D-02, .175000D-02
* ,.178800D-02, .182500D-02, .186300D-02, .190000D-02, .193800D-02
* ,.197500D-02, .201200D-02, .204900D-02, .208500D-02, .212200D-02
* ,.215900D-02/
DATA (AKFM(3,I),I=1,45) /
*      .131000D-03, .161000D-03, .193000D-03, .226000D-03
* ,.261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
* ,.442000D-03, .478000D-03, .515000D-03, .553000D-03, .592000D-03
* ,.634000D-03, .681000D-03, .733000D-03, .795000D-03, .868000D-03
* ,.956000D-03, .106000D-02, .117700D-02, .129400D-02, .139200D-02
* ,.145800D-02, .149900D-02, .152700D-02, .155300D-02, .158200D-02
* ,.161300D-02, .164600D-02, .168100D-02, .171600D-02, .175300D-02
* ,.178900D-02, .182700D-02, .186400D-02, .190100D-02, .193800D-02
* ,.197500D-02, .201200D-02, .204900D-02, .208600D-02, .212200D-02
* ,.215900D-02/
DATA (AKFM(4,I),I=1,45) /
*      .131000D-03, .161000D-03, .193000D-03, .226000D-03
* ,.261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
* ,.442000D-03, .478000D-03, .514000D-03, .551000D-03, .589000D-03
* ,.629000D-03, .671000D-03, .717000D-03, .769000D-03, .828000D-03
* ,.897000D-03, .979000D-03, .107400D-02, .118100D-02, .129300D-02
* ,.139800D-02, .148200D-02, .154000D-02, .157800D-02, .160700D-02
* ,.163400D-02, .166200D-02, .169300D-02, .172500D-02, .175900D-02
* ,.179400D-02, .183000D-02, .186600D-02, .190300D-02, .194000D-02
* ,.197600D-02, .201300D-02, .205000D-02, .208600D-02, .212300D-02
* ,.216000D-02/
DATA (AKFM(5,I),I=1,45) /
*      .131000D-03, .161000D-03, .193000D-03, .226000D-03
```

Appendix G

```

*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .442000D-03, .478000D-03, .514000D-03, .550000D-03, .587000D-03
*, .624000D-03, .664000D-03, .705000D-03, .750000D-03, .800000D-03
*, .855000D-03, .919000D-03, .992000D-03, .107600D-02, .117000D-02
*, .127300D-02, .137800D-02, .147600D-02, .155600D-02, .161600D-02
*, .165900D-02, .169200D-02, .172000D-02, .174800D-02, .177700D-02
*, .180800D-02, .184100D-02, .187400D-02, .190900D-02, .194500D-02
*, .198000D-02, .201600D-02, .205200D-02, .208800D-02, .212400D-02
*, .216100D-02/
DATA (AKFM(6,I),I=1,45) /
*
      .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .441000D-03, .477000D-03, .513000D-03, .549000D-03, .585000D-03
*, .622000D-03, .659000D-03, .698000D-03, .739000D-03, .783000D-03
*, .831000D-03, .883000D-03, .942000D-03, .100900D-02, .108400D-02
*, .116800D-02, .126100D-02, .135900D-02, .145700D-02, .154900D-02
*, .162800D-02, .169000D-02, .173800D-02, .177500D-02, .180600D-02
*, .183500D-02, .186400D-02, .189300D-02, .192500D-02, .195700D-02
*, .199000D-02, .202400D-02, .205800D-02, .209300D-02, .212900D-02
*, .216400D-02/
DATA (AKFM(7,I),I=1,45) /
*
      .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .441000D-03, .477000D-03, .513000D-03, .549000D-03, .584000D-03
*, .620000D-03, .656000D-03, .693000D-03, .731000D-03, .771000D-03
*, .813000D-03, .858000D-03, .907000D-03, .960000D-03, .101900D-02
*, .108500D-02, .115800D-02, .123800D-02, .132500D-02, .141600D-02
*, .150900D-02, .159800D-02, .168000D-02, .175000D-02, .180800D-02
*, .185500D-02, .189300D-02, .192600D-02, .195700D-02, .198600D-02
*, .201600D-02, .204600D-02, .207700D-02, .210900D-02, .214200D-02
*, .217600D-02/
DATA (AKFM(8,I),I=1,45) /
*
      .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .441000D-03, .477000D-03, .513000D-03, .548000D-03, .584000D-03
*, .619000D-03, .654000D-03, .690000D-03, .726000D-03, .754000D-03
*, .802000D-03, .843000D-03, .886000D-03, .931000D-03, .981000D-03
*, .103500D-02, .109300D-02, .115800D-02, .122800D-02, .130400D-02
*, .138500D-02, .147000D-02, .155700D-02, .164300D-02, .172500D-02
*, .180000D-02, .186600D-02, .192200D-02, .197000D-02, .201100D-02

```

Appendix G

```

*, .204700D-02, .207900D-02, .211000D-02, .214000D-02, .217000D-02
*, .220100D-02/
DATA (AKFM(9,I),I=1,45) /
*      .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .441000D-03, .477000D-03, .513000D-03, .548000D-03, .583000D-03
*, .618000D-03, .653000D-03, .688000D-03, .723000D-03, .758000D-03
*, .794000D-03, .832000D-03, .870000D-03, .911000D-03, .953000D-03
*, .998000D-03, .104700D-02, .109800D-02, .115400D-02, .121400D-02
*, .127900D-02, .134800D-02, .142200D-02, .149900D-02, .158000D-02
*, .166100D-02, .174200D-02, .182000D-02, .189400D-02, .196100D-02
*, .202300D-02, .207700D-02, .212400D-02, .216700D-02, .220500D-02
*, .224000D-02/
DATA (AKFM(10,I),I=1,45) /
*      .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .441000D-03, .477000D-03, .513000D-03, .548000D-03, .583000D-03
*, .617000D-03, .652000D-03, .686000D-03, .720000D-03, .755000D-03
*, .790000D-03, .825000D-03, .861000D-03, .898000D-03, .936000D-03
*, .976000D-03, .101800D-02, .106300D-02, .111000D-02, .115900D-02
*, .121200D-02, .126900D-02, .132900D-02, .139200D-02, .146000D-02
*, .153000D-02, .160400D-02, .167900D-02, .175600D-02, .183200D-02
*, .190700D-02, .198000D-02, .204900D-02, .211300D-02, .217300D-02
*, .222700D-02/
DATA (AKFM(11,I),I=1,45) /
*      .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .441000D-03, .477000D-03, .513000D-03, .548000D-03, .583000D-03
*, .617000D-03, .651000D-03, .685000D-03, .719000D-03, .752000D-03
*, .786000D-03, .820000D-03, .854000D-03, .889000D-03, .924000D-03
*, .960000D-03, .998000D-03, .103700D-02, .107700D-02, .111900D-02
*, .116400D-02, .121000D-02, .125900D-02, .131000D-02, .136400D-02
*, .142100D-02, .148100D-02, .154300D-02, .160900D-02, .167600D-02
*, .174600D-02, .181700D-02, .188900D-02, .196100D-02, .203300D-02
*, .210300D-02/
DATA (AKFM(12,I),I=1,45) /
*      .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .441000D-03, .477000D-03, .513000D-03, .548000D-03, .582000D-03
*, .617000D-03, .651000D-03, .684000D-03, .718000D-03, .751000D-03

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Appendix G

```

*, .784000D-03, .817000D-03, .850000D-03, .883000D-03, .917000D-03
*, .951000D-03, .986000D-03, .102100D-02, .105800D-02, .109500D-02
*, .113400D-02, .117400D-02, .121600D-02, .126000D-02, .130500D-02
*, .135200D-02, .140200D-02, .145400D-02, .150700D-02, .156400D-02
*, .162200D-02, .168300D-02, .174600D-02, .181000D-02, .187700D-02
*, .194400D-02/
DATA (AKFM(13,I),I=1,45) /
*, .131000D-03, .161000D-03, .193000D-03, .226000D-03
*, .261000D-03, .296000D-03, .333000D-03, .369000D-03, .405000D-03
*, .441000D-03, .477000D-03, .513000D-03, .548000D-03, .582000D-03
*, .617000D-03, .650000D-03, .684000D-03, .717000D-03, .750000D-03
*, .782000D-03, .815000D-03, .847000D-03, .879000D-03, .911000D-03
*, .944000D-03, .976000D-03, .101000D-02, .104300D-02, .107800D-02
*, .111300D-02, .114800D-02, .118500D-02, .122300D-02, .126200D-02
*, .130200D-02, .134300D-02, .138600D-02, .143100D-02, .147700D-02
*, .152500D-02, .157500D-02, .162600D-02, .168000D-02, .173500D-02
*, .179200D-02/
*
***** END OF BLOCK DATA *
***** THIS IS THE END OF FROZEN PROPERTY CODE FOR HIGH TEMP. STEAM *****
END

```

WARNING! The Frozen property code use data for thermal conductivity by Svehla (1964) which are lower then should be. Since, this are the only available data in literature for frozen thermal conductivity, they are adapted in this work. The estimated inaccuracy of the predictions is in order of -10%.

```
***** PROGRAM IDENTIFICATION *****
```

*

✱

*

*

✱

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209

Appendix G

```
99 CONTINUE
*****      TERMINATION BLOCK      BLOCK 0800 *
*
      CLOSE (1)
*****      END OF MAIN
PROGRAM *
      END
```


Appendix H

Programming Specifications of the UODH2O Code for Effective Properties of Dissociated Steam for Pressure from 0.01 to 100.00MPa and Temperature from 1000. to 5726.85°C

This chapter includes all subroutines, written in FORTRAN77 computer language, of the UODH2O (University of Ottawa Dissociated H₂O) code for prediction of effective high temperature steam properties. The required input data are pressure P(MPa) and temperature T(°C). After the main program calls the subroutine UODH2O(P,T), computations are performed. The results of the calculations are stored in COMMON /THPRO/ block for thermodynamic properties V, CP, H and S, COMMON /TRPRO/ block for transport properties K and MU and COMMON /PRONO/ block for derived properties RHO, NI, TDF and PR.

Appendix H

```
SUBROUTINE UODH2O(PIN,TIN)
***** SUBROUTINE IDENTIFICATION *****
*
* This is University of Ottawa High Temperature Dissociated
* Steam Property code - UODH2O
*
* Code has total 1434 lines.
*
* Code generates Thermodynamic and Transport Properties
* of High Temperature Dissociated Steam
* for Pressures from 0.01 to 100. MPa
* at Temperatures from 1000. to 5726.85 degC.
*
* Written by ALEKSANDAR VASIC'      Revised March /1990
* University of Ottawa
*
*****
*
***** VARIABLE IDENTIFICATION *****
*
* PIN  = Input Pressure (MPa = MN/m**2)
* TIN  = Input Temperature (degC)
*
* Output are stored in COMMON /THPRO/
* V     = Specific Volume (m**3/kg)
* S     = Entropy (J/kg*K)
* H     = Enthalpy (J/kg)
* CP    = Heat Capacity (J/kg*K)
*
* Output are stored in COMMON /TRPRO/
* K     = Thermal Conductivity (W/m*K)
* MU    = Dynamic Viscosity (N*s/m**2)
*
* Output are stored in COMMON /PRONO/
* RHO   = Density (kg/m**3)
* NI    = Kinematic Viscosity (m**2/s)
* TDF   = Thermal diffusivity (m**2/s)
* PR    = Prandtl number (-)
*
*****
```

Appendix H

```
*
*****      TYPE DECLARATION      BLOCK 0000
*
  IMPLICIT REAL*8 (A-H,O-Z)
  REAL*8 PIN,TIN,V,S,H,CP,MU,K,RHO,NI,TDF,PR
  COMMON /THPRO/ V,S,H,CP
  COMMON /TRPRO/ MU,K
  COMMON /PRONO/ RHO,NI,TDF,PR
*
*****
*
*****      COMPUTATION BLOCK      BLOCK 0100 *
*
  CALL PRDH2O (PIN,TIN)
  CALL TPDH2O (PIN,TIN)
  RHO = .1D1 / V
  NI  = MU * V
  TDF = (K * V) / CP
  PR  = (CP * MU) / K
  RETURN
*
*****      END OF SUBPROGRAM *
  END
```

Appendix H

```

SUBROUTINE PRDH2O (PRE,TC)
***** SUBROUTINE IDENTIFICATION *****
*
*   This SUBROUTINE generates Thermodynamic Properties.
*
*****
*
  INTEGER I,J,L
  IMPLICIT REAL*8 (A-H,O-Z)
  REAL*8 PRE,TC,TK,
1    DH2OP(26),DH2OT(26)
2    ,P(2),T(2)
3    ,DH2OV(26,26),DH2OS(26,26),DH2OH0(26),DH2OH(26,26)
4    ,DH2OCP(26,26)
5    ,V4(2,2),S4(2,2),H4(2,2),CP4(2,2)
6    ,V,S,H,CP
  LOGICAL EQUALP,EQUALT
  COMMON /THPTD/ DH2OP,DH2OT
  COMMON /THPROD/ DH2OV,DH2OS,DH2OH0,DH2OH,DH2OCP
  COMMON /WAREA/ V4,S4,H4,CP4
  COMMON /THPRO/ V,S,H,CP
  TK=TC+273.15
  CALL SEARCH(DH2OP,PRE,26,I,EQUALP)
  CALL SEARCH(DH2OT,TK,26,J,EQUALT)
  CALL WORKAR(I,J,EQUALP,EQUALT)
  IF (.NOT.(EQUALP.EQV..TRUE.).AND..NOT.(EQUALT.EQV..TRUE.)) THEN
    DO 5 L=1,2
      P(L)=DH2OP(I-1+L)
      T(L)=DH2OT(J-1+L)
5    CONTINUE
    ELSE IF(EQUALT.EQV..TRUE.) THEN
      T(1)=DH2OT(J)
      DO 6 L=1,2
        P(L)=DH2OP(I-1+L)
6    CONTINUE
    ELSE
      P(1)=DH2OP(I)
      DO 7 L=1,2
        T(L)=DH2OT(J-1+L)
7    CONTINUE

```

Appendix H

```
END IF
IF (EQUALP.EQV..TRUE.) THEN
  IF (EQUALT.EQV..TRUE.) THEN
    V=DH2OV(I,J)
    S=DH2OS(I,J)
    H=DH2OH(I,J)+DH2OH0(I)
    CP=DH2OCP(I,J)
    RETURN
  ELSE
    CALL INTE2P(TK,T,V4,V)
    CALL INTE2P(TK,T,CP4,CP)
    CALL INTE2P(TK,T,H4,H)
    CALL INTE2P(TK,T,S4,S)
    RETURN
  END IF
ELSE
  PR=(PRE*P(2)-P(1)*P(2))/(PRE*P(2)-P(1)*PRE)
  IF (EQUALT.EQV..TRUE.) THEN
    CALL INTE2T(PR,V4,V)
    CALL INTE2T(PR,CP4,CP)
    CALL INTE2T(PR,H4,H)
    CALL INTE2T(PR,S4,S)
    RETURN
  END IF
  CALL INTER4 (PR,TK,T,V4,V)
  CALL INTER4 (PR,TK,T,CP4,CP)
  CALL INTER4 (PR,TK,T,H4,H)
  CALL INTER4 (PR,TK,T,S4,S)
END IF
RETURN
***** END OF SUBPROGRAM *
END
```

Appendix H

```

SUBROUTINE TPDH2O (PRE,TC)
***** SUBROUTINE IDENTIFICATION *****
*
*   This SUBROUTINE generates Transport Properties.
*
*****
*
  INTEGER IT,JT,L
  IMPLICIT REAL*8 (A-H,O-Z)
  REAL*8 PRE,TC,TK
1    ,DH2OPT(17),DH2OTT(25)
2    ,PT(2),TT(2)
3    ,DH2OMU(17,25),DH2OK(17,25)
4    ,MU4(2,2),K4(2,2)
5    ,MU,K
  LOGICAL EQUAPT,EQUATT
  COMMON /TRPTD/ DH2OPT,DH2OTT
  COMMON /TRPROD/ DH2OMU,DH2OK
  COMMON /WAREAT/ MU4,K4
  COMMON /TRPRO/ MU,K
  TK=TC+273.15
  CALL SEARCH(DH2OTT,TK,25,JT,EQUATT)
  CALL SEARCH(DH2OPT,PRE,17,IT,EQUAPT)
  CALL WORKAT(IT,JT,EQUAPT,EQUATT)
  IF (.NOT.(EQUAPT.EQV..TRUE.).AND..NOT.(EQUATT.EQV..TRUE.)) THEN
    DO 8 L=1,2
      PT(L)=DH2OPT(IT-1+L)
      TT(L)=DH2OTT(JT-1+L)
8    CONTINUE
    ELSE IF(EQUATT.EQV..TRUE.) THEN
      TT(1)=DH2OTT(JT)
      DO 9 L=1,2
        PT(L)=DH2OPT(IT-1+L)
9    CONTINUE
    ELSE
      PT(1)=DH2OPT(IT)
      DO 10 L=1,2
        TT(L)=DH2OTT(JT-1+L)
10   CONTINUE
    END IF

```

Appendix H

```
IF (EQUAPT.EQV..TRUE.) THEN
  IF (EQUATT.EQV..TRUE.) THEN
    K=DH2OK(IT,JT)
    MU=DH2OMU(IT,JT)
    RETURN
  ELSE
    CALL INTE2P(TK,TT,K4,K)
    CALL INTE2P(TK,TT,MU4,MU)
    RETURN
  END IF
ELSE
  PRK=(PRE*PT(2)-PT(1)*PT(2))/(PRE*PT(2)-PT(1)*PRE)
  PRMU=(PRE-PT(1))/(PT(2)-PT(1))
  IF (EQUATT.EQV..TRUE.) THEN
    CALL INTE2T(PRK,K4,K)
    CALL INTE2T(PRMU,MU4,MU)
    RETURN
  END IF
  CALL INTER4 (PRK,TK,TT,K4,K)
  CALL INTER4 (PRMU,TK,TT,MU4,MU)
END IF
RETURN
***** END OF SUBPROGRAM *
END
```

Appendix H

```

SUBROUTINE SEARCH (ARR,VAR,MAXARR,I,EQUAL)
***** SUBROUTINE IDENTIFICATION *****
*
* Subroutine which searches accending array ARR for first value
* which is less or equal to given value VAR.
*
*****
*
INTEGER I,MIN,MAX,MAXARR
IMPLICIT REAL*8 (A-H,O-Z)
REAL*8 ARR(MAXARR),VAR
LOGICAL EQUAL
EQUAL=.FALSE.
MIN=1
MAX=MAXARR
WHILE (MIN.LE.MAX)
    I=(MIN+MAX)/2
    IF (ARR(I).EQ.VAR) THEN
        EQUAL=.TRUE.
        RETURN
    ELSE IF (ARR(I).LT.VAR) THEN
        MIN=I+1
    ELSE
        MAX=I-1
    END IF
END WHILE
I=MAX
RETURN
***** END OF SUBPROGRAM *
END
```


Appendix H

```

SUBROUTINE WORKAR(IJ,EQUALP,EQUALT)
***** SUBROUTINE IDENTIFICATION *****
*
* This subroutine indentifies if the given pressure and temperature
* are equal to any of the pressures and temperatures for
* thermodynamic properties data stored in BLOCK DATA DATAD1.
* Should they not correspond, it will indentify values of properties
* from BLOCK DATAD1 for first large and first smaller pressure
* and temperaure then given pressure and temperature.
*
*****
*
  INTEGER I,J,II,JJ,IL,JL
  LOGICAL EQUALP,EQUALT
  IMPLICIT REAL*8 (A-H,O-Z)
  REAL*8 DH2OV(26,26),DH2OS(26,26),DH2OH0(26),DH2OH(26,26)
  1  ,DH2OCP(26,26)
  2  ,V4(2,2),S4(2,2),H4(2,2),CP4(2,2)
  COMMON /THPROD/ DH2OV,DH2OS,DH2OH0,DH2OH,DH2OCP
  COMMON /WAREA/ V4,S4,H4,CP4
  IF (EQUALP.EQV..TRUE.) THEN
    IL=1
  ELSE
    IL=2
  END IF
  IF (EQUALT.EQV..TRUE.) THEN
    JL=1
  ELSE
    JL=2
  END IF
  DO 99 II=1,IL
    DO 9 JJ=1,JL
      V4(II,JJ)=DH2OV(IJ)
      S4(II,JJ)=DH2OS(IJ)
      H4(II,JJ)=DH2OH(IJ)+DH2OH0(I)
      CP4(II,JJ)=DH2OCP(IJ)
      J=J+1
  9  CONTINUE
      J=J-JL
      I=I+1

```

Appendix H

99 CONTINUE

I=I-IL

RETURN

***** END OF SUBPROGRAM *

END

SUBROUTINE WORKAT(IT,JT,EQUAPT,EQUATT)

***** SUBROUTINE IDENTIFICATION *****

*

* This subroutine identifies if the given pressure and temperature
 * are equal to any of the pressures and temperatures for
 * thermodynamic properties data stored in BLOCK DATA DATAD2.
 * If not it will identify values of properties
 * from BLOCK DATAD2 for first large and first smaller pressure
 * and temperature then given pressure and temperature.
 *

*

INTEGER IT,JT,II,JJ,IL,JL

IMPLICIT REAL*8 (A-H,O-Z)

REAL*8 DH2OMU(17,25),DH2OK(17,25)

1 ,MU4(2,2),K4(2,2)

LOGICAL EQUAPT,EQUATT

COMMON /TRPROD/ DH2OMU,DH2OK

COMMON /WAREAT/ MU4,K4

IF (EQUAPT.EQV..TRUE.) THEN

IL=1

ELSE

IL=2

END IF

IF (EQUATT.EQV..TRUE.) THEN

JL=1

ELSE

JL=2

END IF

DO 99 II=1,IL

DO 9 JJ=1,JL

K4(II,JJ)=DH2OK(IT,JT)

MU4(II,JJ)=DH2OMU(IT,JT)

JT=JT+1

9 CONTINUE

Appendix H

```

      JT=JT-JL
      IT=IT+1
      99 CONTINUE
      IT=IT-IL
      RETURN
      ***** END OF SUBPROGRAM *

      END

      SUBROUTINE INTER4(PR,TK,T,PRO4,PRO)
      *****
      SUBROUTINE IDENTIFICATION
      *
      *   This subroutine interpolates the new property value using
      *   four values of the property from BLOCK DATA
      *   neighboring to given pressure and temperature.
      *
      *****
      *
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 PR,TK,T(2),PRO4(2,2),PRO
      PRO=(PRO4(1,1)*(T(2)-TK)+PRO4(1,2)*(TK-T(1))+(PRO4(1,1)*(TK-T(2))
      1   -PRO4(1,2)*(TK-T(1))+PRO4(2,1)*(T(2)-TK)+PRO4(2,2)*(TK-T(1)))
      2   PR)/(T(2)-T(1))
      RETURN
      ***** END OF SUBPROGRAM *

      END

      SUBROUTINE INTE2P(TK,T,PRO4,PRO)
      *****
      SUBROUTINE IDENTIFICATION
      *
      *   This subroutine interpolates the new property value using
      *   two values of the property from BLOCK DATA
      *   neighboring to given temperature, given pressure is same
      *   as pressure in BLOCK DATA.
      *
      *****
      *
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 TK,T(2),PRO4(2,2),PRO
      PRO=PRO4(1,1)+((PRO4(1,2)*(TK-T(1)))-(PRO4(1,1)*(TK-T(1))))/
      1   (T(2)-T(1))
      RETURN
      ***** END OF SUBPROGRAM *

```

Appendix H

```
END
      SUBROUTINE INTE2T(PR,PRO4,PRO)
*****      SUBROUTINE IDENTIFICATION      *****
*
*   This subroutine interpolates the new property value using
*   two values of the property from BLOCK DATA
*   neighboring to given pressure, given temperature is same
*   as temperature in BLOCK DATA.
*
*****
*
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 PR,PRO4(2,2),PRO
      PRO=(PRO4(1,1)*(1.-PR))+(PRO4(2,1)*PR)
      RETURN
*****      END OF SUBPROGRAM      *
END
```

Appendix H

```

BLOCK DATA DATADI
*****
BLOCK DATA IDENTIFICATION
*****
*
*
*   Data stored in this BLOCK DATA are
*   Thermodynamic Properties of Dissociated Steam
*   for Pressures from 0.01 to 100. MN/m**2
*   at Temperatures from 1250. to 6000. K
*   from VARGATIK (1983) and data generated by author.
*
*   Written by ALEKSANDAR VASIC'      Revised  March /1990
*   University of Ottawa
*
*****
*
*****
VARIABLE IDENTIFICATION
*****
*
*   DH2OP = Pressure for Thermodynamic Properties (MN/m**2)
*   DH2OT = Temperature for Thermodynamic Properties (K)
*   DH2OV = Specific Volume (m**3/kg)
*   DH2OS = Entropy (J/kg*K)
*   DH2OH = Enthalpy (J/kg)
*   DH2OCP = Heat Capacity (J/kg*K)
*
*****
*
*****
TYPE DECLARATION                                BLOCK 0000 *
*
INTEGER I
IMPLICIT REAL*8 (A-H,O-Z)
REAL*8 DH2OP(26),DH2OT(26)
1      ,DH2OV(26,26),DH2OS(26,26),DH2OH0(26),DH2OH(26,26)
2      ,DH2OCP(26,26)
COMMON /THPTD/ DH2OP,DH2OT
COMMON /THPROD/ DH2OV,DH2OS,DH2OH0,DH2OH,DH2OCP
*
*****
*
*   PRESSURE (MN/m**2) TABLE FOR THERMODYNAMIC PROPERTIES
*
*   DATA (DH2OP(I),I=1,26)/

```

Appendix H

```
* 0.10000E-01, 0.20000E-01, 0.40000E-01, 0.60000E-01, 0.80000E-01,
* 0.10000E+00, 0.20000E+00, 0.30000E+00, 0.40000E+00, 0.50000E+00,
* 0.60000E+00, 0.80000E+00, 0.10000E+01, 0.20000E+01, 0.30000E+01,
* 0.40000E+01, 0.50000E+01, 0.60000E+01, 0.80000E+01, 0.10000E+02,
* 0.15000E+02, 0.20000E+02, 0.40000E+02, 0.60000E+02, 0.80000E+02,
* 0.10000E+03/
```

*

*

* TEMPERATURE (K) TABLE FOR THERMODYNAMIC PROPERTIES

*

DATA (DH2OT(1),I=1,26)/

```
* 0.12500E+04, 0.13000E+04, 0.14000E+04, 0.15000E+04, 0.16000E+04,
* 0.17000E+04, 0.18000E+04, 0.19000E+04, 0.20000E+04, 0.22000E+04,
* 0.24000E+04, 0.26000E+04, 0.28000E+04, 0.30000E+04, 0.32000E+04,
* 0.34000E+04, 0.36000E+04, 0.38000E+04, 0.40000E+04, 0.42000E+04,
* 0.44000E+04, 0.46000E+04, 0.48000E+04, 0.50000E+04, 0.55000E+04,
* 0.60000E+04/
```

*

*

* SPECIFIC VOLUME (m**3/kg)

*

DATA (DH2OV(1,I),I=1,26)/

```
* 0.57690E+02, 0.60000E+02, 0.64620E+02, 0.69240E+02, 0.73880E+02,
* 0.78550E+02, 0.83270E+02, 0.88080E+02, 0.93030E+02, 0.10380E+03,
* 0.11670E+03, 0.13340E+03, 0.16150E+03, 0.20540E+03, 0.27230E+03,
* 0.35500E+03, 0.43130E+03, 0.48980E+03, 0.54320E+03, 0.57060E+03,
* 0.60280E+03, 0.63300E+03, 0.66220E+03, 0.69070E+03, 0.76090E+03,
* 0.83040E+03/
```

DATA (DH2OV(2,I),I=1,26)/

```
* 0.28840E+02, 0.30000E+02, 0.32310E+02, 0.34620E+02, 0.36940E+02,
* 0.39270E+02, 0.41610E+02, 0.44000E+02, 0.46440E+02, 0.51630E+02,
* 0.57650E+02, 0.65380E+02, 0.76430E+02, 0.93420E+02, 0.11960E+03,
* 0.15570E+03, 0.19580E+03, 0.23110E+03, 0.25860E+03, 0.28040E+03,
* 0.29830E+03, 0.31460E+03, 0.32990E+03, 0.34460E+03, 0.38010E+03,
* 0.41510E+03/
```

DATA (DH2OV(3,I),I=1,26)/

```
* 0.14420E+02, 0.15000E+02, 0.16150E+02, 0.17310E+02, 0.18470E+02,
* 0.19630E+02, 0.20800E+02, 0.21980E+02, 0.23190E+02, 0.25720E+02,
```

Appendix H

* 0.28560E+02, 0.32030E+02, 0.36690E+02, 0.43430E+02, 0.53530E+02,
* 0.68090E+02, 0.86530E+02, 0.10570E+03, 0.12230E+03, 0.13560E+03,
* 0.14630E+03, 0.15550E+03, 0.16380E+03, 0.17150E+03, 0.18970E+03,
* 0.20740E+03/
DATA (DH2OV(4,I),I=1,26)/
* 0.96150E+01, 0.99990E+01, 0.10770E+02, 0.11540E+02, 0.12310E+02,
* 0.13080E+02, 0.13860E+02, 0.14650E+02, 0.15450E+02, 0.17120E+02,
* 0.18960E+02, 0.21150E+02, 0.24000E+02, 0.27980E+02, 0.33800E+02,
* 0.42210E+02, 0.53350E+02, 0.65920E+02, 0.77800E+02, 0.87440E+02,
* 0.95800E+02, 0.10250E+03, 0.10840E+03, 0.11380E+03, 0.12630E+03,
* 0.13820E+03/
DATA (DH2OV(5,I),I=1,26)/
* 0.72110E+01, 0.74990E+01, 0.80770E+01, 0.86540E+01, 0.92330E+01,
* 0.98130E+01, 0.10400E+02, 0.10980E+02, 0.11580E+02, 0.12820E+02,
* 0.14180E+02, 0.15770E+02, 0.17790E+02, 0.20550E+02, 0.24510E+02,
* 0.30190E+02, 0.37860E+02, 0.46960E+02, 0.56990E+02, 0.64070E+02,
* 0.70630E+02, 0.76080E+02, 0.80770E+02, 0.85000E+02, 0.94560E+02,
* 0.10350E+03/
DATA (DH2OV(6,I),I=1,26)/
* 0.57690E+01, 0.59990E+01, 0.64610E+01, 0.69230E+01, 0.73860E+01,
* 0.78500E+01, 0.83160E+01, 0.87870E+01, 0.92630E+01, 0.10250E+02,
* 0.11320E+02, 0.12570E+02, 0.14120E+02, 0.16200E+02, 0.19140E+02,
* 0.23330E+02, 0.29050E+02, 0.36030E+02, 0.43360E+02, 0.50020E+02,
* 0.55610E+02, 0.60240E+02, 0.64190E+02, 0.67710E+02, 0.75530E+02,
* 0.82780E+02/
DATA (DH2OV(7,I),I=1,26)/
* 0.28840E+01, 0.30000E+01, 0.32310E+01, 0.34620E+01, 0.36930E+01,
* 0.39240E+01, 0.41570E+01, 0.43920E+01, 0.46280E+01, 0.51150E+01,
* 0.56350E+01, 0.62190E+01, 0.69160E+01, 0.78040E+01, 0.89950E+01,
* 0.10640E+02, 0.12880E+02, 0.15790E+02, 0.19200E+02, 0.22720E+02,
* 0.25960E+02, 0.28750E+02, 0.31120E+02, 0.33160E+02, 0.37460E+02,
* 0.41250E+02/
DATA (DH2OV(8,I),I=1,26)/
* 0.19220E+01, 0.20000E+01, 0.21540E+01, 0.23080E+01, 0.24620E+01,
* 0.26160E+01, 0.27710E+01, 0.29270E+01, 0.30850E+01, 0.34070E+01,
* 0.37480E+01, 0.41260E+01, 0.45670E+01, 0.51130E+01, 0.58260E+01,
* 0.67850E+01, 0.80830E+01, 0.97850E+01, 0.11870E+02, 0.14140E+02,
* 0.16390E+02, 0.18420E+02, 0.20180E+02, 0.21690E+02, 0.24780E+02,
* 0.27400E+02/
DATA (DH2OV(9,I),I=1,26)/

Appendix H

* 0.14420E+01, 0.15000E+01, 0.16150E+01, 0.17310E+01, 0.18460E+01,
* 0.19620E+01, 0.20780E+01, 0.21950E+01, 0.23130E+01, 0.25540E+01,
* 0.28070E+01, 0.30850E+01, 0.34050E+01, 0.37940E+01, 0.42920E+01,
* 0.49510E+01, 0.58330E+01, 0.69900E+01, 0.84290E+01, 0.10070E+02,
* 0.11760E+02, 0.13350E+02, 0.14750E+02, 0.15980E+02, 0.18450E+02,
* 0.20480E+02/
DATA (DH2OV(10,I),I=1,26)/
* 0.11530E+01, 0.12000E+01, 0.12920E+01, 0.13850E+01, 0.14770E+01,
* 0.15700E+01, 0.16630E+01, 0.17560E+01, 0.18500E+01, 0.20420E+01,
* 0.22440E+01, 0.24630E+01, 0.27130E+01, 0.30130E+01, 0.33910E+01,
* 0.38850E+01, 0.45400E+01, 0.53970E+01, 0.64730E+01, 0.77290E+01,
* 0.90630E+01, 0.11360E+02, 0.11540E+02, 0.12570E+02, 0.14650E+02,
* 0.16330E+02/
DATA (DH2OV(11,I),I=1,26)/
* 0.96110E+00, 0.99960E+00, 0.10770E+01, 0.11540E+01, 0.12310E+01,
* 0.13080E+01, 0.13850E+01, 0.14630E+01, 0.15420E+01, 0.17010E+01,
* 0.18680E+01, 0.20490E+01, 0.22530E+01, 0.24970E+01, 0.28000E+01,
* 0.31910E+01, 0.37050E+01, 0.43760E+01, 0.52220E+01, 0.62250E+01,
* 0.73160E+01, 0.84030E+01, 0.94130E+01, 0.10310E+02, 0.12120E+02,
* 0.13560E+02/
DATA (DH2OV(12,I),I=1,26)/
* 0.72070E+00, 0.74970E+00, 0.80750E+00, 0.86530E+00, 0.92320E+00,
* 0.98110E+00, 0.10390E+01, 0.10970E+01, 0.11560E+01, 0.12750E+01,
* 0.14000E+01, 0.15330E+01, 0.16830E+01, 0.18580E+01, 0.20720E+01,
* 0.23440E+01, 0.26960E+01, 0.31520E+01, 0.37300E+01, 0.44260E+01,
* 0.52090E+01, 0.60200E+01, 0.68000E+01, 0.75130E+01, 0.89670E+01,
* 0.10110E+02/
DATA (DH2OV(13,I),I=1,26)/
* 0.57650E+00, 0.59970E+00, 0.64600E+00, 0.69230E+00, 0.73860E+00,
* 0.78490E+00, 0.83130E+00, 0.87790E+00, 0.92480E+00, 0.10200E+01,
* 0.11190E+01, 0.12250E+01, 0.13420E+01, 0.14780E+01, 0.16420E+01,
* 0.18480E+01, 0.21110E+01, 0.24500E+01, 0.28790E+01, 0.34010E+01,
* 0.39990E+01, 0.46360E+01, 0.52670E+01, 0.58560E+01, 0.70820E+01,
* 0.80350E+01/
DATA (DH2OV(14,I),I=1,26)/
* 0.28800E+00, 0.29970E+00, 0.32290E+00, 0.34610E+00, 0.36930E+00,
* 0.39250E+00, 0.41570E+00, 0.43900E+00, 0.46240E+00, 0.50970E+00,
* 0.55850E+00, 0.60990E+00, 0.66570E+00, 0.72840E+00, 0.80160E+00,
* 0.88990E+00, 0.99880E+00, 0.11350E+01, 0.13050E+01, 0.15150E+01,
* 0.17630E+01, 0.20450E+01, 0.23470E+01, 0.26520E+01, 0.33460E+01,

Appendix H

```
* 0.39010E+01/
DATA (DH2OV(15,I),I=1,26)/
* 0.19190E+00, 0.19970E+00, 0.21520E+00, 0.23070E+00, 0.24620E+00,
* 0.26170E+00, 0.27720E+00, 0.29270E+00, 0.30830E+00, 0.33980E+00,
* 0.37210E+00, 0.40590E+00, 0.44220E+00, 0.48250E+00, 0.52860E+00,
* 0.58300E+00, 0.64890E+00, 0.72990E+00, 0.82980E+00, 0.95200E+00,
* 0.10980E+01, 0.12670E+01, 0.14550E+01, 0.16520E+01, 0.21310E+01,
* 0.25330E+01/
DATA (DH2OV(16,I),I=1,26)/
* 0.14380E+00, 0.14970E+00, 0.16140E+00, 0.17300E+00, 0.18470E+00,
* 0.19630E+00, 0.20790E+00, 0.21960E+00, 0.23130E+00, 0.25480E+00,
* 0.27900E+00, 0.30420E+00, 0.33100E+00, 0.36050E+00, 0.39380E+00,
* 0.43270E+00, 0.47910E+00, 0.53530E+00, 0.60400E+00, 0.68760E+00,
* 0.78770E+00, 0.90450E+00, 0.10360E+01, 0.11770E+01, 0.15280E+01,
* 0.18550E+01/
DATA (DH2OV(17,I),I=1,26)/
* 0.11500E+00, 0.11970E+00, 0.12910E+00, 0.13840E+00, 0.14770E+00,
* 0.15710E+00, 0.16640E+00, 0.17570E+00, 0.18500E+00, 0.20390E+00,
* 0.22320E+00, 0.24320E+00, 0.26440E+00, 0.28760E+00, 0.31360E+00,
* 0.34360E+00, 0.37910E+00, 0.42160E+00, 0.47320E+00, 0.53550E+00,
* 0.61010E+00, 0.69740E+00, 0.79660E+00, 0.90510E+00, 0.11900E+01,
* 0.14520E+01/
DATA (DH2OV(18,I),I=1,26)/
* 0.95750E-01, 0.99700E-01, 0.10750E+00, 0.11530E+00, 0.12310E+00,
* 0.13090E+00, 0.13870E+00, 0.14640E+00, 0.15420E+00, 0.17000E+00,
* 0.18600E+00, 0.20260E+00, 0.22020E+00, 0.23920E+00, 0.26050E+00,
* 0.28480E+00, 0.31330E+00, 0.34730E+00, 0.38810E+00, 0.43730E+00,
* 0.49600E+00, 0.56470E+00, 0.64330E+00, 0.73010E+00, 0.96420E+00,
* 0.11860E+01/
DATA (DH2OV(19,I),I=1,26)/
* 0.71720E-01, 0.74700E-01, 0.80620E-01, 0.86500E-01, 0.92360E-01,
* 0.98200E-01, 0.10400E+00, 0.10990E+00, 0.11570E+00, 0.12750E+00,
* 0.13950E+00, 0.15190E+00, 0.16490E+00, 0.17900E+00, 0.19450E+00,
* 0.21200E+00, 0.23230E+00, 0.25620E+00, 0.28460E+00, 0.31850E+00,
* 0.35870E+00, 0.40590E+00, 0.46000E+00, 0.52060E+00, 0.68970E+00,
* 0.85900E+00/
DATA (DH2OV(20,I),I=1,26)/
* 0.57300E-01, 0.59700E-01, 0.64470E-01, 0.69200E-01, 0.73900E-01,
* 0.78590E-01, 0.83270E-01, 0.87950E-01, 0.92640E-01, 0.10210E+00,
* 0.11170E+00, 0.12150E+00, 0.13190E+00, 0.14300E+00, 0.15510E+00,
```

Appendix H

* 0.16870E+00, 0.18440E+00, 0.20270E+00, 0.22410E+00, 0.24960E+00,
* 0.27970E+00, 0.31490E+00, 0.35540E+00, 0.40100E+00, 0.53120E+00,
* 0.66670E+00/
DATA (DH2OV(21,I),I=1,26)/
* 0.38080E-01, 0.39710E-01, 0.42940E-01, 0.46130E-01, 0.49290E-01,
* 0.52440E-01, 0.55580E-01, 0.58710E-01, 0.61850E-01, 0.68150E-01,
* 0.74530E-01, 0.81080E-01, 0.87890E-01, 0.95130E-01, 0.10300E+00,
* 0.11170E+00, 0.12150E+00, 0.13270E+00, 0.14580E+00, 0.16100E+00,
* 0.17890E+00, 0.19960E+00, 0.22350E+00, 0.25060E+00, 0.33010E+00,
* 0.41820E+00/
DATA (DH2OV(22,I),I=1,26)/
* 0.28470E-01, 0.29720E-01, 0.32180E-01, 0.34600E-01, 0.37000E-01,
* 0.39360E-01, 0.41730E-01, 0.44090E-01, 0.46450E-01, 0.51290E-01,
* 0.55980E-01, 0.60880E-01, 0.65960E-01, 0.71320E-01, 0.77080E-01,
* 0.83410E-01, 0.90490E-01, 0.98520E-01, 0.10770E+00, 0.11840E+00,
* 0.13080E+00, 0.14510E+00, 0.16150E+00, 0.18020E+00, 0.23570E+00,
* 0.29940E+00/
DATA (DH2OV(23,I),I=1,26)/
* 0.14080E-01, 0.14750E-01, 0.16050E-01, 0.17310E-01, 0.18550E-01,
* 0.19770E-01, 0.20980E-01, 0.22180E-01, 0.23380E-01, 0.25770E-01,
* 0.28180E-01, 0.30630E-01, 0.33140E-01, 0.35760E-01, 0.38540E-01,
* 0.41530E-01, 0.44810E-01, 0.48440E-01, 0.52510E-01, 0.57120E-01,
* 0.62350E-01, 0.68300E-01, 0.75050E-01, 0.82670E-01, 0.10560E+00,
* 0.13340E+00/
DATA (DH2OV(24,I),I=1,26)/
* 0.93070E-02, 0.97850E-02, 0.10700E-01, 0.11570E-01, 0.12420E-01,
* 0.13250E-01, 0.14070E-01, 0.14880E-01, 0.15690E-01, 0.17310E-01,
* 0.18920E-01, 0.20560E-01, 0.22240E-01, 0.23970E-01, 0.25800E-01,
* 0.27740E-01, 0.29850E-01, 0.32160E-01, 0.34710E-01, 0.37570E-01,
* 0.40780E-01, 0.44380E-01, 0.48440E-01, 0.53000E-01, 0.66650E-01,
* 0.83450E-01/
DATA (DH2OV(25,I),I=1,26)/
* 0.69400E-02, 0.73180E-02, 0.80330E-02, 0.87100E-02, 0.93620E-02,
* 0.10000E-01, 0.10620E-01, 0.11240E-01, 0.12460E-01, 0.13080E-01,
* 0.14300E-01, 0.15540E-01, 0.16800E-01, 0.18090E-01, 0.19450E-01,
* 0.20890E-01, 0.22440E-01, 0.24120E-01, 0.25970E-01, 0.28010E-01,
* 0.30290E-01, 0.32840E-01, 0.35680E-01, 0.38850E-01, 0.48330E-01,
* 0.60030E-01/
DATA (DH2OV(26,I),I=1,26)/
* 0.55340E-02, 0.58520E-02, 0.64460E-02, 0.70030E-02, 0.75360E-02,

Appendix H

* 0.80550E-02, 0.85640E-02, 0.90660E-02, 0.95630E-02, 0.10550E-01,
* 0.11540E-01, 0.12530E-01, 0.13540E-01, 0.14570E-01, 0.15660E-01,
* 0.16800E-01, 0.18020E-01, 0.19340E-01, 0.20780E-01, 0.22360E-01,
* 0.24120E-01, 0.26070E-01, 0.28240E-01, 0.30640E-01, 0.37790E-01,
* 0.46620E-01/

*

*

* ENTROPY (J/kg*K)

*

DATA (DH2OS(1,I),I=1,26)/

* 0.14517E+05, 0.14615E+05, 0.14804E+05, 0.14986E+05, 0.15163E+05,
* 0.15338E+05, 0.15515E+05, 0.15700E+05, 0.15897E+05, 0.16367E+05,
* 0.17022E+05, 0.18019E+05, 0.19593E+05, 0.22029E+05, 0.25393E+05,
* 0.28983E+05, 0.31696E+05, 0.33280E+05, 0.34133E+05, 0.34621E+05,
* 0.34949E+05, 0.35168E+05, 0.35357E+05, 0.35522E+05, 0.35880E+05,
* 0.36194E+05/

DATA (DH2OS(2,I),I=1,26)/

* 0.14197E+05, 0.14295E+05, 0.14484E+05, 0.14665E+05, 0.14841E+05,
* 0.15014E+05, 0.15187E+05, 0.15364E+05, 0.15550E+05, 0.15976E+05,
* 0.16536E+05, 0.17338E+05, 0.18542E+05, 0.20357E+05, 0.22948E+05,
* 0.26134E+05, 0.29159E+05, 0.31326E+05, 0.32621E+05, 0.33364E+05,
* 0.33814E+05, 0.34117E+05, 0.34344E+05, 0.34530E+05, 0.34910E+05,
* 0.35231E+05/

DATA (DH2OS(3,I),I=1,26)/

* 0.13877E+05, 0.13975E+05, 0.14163E+05, 0.14344E+05, 0.14519E+05,
* 0.14690E+05, 0.14860E+05, 0.15032E+05, 0.15210E+05, 0.15603E+05,
* 0.16092E+05, 0.16753E+05, 0.17698E+05, 0.19068E+05, 0.21016E+05,
* 0.23576E+05, 0.26434E+05, 0.28963E+05, 0.30756E+05, 0.31872E+05,
* 0.32550E+05, 0.32981E+05, 0.33280E+05, 0.33507E+05, 0.33929E+05,
* 0.34263E+05/

DATA (DH2OS(4,I),I=1,26)/

* 0.13690E+05, 0.13788E+05, 0.13976E+05, 0.14157E+05, 0.14331E+05,
* 0.14501E+05, 0.14670E+05, 0.14839E+05, 0.15012E+05, 0.15390E+05,
* 0.15846E+05, 0.16445E+05, 0.17273E+05, 0.18448E+05, 0.20096E+05,
* 0.22294E+05, 0.24898E+05, 0.27454E+05, 0.29482E+05, 0.30850E+05,
* 0.31709E+05, 0.32253E+05, 0.32618E+05, 0.32883E+05, 0.33346E+05,
* 0.33693E+05/

DATA (DH2OS(5,I),I=1,26)/

* 0.13557E+05, 0.13655E+05, 0.13843E+05, 0.14024E+05, 0.14198E+05,

Appendix H

* 0.14368E+05, 0.14535E+05, 0.14702E+05, 0.14873E+05, 0.15241E+05,
* 0.15677E+05, 0.16237E+05, 0.16997E+05, 0.18054E+05, 0.19522E+05,
* 0.21484E+05, 0.23877E+05, 0.26371E+05, 0.28507E+05, 0.30047E+05,
* 0.31053E+05, 0.31696E+05, 0.32122E+05, 0.32424E+05, 0.32928E+05,
* 0.33287E+05/
DATA (DH2OS(6,I),I=1,26)/
* 0.13454E+05, 0.13552E+05, 0.13740E+05, 0.13921E+05, 0.14094E+05,
* 0.14264E+05, 0.14430E+05, 0.14597E+05, 0.14756E+05, 0.15127E+05,
* 0.15549E+05, 0.16082E+05, 0.16794E+05, 0.17772E+05, 0.19116E+05,
* 0.20911E+05, 0.23134E+05, 0.25542E+05, 0.27722E+05, 0.29381E+05,
* 0.30505E+05, 0.31235E+05, 0.31718E+05, 0.32055E+05, 0.32598E+05,
* 0.32970E+05/
DATA (DH2OS(7,I),I=1,26)/
* 0.13133E+05, 0.13232E+05, 0.13420E+05, 0.13600E+05, 0.13773E+05,
* 0.13944E+05, 0.14106E+05, 0.14270E+05, 0.14434E+05, 0.14777E+05,
* 0.15162E+05, 0.15627E+05, 0.16220E+05, 0.16999E+05, 0.18035E+05,
* 0.19398E+05, 0.21121E+05, 0.23140E+05, 0.25235E+05, 0.27111E+05,
* 0.28575E+05, 0.29615E+05, 0.30325E+05, 0.30814E+05, 0.31538E+05,
* 0.31970E+05/
DATA (DH2OS(8,I),I=1,26)/
* 0.12946E+05, 0.13044E+05, 0.13233E+05, 0.13413E+05, 0.13586E+05,
* 0.13753E+05, 0.13917E+05, 0.14079E+05, 0.14241E+05, 0.14575E+05,
* 0.14944E+05, 0.15377E+05, 0.15915E+05, 0.16606E+05, 0.17505E+05,
* 0.18671E+05, 0.20145E+05, 0.21909E+05, 0.23839E+05, 0.25710E+05,
* 0.27302E+05, 0.28518E+05, 0.29388E+05, 0.29997E+05, 0.30880E+05,
* 0.31369E+05/
DATA (DH2OS(9,I),I=1,26)/
* 0.12814E+05, 0.12911E+05, 0.13100E+05, 0.13280E+05, 0.13453E+05,
* 0.13620E+05, 0.13783E+05, 0.13944E+05, 0.14105E+05, 0.14433E+05,
* 0.14791E+05, 0.15205E+05, 0.15710E+05, 0.16347E+05, 0.17164E+05,
* 0.18212E+05, 0.19531E+05, 0.21123E+05, 0.22911E+05, 0.24724E+05,
* 0.26357E+05, 0.27686E+05, 0.28659E+05, 0.29365E+05, 0.30389E+05,
* 0.30931E+05/
DATA (DH2OS(10,I),I=1,26)/
* 0.12710E+05, 0.12808E+05, 0.12996E+05, 0.13176E+05, 0.13349E+05,
* 0.13517E+05, 0.13679E+05, 0.13840E+05, 0.13999E+05, 0.14324E+05,
* 0.14674E+05, 0.15075E+05, 0.15557E+05, 0.16157E+05, 0.16918E+05,
* 0.17885E+05, 0.19096E+05, 0.20562E+05, 0.22233E+05, 0.23978E+05,
* 0.25614E+05, 0.26992E+05, 0.28058E+05, 0.28841E+05, 0.29990E+05,
* 0.30584E+05/

Appendix H

DATA (DH2OS(11,I),I=1,26)/

* 0.12626E+05, 0.12724E+05, 0.12912E+05, 0.13092E+05, 0.13265E+05,
* 0.13432E+05, 0.13595E+05, 0.13754E+05, 0.13913E+05, 0.14235E+05,
* 0.14579E+05, 0.14970E+05, 0.15434E+05, 0.16007E+05, 0.16727E+05,
* 0.17639E+05, 0.18765E+05, 0.20134E+05, 0.21710E+05, 0.23388E+05,
* 0.25008E+05, 0.26419E+05, 0.27544E+05, 0.28391E+05, 0.29651E+05,
* 0.30294E+05/

DATA (DH2OS(12,I),I=1,26)/

* 0.12493E+05, 0.12591E+05, 0.12779E+05, 0.12959E+05, 0.13132E+05,
* 0.13299E+05, 0.13461E+05, 0.13620E+05, 0.13777E+05, 0.14095E+05,
* 0.14431E+05, 0.14807E+05, 0.15247E+05, 0.15781E+05, 0.16441E+05,
* 0.17264E+05, 0.18281E+05, 0.19511E+05, 0.20940E+05, 0.22498E+05,
* 0.24064E+05, 0.25498E+05, 0.26699E+05, 0.27640E+05, 0.29088E+05,
* 0.29822E+05/

DATA (DH2OS(13,I),I=1,26)/

* 0.12389E+05, 0.12487E+05, 0.12676E+05, 0.12856E+05, 0.13028E+05,
* 0.13195E+05, 0.13357E+05, 0.13515E+05, 0.13672E+05, 0.13987E+05,
* 0.14317E+05, 0.14683E+05, 0.15106E+05, 0.15612E+05, 0.16232E+05,
* 0.16998E+05, 0.17936E+05, 0.19068E+05, 0.20388E+05, 0.21849E+05,
* 0.23355E+05, 0.24780E+05, 0.26020E+05, 0.27025E+05, 0.28625E+05,
* 0.29442E+05/

DATA (DH2OS(14,I),I=1,26)/

* 0.12067E+05, 0.12166E+05, 0.12355E+05, 0.12535E+05, 0.12707E+05,
* 0.12874E+05, 0.13035E+05, 0.13192E+05, 0.13346E+05, 0.13653E+05,
* 0.13969E+05, 0.14307E+05, 0.14686E+05, 0.15124E+05, 0.15642E+05,
* 0.16262E+05, 0.17004E+05, 0.17885E+05, 0.18913E+05, 0.20077E+05,
* 0.21388E+05, 0.22631E+05, 0.23872E+05, 0.24988E+05, 0.27024E+05,
* 0.28159E+05/

DATA (DH2OS(15,I),I=1,26)/

* 0.11878E+05, 0.11977E+05, 0.12166E+05, 0.12346E+05, 0.12519E+05,
* 0.12685E+05, 0.12846E+05, 0.13003E+05, 0.13156E+05, 0.13460E+05,
* 0.13767E+05, 0.14093E+05, 0.14451E+05, 0.14851E+05, 0.15329E+05,
* 0.15883E+05, 0.16537E+05, 0.17304E+05, 0.18195E+05, 0.19205E+05,
* 0.20315E+05, 0.21486E+05, 0.22658E+05, 0.23768E+05, 0.25975E+05,
* 0.27317E+05/

DATA (DH2OS(16,I),I=1,26)/

* 0.11743E+05, 0.11842E+05, 0.12032E+05, 0.12213E+05, 0.12386E+05,
* 0.12552E+05, 0.12712E+05, 0.12869E+05, 0.13021E+05, 0.13322E+05,
* 0.13626E+05, 0.13943E+05, 0.14289E+05, 0.14675E+05, 0.15118E+05,
* 0.15633E+05, 0.16233E+05, 0.16932E+05, 0.17738E+05, 0.18652E+05,

Appendix H

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* 0.19662E+05, 0.20740E+05, 0.21844E+05, 0.22920E+05, 0.25191E+05,
* 0.26674E+05/
DATA (DH2OS(17,I),I=1,26)/
* 0.11639E+05, 0.11737E+05, 0.11928E+05, 0.12109E+05, 0.12282E+05,
* 0.12448E+05, 0.12608E+05, 0.12764E+05, 0.12916E+05, 0.13216E+05,
* 0.13516E+05, 0.13828E+05, 0.14165E+05, 0.14538E+05, 0.14961E+05,
* 0.15448E+05, 0.16012E+05, 0.16664E+05, 0.17411E+05, 0.18257E+05,
* 0.19194E+05, 0.20201E+05, 0.21246E+05, 0.22284E+05, 0.24568E+05,
* 0.26148E+05/
DATA (DH2OS(18,I),I=1,26)/
* 0.11552E+05, 0.11651E+05, 0.11843E+05, 0.12024E+05, 0.12197E+05,
* 0.12363E+05, 0.12523E+05, 0.12679E+05, 0.12831E+05, 0.13130E+05,
* 0.13427E+05, 0.13735E+05, 0.13981E+05, 0.14427E+05, 0.14836E+05,
* 0.15303E+05, 0.15839E+05, 0.16456E+05, 0.17160E+05, 0.17954E+05,
* 0.18835E+05, 0.19786E+05, 0.20781E+05, 0.21782E+05, 0.24055E+05,
* 0.25703E+05/
DATA (DH2OS(19,I),I=1,26)/
* 0.11415E+05, 0.11515E+05, 0.11707E+05, 0.11889E+05, 0.12062E+05,
* 0.12229E+05, 0.12389E+05, 0.12545E+05, 0.12697E+05, 0.12993E+05,
* 0.13237E+05, 0.13589E+05, 0.13908E+05, 0.14256E+05, 0.14644E+05,
* 0.15081E+05, 0.15579E+05, 0.16146E+05, 0.16789E+05, 0.17510E+05,
* 0.18309E+05, 0.19176E+05, 0.20091E+05, 0.21028E+05, 0.23248E+05,
* 0.24975E+05/
DATA (DH2OS(20,I),I=1,26)/
* 0.11308E+05, 0.11409E+05, 0.11601E+05, 0.11784E+05, 0.11958E+05,
* 0.12124E+05, 0.12285E+05, 0.12440E+05, 0.12592E+05, 0.12887E+05,
* 0.13179E+05, 0.13476E+05, 0.13789E+05, 0.14129E+05, 0.14499E+05,
* 0.14917E+05, 0.15387E+05, 0.15920E+05, 0.16520E+05, 0.17191E+05,
* 0.17933E+05, 0.18738E+05, 0.19594E+05, 0.20478E+05, 0.22630E+05,
* 0.24394E+05/
DATA (DH2OS(21,I),I=1,26)/
* 0.11110E+05, 0.11213E+05, 0.11408E+05, 0.11592E+05, 0.11767E+05,
* 0.11934E+05, 0.12095E+05, 0.12250E+05, 0.12401E+05, 0.12695E+05,
* 0.12982E+05, 0.13273E+05, 0.13574E+05, 0.13896E+05, 0.14245E+05,
* 0.14630E+05, 0.15058E+05, 0.15536E+05, 0.16069E+05, 0.16661E+05,
* 0.17311E+05, 0.18017E+05, 0.18769E+05, 0.19557E+05, 0.21550E+05,
* 0.23322E+05/
DATA (DH2OS(22,I),I=1,26)/
* 0.10967E+05, 0.11071E+05, 0.11268E+05, 0.11454E+05, 0.11630E+05,
* 0.11798E+05, 0.11959E+05, 0.12115E+05, 0.12266E+05, 0.12558E+05,
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Appendix H

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* 0.12843E+05, 0.13129E+05, 0.13424E+05, 0.13735E+05, 0.14069E+05,
* 0.14435E+05, 0.14837E+05, 0.15282E+05, 0.15775E+05, 0.16318E+05,
* 0.16912E+05, 0.17555E+05, 0.18243E+05, 0.18965E+05, 0.20829E+05,
* 0.22563E+05/
DATA (DH2OS(23.I),I=1,26)/
* 0.10604E+05, 0.10715E+05, 0.10923E+05, 0.11115E+05, 0.11295E+05,
* 0.11465E+05, 0.11628E+05, 0.11785E+05, 0.11936E+05, 0.12227E+05,
* 0.12508E+05, 0.12786E+05, 0.13066E+05, 0.13357E+05, 0.13662E+05,
* 0.13988E+05, 0.14339E+05, 0.14720E+05, 0.15134E+05, 0.15583E+05,
* 0.16068E+05, 0.16589E+05, 0.17143E+05, 0.17727E+05, 0.19273E+05,
* 0.20825E+05/
DATA (DH2OS(24.I),I=1,26)/
* 0.10375E+05, 0.10493E+05, 0.10710E+05, 0.10909E+05, 0.11093E+05,
* 0.11266E+05, 0.11431E+05, 0.11588E+05, 0.11740E+05, 0.12031E+05,
* 0.12311E+05, 0.12585E+05, 0.12859E+05, 0.13139E+05, 0.13431E+05,
* 0.13739E+05, 0.14066E+05, 0.14417E+05, 0.14795E+05, 0.15201E+05,
* 0.15635E+05, 0.16099E+05, 0.16591E+05, 0.17108E+05, 0.18484E+05,
* 0.19900E+05/
DATA (DH2OS(25.I),I=1,26)/
* 0.10199E+05, 0.10324E+05, 0.10552E+05, 0.10757E+05, 0.10946E+05,
* 0.11122E+05, 0.11288E+05, 0.11447E+05, 0.11599E+05, 0.11891E+05,
* 0.12170E+05, 0.12441E+05, 0.12712E+05, 0.12986E+05, 0.13270E+05,
* 0.13566E+05, 0.13879E+05, 0.14212E+05, 0.14567E+05, 0.14946E+05,
* 0.15350E+05, 0.15770E+05, 0.16233E+05, 0.16709E+05, 0.17976E+05,
* 0.19294E+05/
DATA (DH2OS(26.I),I=1,26)/
* 0.10054E+05, 0.10187E+05, 0.10425E+05, 0.10636E+05, 0.10828E+05,
* 0.11007E+05, 0.11176E+05, 0.11335E+05, 0.11489E+05, 0.11731E+05,
* 0.12059E+05, 0.12330E+05, 0.12598E+05, 0.12868E+05, 0.13146E+05,
* 0.13433E+05, 0.13736E+05, 0.14056E+05, 0.14396E+05, 0.14756E+05,
* 0.15139E+05, 0.15545E+05, 0.15971E+05, 0.16418E+05, 0.17608E+05,
* 0.18852E+05/
*
*****
*
* ENTHALPY (J/kg)
*
* Correction factor for enthalpy such that the zero value
* of water enthalpy is at triple point, i.e. value of enthalpy
* from Vukalovitch (1967) and this table are equal at 1000 degC.

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Appendix H

*

DATA (DH2OH(1),I=1,26)/ 26*0.15250E+08/

*

DATA (DH2OH(1,I),I=1,26)/

*-0.10670E+08,-0.10546E+08,-0.10290E+08,-0.10027E+08,-0.97520E+07,
*-0.94630E+07,-0.91530E+07,-0.88120E+07,-0.84270E+07,-0.74390E+07,
*-0.59270E+07,-0.34280E+07,-0.83400E+06, 0.79160E+07, 0.18357E+08,
* 0.30196E+08, 0.39669E+08, 0.45512E+08, 0.48834E+08, 0.50829E+08,
* 0.52182E+08, 0.53224E+08, 0.54112E+08, 0.54921E+08, 0.56798E+08,
* 0.58603E+08/

DATA (DH2OH(2,I),I=1,26)/

*-0.10670E+08,-0.10546E+08,-0.10291E+08,-0.10028E+08,-0.97560E+07,
*-0.94700E+07,-0.91670E+07,-0.88390E+07,-0.84760E+07,-0.75800E+07,
*-0.62900E+07,-0.42790E+07,-0.10200E+07, 0.42540E+07, 0.12298E+08,
* 0.22817E+08, 0.33395E+08, 0.41395E+08, 0.46435E+08, 0.49472E+08,
* 0.51404E+08, 0.52765E+08, 0.53832E+08, 0.54744E+08, 0.56733E+08,
* 0.58576E+08/

DATA (DH2OH(3,I),I=1,26)/

*-0.10670E+08,-0.10546E+08,-0.10291E+08,-0.10029E+08,-0.97580E+07,
*-0.94760E+07,-0.91790E+07,-0.88610E+07,-0.85140E+07,-0.76880E+07,
*-0.65610E+07,-0.49030E+07,-0.23480E+07, 0.16350E+07, 0.76850E+07,
* 0.16139E+08, 0.26142E+08, 0.35487E+08, 0.42467E+08, 0.47035E+08,
* 0.49493E+08, 0.51881E+08, 0.53284E+08, 0.54395E+08, 0.56604E+08,
* 0.58520E+08/

DATA (DH2OH(4,I),I=1,26)/

*-0.10671E+08,-0.10546E+08,-0.10292E+08,-0.10030E+08,-0.97590E+07,
*-0.94790E+07,-0.91840E+07,-0.88710E+07,-0.85330E+07,-0.77400E+07,
*-0.66880E+07,-0.51890E+07,-0.29470E+07, 0.46600E+06, 0.55860E+07,
* 0.12845E+08, 0.21963E+08, 0.31415E+08, 0.39311E+08, 0.44909E+08,
* 0.48596E+08, 0.51039E+08, 0.52753E+08, 0.54052E+08, 0.56477E+08,
* 0.58465E+08/

DATA (DH2OH(5,I),I=1,26)/

*-0.10671E+08,-0.10546E+08,-0.10292E+08,-0.10030E+08,-0.97600E+07,
*-0.94800E+07,-0.91880E+07,-0.88780E+07,-0.85440E+07,-0.77720E+07,
*-0.67670E+07,-0.53640E+07,-0.33090E+07,-0.23700E+06, 0.43220E+07,
* 0.10805E+08, 0.19183E+08, 0.28408E+08, 0.36730E+08, 0.43038E+08,
* 0.47349E+08, 0.50237E+08, 0.52238E+08, 0.53717E+08, 0.56351E+08,
* 0.58411E+08/

DATA (DH2OH(6,I),I=1,26)/

*-0.10671E+08,-0.10546E+08,-0.10292E+08,-0.10030E+08,-0.97610E+07,

Appendix H

*-0.94820E+07,-0.91900E+07,-0.88820E+07,-0.85520E+07,-0.77940E+07,
*-0.68220E+07,-0.54860E+07,-0.35600E+07,-0.72000E+06, 0.34550E+07,
* 0.93850E+07, 0.17170E+08, 0.26079E+08, 0.34573E+08, 0.41365E+08,
* 0.46190E+08, 0.49471E+08, 0.51737E+08, 0.53388E+08, 0.56225E+08,
* 0.58356E+08/

DATA (DH2OH(7,I),I=1,26)/

*-0.10671E+08,-0.10546E+08,-0.10292E+08,-0.10031E+08,-0.97630E+07,
*-0.94850E+07,-0.91970E+07,-0.88950E+07,-0.95740E+07,-0.78540E+07,
*-0.69660E+07,-0.58020E+07,-0.42000E+07,-0.19360E+07, 0.12810E+07,
* 0.57830E+07, 0.11820E+08, 0.19290E+08, 0.27460E+08, 0.35146E+08,
* 0.41433E+08, 0.46106E+08, 0.49440E+08, 0.51832E+08, 0.55612E+08,
* 0.58086E+08/

DATA (DH2OH(8,I),I=1,26)/

*-0.10672E+08,-0.10547E+08,-0.10293E+08,-0.10032E+08,-0.97630E+07,
*-0.94870E+07,-0.92000E+07,-0.89010E+07,-0.85850E+07,-0.78830E+07,
*-0.70350E+07,-0.59500E+07,-0.44950E+07,-0.24900E+07, 0.30200E+06,
* 0.41540E+07, 0.93170E+07, 0.15849E+08, 0.23378E+08, 0.31044E+08,
* 0.37883E+08, 0.43848E+08, 0.47430E+08, 0.50411E+08, 0.55020E+08,
* 0.57819E+08/

DATA (DH2OH(9,I),I=1,26)/

*-0.10672E+08,-0.10547E+08,-0.10293E+08,-0.10032E+08,-0.97640E+07,
*-0.94880E+07,-0.92020E+07,-0.89040E+07,-0.85910E+07,-0.79010E+07,
*-0.70780E+07,-0.60410E+07,-0.46760E+07,-0.28260E+07,-0.29000E+06,
* 0.31730E+07, 0.77940E+07, 0.13686E+08, 0.20660E+08, 0.28092E+08,
* 0.35111E+08, 0.41037E+08, 0.45653E+08, 0.49106E+08, 0.54448E+08,
* 0.57558E+08/

DATA (DH2OH(10,I),I=1,26)/

*-0.10672E+08,-0.10547E+08,-0.10293E+08,-0.10032E+08,-0.97640E+07,
*-0.94890E+07,-0.92040E+07,-0.89070E+07,-0.85960E+07,-0.79140E+07,
*-0.71080E+07,-0.61050E+07,-0.48030E+07, 0.30600E+07, 0.69800E+06,
* 0.24980E+07, 0.67410E+07, 0.12169E+08, 0.18689E+08, 0.25841E+08,
* 0.32872E+08, 0.39066E+08, 0.44069E+08, 0.47903E+08, 0.53897E+08,
* 0.57300E+08/

DATA (DH2OH(11,I),I=1,26)/

*-0.10672E+08,-0.10548E+08,-0.10293E+08,-0.10033E+08,-0.97650E+07,
*-0.94890E+07,-0.92050E+07,-0.89090E+07,-0.86000E+07,-0.79230E+07,
*-0.71310E+07,-0.61540E+07,-0.48980E+07,-0.32350E+07,-0.10020E+07,
* 0.19950E+07, 0.59570E+07, 0.11029E+08, 0.17175E+08, 0.24054E+08,
* 0.31016E+08, 0.37360E+08, 0.42645E+08, 0.46789E+08, 0.53363E+08,
* 0.57046E+08/

Appendix H

DATA (DH2OH(12,I),I=1,26)/

*-0.10673E+08,-0.10548E+08,-0.10294E+08,-0.10033E+08,-0.97650E+07,
*-0.94900E+07,-0.92060E+07,-0.89120E+07,-0.86050E+07,-0.79380E+07,
*-0.71640E+07,-0.62340E+07,-0.50350E+07,-0.34350E+07,-0.14340E+07,
* 0.12840E+07, 0.48470E+07, 0.94010E+07, 0.14974E+08, 0.21366E+08,
* 0.28098E+08, 0.34542E+08, 0.40182E+08, 0.44789E+08, 0.52347E+08,
* 0.56550E+08/

DATA (DH2OH(13,I),I=1,26)/

*-0.10674E+08,-0.10549E+08,-0.10294E+08,-0.10033E+08,-0.97660E+07,
*-0.94910E+07,-0.92080E+07,-0.89150E+07,-0.86090E+07,-0.79480E+07,
*-0.71870E+07,-0.62730E+07,-0.51300E+07,-0.36590E+07,-0.17340E+07,
* 0.79300E+06, 0.40810E+07, 0.82720E+07, 0.13423E+08, 0.19414E+08,
* 0.25886E+08, 0.32297E+08, 0.38120E+08, 0.43040E+08, 0.51393E+08,
* 0.56069E+08/

DATA (DH2OH(14,I),I=1,26)/

*-0.10677E+08,-0.10551E+08,-0.10296E+08,-0.10035E+08,-0.97680E+07,
*-0.94930E+07,-0.92120E+07,-0.89210E+07,-0.86190E+07,-0.79750E+07,
*-0.72490E+07,-0.64030E+07,-0.53800E+07,-0.41080E+07,-0.25010E+07,
*-0.45400E+06, 0.21460E+07, 0.54090E+07, 0.94210E+07, 0.14193E+08,
* 0.19617E+08, 0.25433E+08, 0.31265E+08, 0.36730E+08, 0.47372E+08,
* 0.53865E+08/

DATA (DH2OH(15,I),I=1,26)/

*-0.10680E+08,-0.10554E+08,-0.10298E+08,-0.10037E+08,-0.97690E+07,
*-0.94950E+07,-0.92140E+07,-0.89240E+07,-0.86250E+07,-0.79880E+07,
*-0.72800E+07,-0.64650E+07,-0.54980E+07,-0.43190E+07,-0.28560E+07,
*-0.10260E+07, 0.12640E+07, 0.41060E+07, 0.75800E+07, 0.11723E+08,
* 0.16500E+08, 0.21768E+08, 0.27276E+08, 0.32690E+08, 0.44255E+08,
* 0.51941E+08/

DATA (DH2OH(16,I),I=1,26)/

*-0.10683E+08,-0.10557E+08,-0.10300E+08,-0.10038E+08,-0.97710E+07,
*-0.94970E+07,-0.92150E+07,-0.89260E+07,-0.86280E+07,-0.79960E+07,
*-0.72990E+07,-0.65040E+07,-0.55710E+07,-0.44490E+07,-0.30740E+07,
*-0.13750E+07, 0.72800E+06, 0.38160E+07, 0.64600E+07, 0.10207E+08,
* 0.14550E+08, 0.19404E+08, 0.24592E+08, 0.29863E+08, 0.41748E+08,
* 0.50243E+08/

DATA (DH2OH(17,I),I=1,26)/

*-0.10686E+08,-0.10559E+08,-0.10302E+08,-0.10040E+08,-0.97720E+07,
*-0.94980E+07,-0.92170E+07,-0.89280E+07,-0.86310E+07,-0.80020E+07,
*-0.73120E+07,-0.65310E+07,-0.56230E+07,-0.45410E+07,-0.32270E+07,
*-0.16190E+07, 0.35600E+06, 0.27690E+07, 0.56860E+07, 0.91540E+07,

Appendix H

* 0.13183E+08, 0.17717E+08, 0.22628E+08, 0.27714E+08, 0.39676E+08,
* 0.48729E+08/
DATA (DH2OH(18,I),I=1,26)/
*-0.10689E+08,-0.10562E+08,-0.10304E+08,-0.10042E+08,-0.97730E+07,
*-0.94990E+07,-0.92180E+07,-0.89300E+07,-0.86330E+07,-0.80070E+07,
*-0.73220E+07,-0.65520E+07,-0.56630E+07,-0.46100E+07,-0.33420E+07,
*-0.18020E+07, 0.77000E+05, 0.23600E+07, 0.51080E+07, 0.83670E+07,
* 0.12154E+08, 0.16434E+08, 0.21110E+08, 0.26017E+08, 0.37925E+08,
* 0.47369E+08/
DATA (DH2OH(19,I),I=1,26)/
*-0.10695E+08,-0.10567E+08,-0.10308E+08,-0.10045E+08,-0.97760E+07,
*-0.95000E+07,-0.92200E+07,-0.89320E+07,-0.86370E+07,-0.80140E+07,
*-0.73380E+07,-0.65830E+07,-0.57200E+07,-0.47100E+07,-0.35080E+07,
*-0.20640E+07,-0.32100E+06, 0.17770E+07, 0.42850E+07, 0.72460E+07,
* 0.10682E+08, 0.14582E+08, 0.18884E+08, 0.23475E+08, 0.35109E+08,
* 0.45015E+08/
DATA (DH2OH(20,I),I=1,26)/
*-0.10701E+08,-0.10572E+08,-0.10312E+08,-0.10048E+08,-0.97780E+07,
*-0.95030E+07,-0.92220E+07,-0.89350E+07,-0.86390E+07,-0.80200E+07,
*-0.73480E+07,-0.66050E+07,-0.57600E+07,-0.47800E+07,-0.36250E+07,
*-0.22470E+07,-0.59800E+06, 0.13730E+07, 0.37150E+07, 0.64680E+07,
* 0.96580E+07, 0.13283E+08, 0.17303E+08, 0.21634E+08, 0.32924E+08,
* 0.43042E+08/
DATA (DH2OH(21,I),I=1,26)/
*-0.10716E+08,-0.10585E+08,-0.10322E+08,-0.10055E+08,-0.97840E+07,
*-0.95080E+07,-0.92270E+07,-0.89390E+07,-0.86450E+07,-0.80290E+07,
*-0.73670E+07,-0.66400E+07,-0.58260E+07,-0.48940E+07,-0.38120E+07,
*-0.25410E+07,-0.10410E+07, 0.72900E+06, 0.28100E+07, 0.52360E+07,
* 0.80320E+07, 0.11207E+08, 0.14746E+08, 0.18604E+08, 0.29066E+08,
* 0.39231E+08/
DATA (DH2OH(22,I),I=1,26)/
*-0.10731E+08,-0.10597E+08,-0.10331E+08,-0.10062E+08,-0.97900E+07,
*-0.95130E+07,-0.92310E+07,-0.89450E+07,-0.86490E+07,-0.80350E+07,
*-0.73790E+07,-0.66630E+07,-0.58680E+07,-0.49660E+07,-0.39290E+07,
*-0.27230E+07,-0.13140E+07, 0.33400E+06, 0.22560E+07, 0.44830E+07,
* 0.70390E+07, 0.89340E+07, 0.13165E+08, 0.16702E+08, 0.26486E+08,
* 0.36448E+08/
DATA (DH2OH(23,I),I=1,26)/
*-0.10790E+08,-0.10649E+08,-0.10369E+08,-0.10091E+08,-0.98120E+07,
*-0.95310E+07,-0.92460E+07,-0.89570E+07,-0.86620E+07,-0.80510E+07,

Appendix H

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*-0.74050E+07,-0.67110E+07,-0.59530E+07,-0.51110E+07,-0.41640E+07,
*-0.30880E+07,-0.18580E+07,-0.48800E+06, 0.11670E+07, 0.30070E+07,
* 0.50930E+07, 0.74360E+07, 0.10041E+08, 0.12902E+08, 0.21020E+08,
* 0.29940E+08/
DATA (DH2OH(24,I),I=1,26)/
*-0.10848E+08,-0.10698E+08,-0.10405E+08,-0.10118E+08,-0.98330E+07,
*-0.95470E+07,-0.92600E+07,-0.89680E+07,-0.86720E+07,-0.80620E+07,
*-0.74200E+07,-0.67350E+07,-0.59940E+07,-0.51810E+07,-0.42760E+07,
*-0.32610E+07,-0.21140E+07,-0.81500E+06, 0.65800E+06, 0.23210E+07,
* 0.41910E+07, 0.62790E+07, 0.85910E+07, 0.11125E+08, 0.18352E+08,
* 0.26493E+08/
DATA (DH2OH(25,I),I=1,26)/
*-0.10904E+08,-0.10745E+08,-0.10439E+08,-0.10142E+08,-0.98520E+07,
*-0.95620E+07,-0.92720E+07,-0.89780E+07,-0.86810E+07,-0.80690E+07,
*-0.74290E+07,-0.67500E+07,-0.60200E+07,-0.52240E+07,-0.43460E+07,
*-0.33690E+07,-0.22730E+07,-0.10420E+07, 0.34300E+06, 0.18990E+07,
* 0.36370E+07, 0.55690E+07, 0.77000E+07, 0.10032E+08, 0.16686E+08,
* 0.24266E+08/
DATA (DH2OH(26,I),I=1,26)/
*-0.10958E+08,-0.10790E+08,-0.10471E+08,-0.10167E+08,-0.98700E+07,
*-0.95760E+07,-0.92830E+07,-0.89670E+07,-0.86880E+07,-0.80760E+07,
*-0.74360E+07,-0.67610E+07,-0.60380E+07,-0.52540E+07,-0.43950E+07,
*-0.34440E+07,-0.23850E+07,-0.12010E+07, 0.12300E+06, 0.16020E+07,
* 0.32490E+07, 0.50730E+07, 0.70790E+07, 0.92690E+07, 0.15515E+08,
* 0.22670E+08/
*
*****
*
* HEAT CAPACITY (J/kg*K)
*
DATA (DH2OCP(1,I),I=1,26)/
* 0.24830E+04, 0.25240E+04, 0.26190E+04, 0.27470E+04, 0.29280E+04,
* 0.31930E+04, 0.35780E+04, 0.41270E+04, 0.48900E+04, 0.72950E+04,
* 0.11340E+05, 0.17640E+05, 0.26990E+05, 0.40310E+05, 0.55540E+05,
* 0.59480E+05, 0.44620E+05, 0.26470E+05, 0.14960E+05, 0.91200E+04,
* 0.63300E+04, 0.49800E+04, 0.43200E+04, 0.39700E+04, 0.36600E+04,
* 0.35900E+04/
DATA (DH2OCP(2,I),I=1,26)/
* 0.24810E+04, 0.25200E+04, 0.26080E+04, 0.27220E+04, 0.28770E+04,
* 0.30970E+04, 0.34120E+04, 0.38580E+04, 0.44590E+04, 0.63390E+04,
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Appendix H

* 0.94400E+04, 0.14200E+05, 0.21090E+05, 0.30760E+05, 0.43360E+05,
* 0.54100E+05, 0.51870E+05, 0.37380E+05, 0.22920E+05, 0.13770E+05,
* 0.88700E+04, 0.63700E+04, 0.50900E+04, 0.44200E+04, 0.37900E+04,
* 0.36400E+04/
DATA (DH2OCP(3,I),I=1,26)/
* 0.24790E+04, 0.25160E+04, 0.26000E+04, 0.27020E+04, 0.28360E+04,
* 0.30220E+04, 0.32800E+04, 0.36380E+04, 0.41220E+04, 0.56010E+04,
* 0.79980E+04, 0.11610E+05, 0.16760E+05, 0.23820E+05, 0.33180E+05,
* 0.43910E+05, 0.50210E+05, 0.45170E+05, 0.32540E+05, 0.20870E+05,
* 0.13250E+05, 0.80210E+04, 0.65670E+04, 0.52870E+04, 0.40470E+04,
* 0.37260E+04/
DATA (DH2OCP(4,I),I=1,26)/
* 0.24780E+04, 0.25150E+04, 0.25950E+04, 0.26920E+04, 0.28170E+04,
* 0.29850E+04, 0.32170E+04, 0.35340E+04, 0.39600E+04, 0.52500E+04,
* 0.73170E+04, 0.10700E+05, 0.14760E+05, 0.20660E+05, 0.28440E+05,
* 0.37910E+05, 0.46020E+05, 0.46330E+05, 0.37430E+05, 0.25860E+05,
* 0.16840E+05, 0.11190E+05, 0.79370E+04, 0.61130E+04, 0.42980E+04,
* 0.38140E+04/
DATA (DH2OCP(5,I),I=1,26)/
* 0.24770E+04, 0.25140E+04, 0.25930E+04, 0.26860E+04, 0.28040E+04,
* 0.29620E+04, 0.31770E+04, 0.34680E+04, 0.38580E+04, 0.50300E+04,
* 0.68940E+04, 0.96630E+04, 0.13540E+05, 0.18750E+05, 0.25570E+05,
* 0.34030E+05, 0.42380E+05, 0.45510E+05, 0.39880E+05, 0.29390E+05,
* 0.19790E+05, 0.13210E+05, 0.92100E+04, 0.69040E+04, 0.45460E+04,
* 0.39030E+04/
DATA (DH2OCP(6,I),I=1,26)/
* 0.24770E+04, 0.25130E+04, 0.25910E+04, 0.26820E+04, 0.27950E+04,
* 0.29460E+04, 0.31480E+04, 0.34220E+04, 0.37860E+04, 0.48740E+04,
* 0.65970E+04, 0.91420E+04, 0.12690E+05, 0.17430E+05, 0.23580E+05,
* 0.31280E+05, 0.39430E+05, 0.44070E+05, 0.40990E+05, 0.31910E+05,
* 0.22240E+05, 0.15010E+05, 0.10400E+05, 0.76600E+04, 0.47890E+04,
* 0.39900E+04/
DATA (DH2OCP(7,I),I=1,26)/
* 0.24770E+04, 0.25120E+04, 0.25860E+04, 0.26700E+04, 0.27720E+04,
* 0.29030E+04, 0.30730E+04, 0.32980E+04, 0.35940E+04, 0.44640E+04,
* 0.58160E+04, 0.77830E+04, 0.10490E+05, 0.14040E+05, 0.18570E+05,
* 0.24200E+05, 0.30800E+05, 0.37060E+05, 0.39860E+05, 0.36830E+05,
* 0.29520E+05, 0.21600E+05, 0.15290E+05, 0.10980E+05, 0.59500E+04,
* 0.44190E+04/
DATA (DH2OCP(8,I),I=1,26)/

Appendix H

* 0.24770E+04, 0.25120E+04, 0.25840E+04, 0.26650E+04, 0.27610E+04,
* 0.28810E+04, 0.30360E+04, 0.32380E+04, 0.35020E+04, 0.42660E+04,
* 0.54430E+04, 0.71420E+04, 0.94580E+04, 0.12470E+05, 0.16270E+05,
* 0.20960E+05, 0.26540E+05, 0.32440E+05, 0.36760E+05, 0.36950E+05,
* 0.32430E+05, 0.25490E+05, 0.18810E+05, 0.13670E+05, 0.70210E+04,
* 0.48330E+04/

DATA (DH2OCP(9.I),I=1.26)/

* 0.24770E+04, 0.25120E+04, 0.25830E+04, 0.26620E+04, 0.27540E+04,
* 0.28680E+04, 0.30130E+04, 0.32010E+04, 0.34430E+04, 0.41430E+04,
* 0.52110E+04, 0.67430E+04, 0.88210E+04, 0.11510E+05, 0.14880E+05,
* 0.19000E+05, 0.23910E+05, 0.29330E+05, 0.34020E+05, 0.35860E+05,
* 0.33440E+05, 0.27820E+05, 0.21380E+05, 0.15860E+05, 0.80100E+04,
* 0.52320E+04/

DATA (DH2OCP(10.I),I=1.26)/

* 0.24770E+04, 0.25120E+04, 0.25830E+04, 0.26600E+04, 0.27490E+04,
* 0.28580E+04, 0.29960E+04, 0.31740E+04, 0.34020E+04, 0.40550E+04,
* 0.50460E+04, 0.64620E+04, 0.83730E+04, 0.10840E+05, 0.13910E+05,
* 0.17640E+05, 0.22090E+05, 0.27080E+05, 0.31790E+05, 0.34500E+05,
* 0.33570E+05, 0.29200E+05, 0.23270E+05, 0.17660E+05, 0.89260E+04,
* 0.56190E+04/

DATA (DH2OCP(11.I),I=1.26)/

* 0.24780E+04, 0.25120E+04, 0.25820E+04, 0.26580E+04, 0.27450E+04,
* 0.28510E+04, 0.29840E+04, 0.31540E+04, 0.33700E+04, 0.39880E+04,
* 0.49220E+04, 0.62490E+04, 0.80860E+04, 0.10330E+05, 0.13180E+05,
* 0.16630E+05, 0.20720E+05, 0.25370E+05, 0.29970E+05, 0.33140E+05,
* 0.33260E+05, 0.29980E+05, 0.24660E+05, 0.19130E+05, 0.97740E+04,
* 0.59920E+04/

DATA (DH2OCP(12.I),I=1.26)/

* 0.24790E+04, 0.25130E+04, 0.25820E+04, 0.26560E+04, 0.27400E+04,
* 0.28410E+04, 0.29660E+04, 0.31370E+04, 0.33250E+04, 0.38910E+04,
* 0.47410E+04, 0.59410E+04, 0.75490E+04, 0.96050E+04, 0.12140E+05,
* 0.15190E+05, 0.18780E+05, 0.22900E+05, 0.27200E+05, 0.30740E+05,
* 0.32150E+05, 0.30530E+05, 0.26430E+05, 0.21360E+05, 0.11290E+05,
* 0.67010E+04/

DATA (DH2OCP(13.I),I=1.26)/

* 0.24800E+04, 0.25140E+04, 0.25820E+04, 0.26550E+04, 0.27370E+04,
* 0.28340E+04, 0.29580E+04, 0.31030E+04, 0.32920E+04, 0.38220E+04,
* 0.46120E+04, 0.57240E+04, 0.72070E+04, 0.90950E+04, 0.11410E+05,
* 0.14130E+05, 0.17440E+05, 0.21170E+05, 0.25170E+05, 0.28780E+05,
* 0.30860E+05, 0.30380E+05, 0.27360E+05, 0.22880E+05, 0.12598E+05,

Appendix H

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* 0.73640E+04/
DATA (DH2OCP(14,I),I=1,26)/
* 0.24860E+04, 0.25190E+04, 0.25850E+04, 0.26530E+04, 0.27280E+04,
* 0.28150E+04, 0.29200E+04, 0.30480E+04, 0.32060E+04, 0.36400E+04,
* 0.42740E+04, 0.51520E+04, 0.63100E+04, 0.77680E+04, 0.95380E+04,
* 0.11620E+05, 0.14030E+05, 0.16770E+05, 0.19800E+05, 0.22930E+05,
* 0.25710E+05, 0.27420E+05, 0.27400E+05, 0.25550E+05, 0.16960E+05,
* 0.10100E+05/
DATA (DH2OCP(15,I),I=1,26)/
* 0.24920E+04, 0.25250E+04, 0.25880E+04, 0.26540E+04, 0.27260E+04,
* 0.28080E+04, 0.29040E+04, 0.30210E+04, 0.31640E+04, 0.35520E+04,
* 0.41110E+04, 0.48790E+04, 0.58840E+04, 0.71410E+04, 0.86580E+04,
* 0.10430E+05, 0.12460E+05, 0.14750E+05, 0.17280E+05, 0.19980E+05,
* 0.22610E+05, 0.24720E+05, 0.25770E+05, 0.25350E+05, 0.19190E+05,
* 0.12100E+05/
DATA (DH2OCP(16,I),I=1,26)/
* 0.24990E+04, 0.25310E+04, 0.25930E+04, 0.26560E+04, 0.27250E+04,
* 0.28040E+04, 0.28950E+04, 0.30050E+04, 0.31390E+04, 0.34970E+04,
* 0.40090E+04, 0.47080E+04, 0.56170E+04, 0.67510E+04, 0.81130E+04,
* 0.96990E+04, 0.11500E+05, 0.13520E+05, 0.15760E+05, 0.18150E+05,
* 0.20570E+05, 0.22720E+05, 0.24170E+05, 0.24520E+05, 0.20320E+05,
* 0.13590E+05/
DATA (DH2OCP(17,I),I=1,26)/
* 0.25050E+04, 0.25370E+04, 0.25980E+04, 0.26590E+04, 0.27260E+04,
* 0.28010E+04, 0.28890E+04, 0.29940E+04, 0.31210E+04, 0.34580E+04,
* 0.39360E+04, 0.45860E+04, 0.54290E+04, 0.64770E+04, 0.77300E+04,
* 0.91850E+04, 0.10830E+05, 0.12670E+05, 0.14690E+05, 0.16870E+05,
* 0.19110E+05, 0.21200E+05, 0.22820E+05, 0.23590E+05, 0.20870E+05,
* 0.14700E+05/
DATA (DH2OCP(18,I),I=1,26)/
* 0.25120E+04, 0.25430E+04, 0.26020E+04, 0.26620E+04, 0.27270E+04,
* 0.28000E+04, 0.28850E+04, 0.29860E+04, 0.31070E+04, 0.34280E+04,
* 0.38810E+04, 0.44940E+04, 0.52870E+04, 0.62690E+04, 0.74410E+04,
* 0.87980E+04, 0.10330E+05, 0.12030E+05, 0.13900E+05, 0.15910E+05,
* 0.18000E+05, 0.20010E+05, 0.21680E+05, 0.22690E+05, 0.21080E+05,
* 0.15540E+05/
DATA (DH2OCP(19,I),I=1,26)/
* 0.25250E+04, 0.25550E+04, 0.26110E+04, 0.26680E+04, 0.27300E+04,
* 0.27990E+04, 0.28800E+04, 0.29750E+04, 0.30880E+04, 0.33860E+04,
* 0.38020E+04, 0.43610E+04, 0.50800E+04, 0.59680E+04, 0.70240E+04,
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Appendix H

* 0.82410E+04, 0.96110E+04, 0.11120E+05, 0.12770E+05, 0.14540E+05,
* 0.16390E+05, 0.18240E+05, 0.19900E+05, 0.21140E+05, 0.20990E+05,
* 0.16660E+05/
DATA (DH2OCP(20,I),I=1,26)/
* 0.25380E+04, 0.25670E+04, 0.26200E+04, 0.26750E+04, 0.27340E+04,
* 0.28000E+04, 0.28770E+04, 0.29680E+04, 0.30750E+04, 0.33560E+04,
* 0.37450E+04, 0.42670E+04, 0.49340E+04, 0.57560E+04, 0.67300E+04,
* 0.78500E+04, 0.91060E+04, 0.10490E+05, 0.11990E+05, 0.13590E+05,
* 0.15280E+05, 0.16980E+05, 0.18580E+05, 0.19890E+05, 0.20610E+05,
* 0.17300E+05/
DATA (DH2OCP(21,I),I=1,26)/
* 0.25710E+04, 0.25980E+04, 0.26440E+04, 0.26920E+04, 0.27450E+04,
* 0.28050E+04, 0.28760E+04, 0.29580E+04, 0.30560E+04, 0.33080E+04,
* 0.36550E+04, 0.41140E+04, 0.46980E+04, 0.54120E+04, 0.62550E+04,
* 0.72190E+04, 0.82950E+04, 0.94710E+04, 0.10740E+05, 0.12080E+05,
* 0.13500E+05, 0.14950E+05, 0.16370E+05, 0.17660E+05, 0.19370E+05,
* 0.17820E+05/
DATA (DH2OCP(22,I),I=1,26)/
* 0.26050E+04, 0.26290E+04, 0.26690E+04, 0.27100E+04, 0.27570E+04,
* 0.28150E+04, 0.28770E+04, 0.29550E+04, 0.30460E+04, 0.32800E+04,
* 0.35990E+04, 0.40190E+04, 0.45500E+04, 0.51970E+04, 0.59590E+04,
* 0.68270E+04, 0.77930E+04, 0.88450E+04, 0.99710E+04, 0.11160E+05,
* 0.12410E+05, 0.13690E+05, 0.14970E+05, 0.16180E+05, 0.18210E+05,
* 0.17700E+05/
DATA (DH2OCP(23,I),I=1,26)/
* 0.27380E+04, 0.27520E+04, 0.27660E+04, 0.27820E+04, 0.28090E+04,
* 0.28470E+04, 0.28970E+04, 0.29600E+04, 0.30350E+04, 0.32300E+04,
* 0.34910E+04, 0.38300E+04, 0.42540E+04, 0.47660E+04, 0.53640E+04,
* 0.60410E+04, 0.67890E+04, 0.75970E+04, 0.84540E+04, 0.93520E+04,
* 0.10280E+05, 0.11230E+05, 0.12190E+05, 0.13140E+05, 0.15200E+05,
* 0.16140E+05/
DATA (DH2OCP(24,I),I=1,26)/
* 0.28720E+04, 0.28760E+04, 0.28630E+04, 0.28550E+04, 0.28620E+04,
* 0.28850E+04, 0.29230E+04, 0.29760E+04, 0.30410E+04, 0.32130E+04,
* 0.34450E+04, 0.37450E+04, 0.41160E+04, 0.45620E+04, 0.50810E+04,
* 0.56670E+04, 0.63120E+04, 0.70070E+04, 0.77410E+04, 0.85060E+04,
* 0.92930E+04, 0.10090E+05, 0.10900E+05, 0.11700E+05, 0.13560E+05,
* 0.14780E+05/
DATA (DH2OCP(25,I),I=1,26)/
* 0.30050E+04, 0.29970E+04, 0.29580E+04, 0.29260E+04, 0.29140E+04,

Appendix H

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* 0.29230E+04, 0.29510E+04, 0.29950E+04, 0.30520E+04, 0.32090E+04,  
* 0.34220E+04, 0.36950E+04, 0.40330E+04, 0.44380E+04, 0.49070E+04,  
* 0.54350E+04, 0.60160E+04, 0.66410E+04, 0.72990E+04, 0.79880E+04,  
* 0.86840E+04, 0.93660E+04, 0.10110E+05, 0.10830E+05, 0.12500E+05,  
* 0.13770E+05/  
DATA (DH2OCP(26,I),I=1,26)/  
* 0.31350E+04, 0.31170E+04, 0.30520E+04, 0.29960E+04, 0.29660E+04,  
* 0.29620E+04, 0.29790E+04, 0.30150E+04, 0.30660E+04, 0.32100E+04,  
* 0.34080E+04, 0.36680E+04, 0.39770E+04, 0.43510E+04, 0.47850E+04,  
* 0.52730E+04, 0.58080E+04, 0.63830E+04, 0.69880E+04, 0.76160E+04,  
* 0.82570E+04, 0.89070E+04, 0.95590E+04, 0.10200E+05, 0.11750E+05,  
* 0.13010E+05/  
*  
***** END OF BLOCK DATA *  
END
```

Appendix H

```

      BLOCK DATA DATAD2
*****
      BLOCK DATA IDENTIFICATION
*****
*
*
*   Data stored in this BLOCK DATA are
*   Transport Properties of Dissociated Steam
*   for Pressures from 0.01 to 100. MN/m**2
*   at Temperatures from 1200. to 6000. K
*   from VARGATIK (1983) and data generated by author.
*
*   Written by ALEKSANDAR VASIC'      Revised  March /1990
*   University of Ottawa
*
*****
*****
*
*****
      VARIABLE IDENTIFICATION
*****
*
*   DH2OPT = Pressure for Transport Properties (MN/m**2)
*   DH2OTT = Temperature for Transport Properties (K)
*   DH2OMU = Dynamic Viscosity (N*s/m**2)
*   DH2OK  = Thermal Conductivity (W/m*K)
*
*****
*****
*
*****
      TYPE DECLARATION                                BLOCK 0000 *
*
      INTEGER I
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 DH2OPT(17),DH2OTT(25)
      1      ,DH2OMU(17,25),DH2OK(17,25)
      COMMON /TRPTD/ DH2OPT,DH2OTT
      COMMON /TRPROD/ DH2OMU,DH2OK
*
*****
*****
*
*   PRESSURE (MN/m**2) TABLE FOR TRANSPORT PROPERTIES
*
*   DATA (DH2OPT(I),I=1,17)/
*   0.10000D-01, 0.20000D-01, 0.40000D-01, 0.60000D-01, 0.80000D-01,
*   0.10000D+00, 0.20000D+00, 0.50000D+00, 0.10000D+01, 0.20000D+01,
*   0.30000D+01, 0.40000D+01, 0.50000D+01, 0.60000D+01, 0.80000D+01,

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Appendix H

* 0.10000D+02, 0.10000D+03/

*

*

* TEMPERATURE (K) TABLE FOR TRANSPORT PROPERTIES

*

DATA (DH2OTT(1),I=1,25)/ 0.12000D+04
*, 0.14000D+04, 0.16000D+04, 0.18000D+04, 0.20000D+04, 0.22000D+04
*, 0.24000D+04, 0.26000D+04, 0.28000D+04, 0.30000D+04, 0.32000D+04
*, 0.34000D+04, 0.36000D+04, 0.38000D+04, 0.40000D+04, 0.42000D+04
*, 0.44000D+04, 0.46000D+04, 0.48000D+04, 0.50000D+04, 0.52000D+04
*, 0.54000D+04, 0.56000D+04, 0.58000D+04, 0.60000D+04/

*

*

* DYNAMIC VISCOSITY (N*s/m**2)

*

DATA (DH2OMU(1,I),I=1,25)/ 0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.65700E-04, 0.69800E-04
*, 0.73100E-04, 0.75200E-04, 0.75400E-04, 0.75600E-04, 0.76300E-04
*, 0.79500E-04, 0.80400E-04, 0.90300E-04, 0.95300E-04, 0.99700E-04
*, 0.10300E-03, 0.10800E-03, 0.11150E-03, 0.11550E-03, 0.11900E-03
*, 0.12300E-03, 0.12650E-03, 0.13000E-03, 0.13400E-03/
DATA (DH2OMU(2,I),I=1,25)/ 0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.65800E-04, 0.70000E-04
*, 0.73500E-04, 0.76000E-04, 0.77200E-04, 0.77400E-04, 0.77400E-04
*, 0.79100E-04, 0.83200E-04, 0.88600E-04, 0.94000E-04, 0.98900E-04
*, 0.10350E-03, 0.10750E-03, 0.11150E-03, 0.11550E-03, 0.11900E-03
*, 0.12300E-03, 0.12650E-03, 0.13000E-03, 0.13400E-03/
DATA (DH2OMU(3,I),I=1,25)/ 0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.65800E-04, 0.70200E-04
*, 0.73900E-04, 0.76700E-04, 0.78400E-04, 0.79000E-04, 0.77800E-04
*, 0.79600E-04, 0.82200E-04, 0.86700E-04, 0.92200E-04, 0.97600E-04
*, 0.10250E-03, 0.10700E-03, 0.11100E-03, 0.11600E-03, 0.11900E-03
*, 0.12250E-03, 0.12650E-03, 0.13000E-03, 0.13400E-03/
DATA (DH2OMU(4,I),I=1,25)/ 0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.65900E-04, 0.70200E-04
*, 0.74000E-04, 0.77100E-04, 0.79100E-04, 0.80000E-04, 0.80100E-04
*, 0.80400E-04, 0.82100E-04, 0.85100E-04, 0.91000E-04, 0.96500E-04
*, 0.10550E-03, 0.10650E-03, 0.10050E-03, 0.11450E-03, 0.11850E-03

Appendix H

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*, 0.12250E-03, 0.12650E-03, 0.13000E-03, 0.13400E-03/
DATA (DH2OMU(5,I),I=1,25)/                                0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.65900E-04, 0.70200E-04
*, 0.74200E-04, 0.77600E-04, 0.79500E-04, 0.80600E-04, 0.80900E-04
*, 0.81000E-04, 0.82200E-04, 0.85400E-04, 0.90100E-04, 0.95600E-04
*, 0.10100E-03, 0.10600E-03, 0.11050E-03, 0.10800E-03, 0.11850E-03
*, 0.12250E-03, 0.12600E-03, 0.13000E-03, 0.13350E-03/
DATA (DH2OMU(6,I),I=1,25)/                                0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.65900E-04, 0.70300E-04
*, 0.74200E-04, 0.77500E-04, 0.79800E-04, 0.81000E-04, 0.81400E-04
*, 0.81600E-04, 0.82500E-04, 0.85100E-04, 0.89500E-04, 0.94900E-04
*, 0.10050E-03, 0.10550E-03, 0.11000E-03, 0.11450E-03, 0.11850E-03
*, 0.12200E-03, 0.12600E-03, 0.13000E-03, 0.13350E-03/
DATA (DH2OMU(7,I),I=1,25)/                                0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.65900E-04, 0.70400E-04
*, 0.74400E-04, 0.77900E-04, 0.80600E-04, 0.82400E-04, 0.83200E-04
*, 0.83400E-04, 0.83800E-04, 0.85200E-04, 0.88200E-04, 0.92700E-04
*, 0.98000E-04, 0.10350E-03, 0.10850E-03, 0.11300E-03, 0.11750E-03
*, 0.12150E-03, 0.12550E-03, 0.12950E-03, 0.13350E-03/
DATA (DH2OMU(8,I),I=1,25)/                                0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.65900E-04, 0.70400E-04
*, 0.74600E-04, 0.78400E-04, 0.81500E-04, 0.83800E-04, 0.85200E-04
*, 0.85900E-04, 0.86300E-04, 0.86800E-04, 0.88200E-04, 0.90900E-04
*, 0.95000E-04, 0.99900E-04, 0.10550E-03, 0.11050E-03, 0.11550E-03
*, 0.12000E-03, 0.12450E-03, 0.12850E-03, 0.13200E-03/
DATA (DH2OMU(9,I),I=1,25)/                                0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66000E-04, 0.70500E-04
*, 0.74800E-04, 0.78800E-04, 0.82000E-04, 0.84600E-04, 0.86600E-04
*, 0.87700E-04, 0.88300E-04, 0.88700E-04, 0.89400E-04, 0.91000E-04
*, 0.93700E-04, 0.97600E-04, 0.10250E-03, 0.10750E-03, 0.11300E-03
*, 0.11800E-03, 0.12250E-03, 0.12700E-03, 0.13150E-03/
DATA (DH2OMU(10,I),I=1,25)/                                0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66000E-04, 0.70500E-04
*, 0.74900E-04, 0.78900E-04, 0.82400E-04, 0.85400E-04, 0.87700E-04
*, 0.89300E-04, 0.90300E-04, 0.90800E-04, 0.91400E-04, 0.92200E-04
*, 0.93900E-04, 0.96500E-04, 0.10000E-03, 0.10450E-03, 0.10950E-03
*, 0.11500E-03, 0.12000E-03, 0.12500E-03, 0.12950E-03/
DATA (DH2OMU(11,I),I=1,25)/                                0.45056E-04
*, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66000E-04, 0.70600E-04
*, 0.74900E-04, 0.79000E-04, 0.82600E-04, 0.85800E-04, 0.88200E-04

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Appendix H

*, 0.90100E-04, 0.91300E-04, 0.92100E-04, 0.93200E-04, 0.93300E-04
 *, 0.94500E-04, 0.96500E-04, 0.99500E-04, 0.10350E-03, 0.10800E-03
 *, 0.11300E-03, 0.11800E-03, 0.12300E-03, 0.12800E-03/
 DATA (DH2OMU(12,I),I=1,25)/ 0.45056E-04
 *, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66000E-04, 0.70600E-04
 *, 0.74900E-04, 0.79000E-04, 0.82800E-04, 0.86000E-04, 0.88600E-04
 *, 0.90600E-04, 0.92000E-04, 0.92900E-04, 0.93600E-04, 0.94200E-04
 *, 0.95200E-04, 0.96800E-04, 0.99300E-04, 0.10250E-03, 0.10700E-03
 *, 0.11150E-03, 0.11650E-03, 0.12150E-03, 0.12650E-03/
 DATA (DH2OMU(13,I),I=1,25)/ 0.45056E-04
 *, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66000E-04, 0.70600E-04
 *, 0.75000E-04, 0.79100E-04, 0.82800E-04, 0.86100E-04, 0.88900E-04
 *, 0.91000E-04, 0.92600E-04, 0.93600E-04, 0.94300E-04, 0.94900E-04
 *, 0.95800E-04, 0.97200E-04, 0.99300E-04, 0.10250E-03, 0.10600E-03
 *, 0.11050E-03, 0.11500E-04, 0.12050E-03, 0.12550E-03/
 DATA (DH2OMU(14,I),I=1,25)/ 0.45056E-04
 *, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66000E-04, 0.70600E-04
 *, 0.75000E-04, 0.79100E-04, 0.82900E-04, 0.86300E-04, 0.89100E-04
 *, 0.91300E-04, 0.93000E-04, 0.94100E-04, 0.94900E-04, 0.95500E-04
 *, 0.96300E-04, 0.97500E-04, 0.99400E-04, 0.10200E-03, 0.10550E-03
 *, 0.11000E-03, 0.11450E-03, 0.11950E-03, 0.12450E-03/
 DATA (DH2OMU(15,I),I=1,25)/ 0.45056E-04
 *, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66000E-04, 0.70600E-04
 *, 0.75000E-04, 0.79200E-04, 0.83000E-04, 0.86500E-04, 0.89400E-04
 *, 0.91800E-04, 0.93600E-04, 0.94900E-04, 0.95800E-04, 0.96500E-04
 *, 0.97200E-04, 0.98300E-04, 0.99800E-04, 0.10200E-03, 0.10500E-03
 *, 0.10900E-03, 0.11300E-03, 0.11800E-03, 0.12300E-03/
 DATA (DH2OMU(16,I),I=1,25)/ 0.45056E-04
 *, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66000E-04, 0.70600E-04
 *, 0.75000E-04, 0.79200E-04, 0.83100E-04, 0.86500E-04, 0.89600E-04
 *, 0.92100E-04, 0.94100E-04, 0.95500E-04, 0.96500E-04, 0.97300E-04
 *, 0.98000E-04, 0.98900E-04, 0.10050E-03, 0.10200E-03, 0.10500E-03
 *, 0.10800E-03, 0.11250E-03, 0.11700E-03, 0.12150E-03/
 * Data added by author (graphical extrapolation of above data).
 DATA (DH2OMU(17,I),I=1,25)/ 0.45056E-04
 *, 0.51200E-04, 0.56300E-04, 0.61200E-04, 0.66200E-04, 0.70800E-04
 *, 0.75200E-04, 0.79400E-04, 0.83400E-04, 0.87000E-04, 0.91000E-04
 *, 0.95000E-04, 0.97000E-04, 0.99000E-04, 0.10000E-03, 0.10080E-03
 *, 0.10110E-03, 0.10200E-03, 0.10350E-03, 0.10500E-03, 0.10800E-03
 *, 0.10900E-03, 0.11000E-03, 0.11500E-03, 0.12000E-03/

Appendix H

*

* THERMAL CONDUCTIVITY (W/m*K)

*

```
DATA (DH2OK(1,I),I=1,25)/                                0.14500E+00
*, 0.18800E+00, 0.22700E+00, 0.29100E+00, 0.42300E+00, 0.71100E+00
*, 0.13300E+01, 0.25900E+01, 0.46100E+01, 0.74500E+01, 0.93800E+01
*, 0.84700E+01, 0.68700E+01, 0.34400E+01, 0.21600E+01, 0.15350E+01
*, 0.12400E+01, 0.11100E+01, 0.10550E+01, 0.10420E+01, 0.10500E+01
*, 0.10650E+01, 0.10900E+01, 0.11150E+01, 0.11450E+01/

DATA (DH2OK(2,I),I=1,25)/                                0.14500E+00
*, 0.18800E+00, 0.22400E+00, 0.28000E+00, 0.38700E+00, 0.60600E+00
*, 0.10600E+01, 0.19350E+01, 0.34650E+01, 0.50900E+01, 0.80600E+01
*, 0.89350E+01, 0.74600E+01, 0.50550E+01, 0.32100E+01, 0.21400E+01
*, 0.15800E+01, 0.13050E+01, 0.11700E+01, 0.11100E+01, 0.10900E+01
*, 0.10900E+01, 0.11050E+01, 0.11300E+01, 0.15550E+01/

DATA (DH2OK(3,I),I=1,25)/                                0.14500E+00
*, 0.18800E+00, 0.22200E+00, 0.27100E+00, 0.35900E+00, 0.53000E+00
*, 0.86500E+00, 0.14950E+01, 0.25950E+01, 0.42950E+01, 0.59450E+01
*, 0.81550E+01, 0.83000E+01, 0.67200E+01, 0.46850E+01, 0.31350E+01
*, 0.21900E+01, 0.16650E+01, 0.13850E+01, 0.12450E+01, 0.11750E+01
*, 0.11450E+01, 0.11450E+01, 0.11550E+01, 0.19050E+01/

DATA (DH2OK(4,I),I=1,25)/                                0.14500E+00
*, 0.18700E+00, 0.22000E+00, 0.26700E+00, 0.34700E+00, 0.49500E+00
*, 0.77900E+00, 0.13050E+01, 0.22100E+01, 0.36250E+01, 0.55050E+01
*, 0.73650E+01, 0.82100E+01, 0.68250E+01, 0.56200E+01, 0.39050E+01
*, 0.30400E+01, 0.20000E+01, 0.15950E+01, 0.13700E+01, 0.12550E+01
*, 0.12000E+01, 0.11800E+01, 0.11750E+01, 0.11900E+01/

DATA (DH2OK(5,I),I=1,25)/                                0.14500E+00
*, 0.18700E+00, 0.22000E+00, 0.26500E+00, 0.33900E+00, 0.47400E+00
*, 0.72600E+00, 0.15450E+01, 0.19800E+01, 0.32200E+01, 0.49150E+01
*, 0.67450E+01, 0.79250E+01, 0.76900E+01, 0.62350E+01, 0.73950E+01
*, 0.31700E+01, 0.23000E+01, 0.17900E+01, 0.15250E+01, 0.13350E+01
*, 0.12550E+01, 0.12150E+01, 0.12000E+01, 0.12050E+01/

DATA (DH2OK(6,I),I=1,25)/                                0.14500E+00
*, 0.18700E+00, 0.21900E+00, 0.26300E+00, 0.33300E+00, 0.45900E+00
*, 0.69000E+00, 0.11100E+01, 0.18200E+01, 0.29400E+01, 0.44950E+01
*, 0.62650E+01, 0.76100E+01, 0.77650E+01, 0.66350E+01, 0.49950E+01
*, 0.35650E+01, 0.25800E+01, 0.19750E+01, 0.16150E+01, 0.14150E+01
*, 0.13050E+01, 0.12450E+01, 0.12250E+01, 0.12200E+01/
```

Appendix H

DATA (DH2OK(7,I),I=1,25)/ 0.14500E+00
*, 0.18700E+00, 0.21800E+00, 0.25800E+00, 0.31600E+00, 0.42100E+00
*, 0.59900E+00, 0.91000E+00, 0.14300E+01, 0.22400E+01, 0.34000E+01
*, 0.48550E+01, 0.63350E+01, 0.73050E+01, 0.72800E+01, 0.63000E+01
*, 0.49300E+01, 0.36850E+01, 0.27700E+01, 0.21600E+01, 0.17800E+01
*, 0.18500E+01, 0.14150E+01, 0.13400E+01, 0.13050E+01/
DATA (DH2OK(8,I),I=1,25)/ 0.14500E+00
*, 0.18700E+00, 0.21700E+00, 0.25300E+00, 0.30400E+00, 0.38400E+00
*, 0.51500E+00, 0.73000E+00, 0.10450E+01, 0.16050E+01, 0.23750E+01
*, 0.33850E+01, 0.46000E+01, 0.57950E+01, 0.66500E+01, 0.68400E+01
*, 0.63150E+01, 0.53350E+01, 0.42700E+01, 0.33550E+01, 0.26650E+01
*, 0.21900E+01, 0.18700E+01, 0.16650E+01, 0.15550E+01/
DATA (DH2OK(9,I),I=1,25)/ 0.14500E+00
*, 0.18600E+00, 0.21600E+00, 0.25100E+00, 0.29600E+00, 0.30400E+00
*, 0.46900E+00, 0.63600E+00, 0.89600E+00, 0.12850E+01, 0.18450E+01
*, 0.26000E+01, 0.35350E+01, 0.45800E+01, 0.55650E+01, 0.62550E+01
*, 0.64450E+01, 0.60950E+01, 0.53550E+01, 0.44800E+01, 0.36600E+01
*, 0.29900E+01, 0.24850E+01, 0.21300E+01, 0.18850E+01/
DATA (DH2OK(10,I),I=1,25)/ 0.14500E+00
*, 0.18600E+00, 0.21500E+00, 0.24800E+00, 0.29000E+00, 0.34800E+00
*, 0.43500E+00, 0.56600E+00, 0.76500E+00, 0.10550E+01, 0.14700E+01
*, 0.20200E+01, 0.27250E+01, 0.35500E+01, 0.44350E+01, 0.52500E+01
*, 0.58350E+01, 0.60600E+01, 0.58750E+01, 0.53650E+01, 0.48850E+01
*, 0.39850E+01, 0.33550E+01, 0.28450E+01, 0.24550E+01/
DATA (DH2OK(11,I),I=1,25)/ 0.14500E+00
*, 0.18600E+00, 0.21500E+00, 0.24700E+00, 0.28700E+00, 0.34100E+00
*, 0.41900E+00, 0.53400E+00, 0.70600E+00, 0.95300E+00, 0.13000E+01
*, 0.17600E+01, 0.23450E+01, 0.30600E+01, 0.38800E+01, 0.46300E+01
*, 0.52950E+01, 0.57250E+01, 0.58300E+01, 0.58050E+01, 0.51350E+01
*, 0.45300E+01, 0.39150E+01, 0.33600E+01, 0.28950E+01/
DATA (DH2OK(12,I),I=1,25)/ 0.14500E+00
*, 0.18600E+00, 0.21500E+00, 0.24700E+00, 0.28500E+00, 0.33600E+00
*, 0.40900E+00, 0.51500E+00, 0.66900E+00, 0.89000E+00, 0.11950E+01
*, 0.16050E+01, 0.21250E+01, 0.27550E+01, 0.34650E+01, 0.42050E+01
*, 0.48850E+01, 0.54000E+01, 0.55600E+01, 0.56250E+01, 0.53250E+01
*, 0.48450E+01, 0.42850E+01, 0.37350E+01, 0.32450E+01/
DATA (DH2OK(13,I),I=1,25)/ 0.14500E+00
*, 0.18600E+00, 0.21500E+00, 0.24600E+00, 0.26400E+00, 0.33300E+00
*, 0.40200E+00, 0.50100E+00, 0.64400E+00, 0.84600E+00, 0.11250E+01
*, 0.14950E+01, 0.19700E+01, 0.25400E+01, 0.32000E+01, 0.38950E+01

Appendix H

```
* , 0.45650E+01, 0.51200E+01, 0.54700E+01, 0.55600E+01, 0.53950E+01
* , 0.50300E+01, 0.45400E+01, 0.40200E+01, 0.35250E+01/
  DATA (DH2OK(14,I),I=1,25)/                                0.14500E+00
* , 0.18600E+00, 0.21500E+00, 0.24600E+00, 0.28300E+00, 0.33100E+00
* , 0.39600E+00, 0.49000E+00, 0.62500E+00, 0.81400E+00, 0.10750E+01
* , 0.14150E+01, 0.18500E+01, 0.23850E+01, 0.29950E+01, 0.36600E+01
* , 0.43100E+01, 0.48800E+01, 0.52800E+01, 0.54650E+01, 0.54000E+01
* , 0.51300E+01, 0.47100E+01, 0.42300E+01, 0.37100E+01/
  DATA (DH2OK(15,I),I=1,25)/                                0.14500E+00
* , 0.18600E+00, 0.21500E+00, 0.24500E+00, 0.28100E+00, 0.32700E+00
* , 0.38900E+00, 0.47600E+00, 0.59800E+00, 0.76800E+00, 0.99900E+00
* , 0.13050E+01, 0.16900E+01, 0.21600E+01, 0.27050E+01, 0.33100E+01
* , 0.39250E+01, 0.44950E+01, 0.49500E+01, 0.52400E+01, 0.53200E+01
* , 0.52000E+01, 0.49100E+01, 0.45150E+01, 0.40800E+01/
  DATA (DH2OK(16,I),I=1,25)/                                0.14500E+00
* , 0.18600E+00, 0.21400E+00, 0.24500E+00, 0.28000E+00, 0.32400E+00
* , 0.38300E+00, 0.46500E+00, 0.57900E+00, 0.75100E+00, 0.94800E+00
* , 0.12250E+01, 0.15750E+01, 0.20050E+01, 0.25050E+01, 0.30600E+01
* , 0.36400E+01, 0.41200E+01, 0.46400E+01, 0.50250E+01, 0.51950E+01
* , 0.51900E+01, 0.49950E+01, 0.46800E+01, 0.43000E+01/
* Data added by author (graphical extrapolation of above data).
  DATA (DH2OK(17,I),I=1,25)/                                0.14500E+00
* , 0.17000E+00, 0.18800E+00, 0.20900E+00, 0.25100E+00, 0.29300E+00
* , 0.33500E+00, 0.41900E+00, 0.48100E+00, 0.58600E+00, 0.67000E+00
* , 0.81600E+00, 0.13000E+01, 0.17000E+01, 0.21000E+01, 0.25000E+01
* , 0.29000E+01, 0.34000E+01, 0.39000E+01, 0.41500E+01, 0.44000E+01
* , 0.48000E+01, 0.50000E+01, 0.49000E+01, 0.47000E+01/
*
***** END OF BLOCK DATA *
***** THIS IS THE END OF U.O.HIGH TEMPERATURE STEAM PROPERTY CODE *****
END
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## BLOCK 0000 \*

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## Appendix H

```
*****      COMPUTATION AND PRINTING      BLOCK 0100 *
*
  OPEN(UNIT=1,FILE='DSPRO1.DAT')
  OPEN(UNIT=2,FILE='DSPRO2.DAT')
  PMP=0.01D0
  DO 19 I=1,5
    WRITE(1,1) PMP
    WRITE(2,1) PMP
1    FORMAT (/,T20,4HP = ,1F6,2,3HMPa,/)
    DO 9 TC=1000,D0,3000,D0,100,D0
      CALL UODH2O(PMP,TC)
      WRITE(1,7) TC,V,S,H,CP,MU,K
      WRITE(2,8) TC,RHO,NI,TDF,PR
7    FORMAT (T2,1F8,1,1F9,4,1F9,1,1F12,1,1F9,1,1F11,7,1F8,4)
8    FORMAT (T2,1F7,0,4D12,4)
9    CONTINUE
      PMP=10.D0*PMP
19  CONTINUE
*
*****      TERMINATION BLOCK      BLOCK 0800 *
*
  CLOSE (1)
  CLOSE (2)
*
***** END OF MAIN PROGRAM *
END
```

## Appendix I

# Programming Specifications of the High Temperature Steam Heat Transfer Code (VASICA)

This chapter includes subroutines, written in FORTRAN77 computer language, of the VASICA (VASIĆ Aleksandar) code to predict heat transfer for high temperature steam. A main program has to call the subroutine VASICA(TB,G,D,P,QW,TW,HTC,F). The input parameters are temperature TB(°C) in the range 726.85 to 4726.85°C, mass velocity G(kg m<sup>-2</sup> s<sup>-1</sup>), pipe diameter D(m), pressure P(MPa) in the range 0.01 to 100MPa, and constant heat flux at the wall QW(MW m<sup>-2</sup>). The results of calculations are wall temperature TW(°C), local heat transfer coefficient HTC(W m<sup>-2</sup> K<sup>-1</sup>) and Fanning friction factor F. Accompanying subroutines are FROZPROP, JANAF, MOLARMAS, FRENTA, FRCOND, PARFAN, NEWTON and functions are YG and F.

For performing a computation of heat transfer for high temperature steam, the required subroutines are all listed: the Fraction code at Appendix F, the Frozen Properties code at Appendix G, the UODH2O code at Appendix H and the VASICA code listed in this Appendix I. If computation requires temperatures lower than 1000°C, the IAPS Property code\* listed by Haar et al. (1984) or the UOH2O code by Cheng et al. (1989) must be incorporated.

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\* In this work, for temperatures <1000°C properties are evaluated using the IAPS code.

## Appendix I

```
      SUBROUTINE VASICA(TB,G,D,P,QW,TW,HTC,F)
***** BEGINNING OF VASICA CODE (TOTAL ~488 LINES) *****
*
      IMPLICIT REAL*8 (A-H,O-Z)
      INTEGER ACO
      REAL*8 KFB,LEFB(6),MMOL,MM(6),MASJ,MAS(4),MUB,NUB,NUFB,T1,T2,SUM
1      ,MUW,NUCR(4),NU1,NU4,NU5,NU6,HTC1,HTC4,HTC5,HTC6,NUFBVP
2      ,YWC,BET(6),BL(6),NUJCR(4)
      DIMENSION Y(6),YB(6),YW(6),DMIX(6),ACO(4,6),QP(4)
1      ,SC(6),SH(6)
      COMMON /FRACT/ Y
      COMMON /FRPRO/ MMOL,MM,HFM,CPFM,KFB
      COMMON /PROP/ VF, VG, VL, RHOF, RHOG, RHOL
1      ,HF, HG, HL, CPF, CPG, CPL, SL
2      ,UF, UG, UL, AKF, AKG, AKL
3      ,PRF, PRG, PRL, HFG, PSAT, TSAT
4      ,SIGMA
      COMMON /DIFMIX/ DMIX
      COMMON /LEWNUM/ LEFB
      COMMON /AJI/ ACO
      DATA E/.1D-6/
      CALL FRACTION(P,TB)
      DO 1 I=1,6
          YB(I) = Y(I)
1  CONTINUE
      TBK=TB+.27315D3
      CALL FROZPROP(P,TB)
      CPFB=CPFM/MMOL
      IF (TB.LE.1000.D0) THEN
          CALL IAPS(P,TB)
      ELSE
          CALL UODH2O(P,TB)
      END IF
      ROB=RHOL
      MUB=UL
      CALL PRN(MUB,CPFB,KFB,PRFB)
      CALL REN(G,D,MUB,REFB)
      N=1
      CALL NUKAKAC(N,PRFB,REFB,NUFB,FCP)
      CALL LEWIS(P,TB,KFB,ROB,CPFB)
```

## Appendix I

---

```

DO 2 I=1,6
  SC(I)=MUB/(ROB*DMIX(I))
  SCN=SC(I)
  N=2
  CALL NUKAKAC(N,SCN,REFB,SHN,Z)
  SH(I)=SHN
2 CONTINUE
CALL HEATEFF(1,HECR)
QP(1)=HECR
MASJ=(HECR*SH(1))/(ACO(1,1)*CPFM*LEFB(1))
MAS(1)=MASJ
DO 3 J=2,4
  L=J+2
  CALL HEATEFF(J,HECR)
  QP(J)=HECR
  MASJ=(HECR*SH(L))/(ACO(J,L)*CPFM*LEFB(L))
  MAS(J)=MASJ
3 CONTINUE
* This block is only for plotting purpose *****
*
C   TDFB=KFB/(ROB*CPFB)
C   TDE=AKL/(ROB*CPL)
C   WRITE(9,4) TB,TDFB,TDE
C   WRITE(9,4) TB,(Y(I),I=1,6)
C 4  FORMAT(T2,1F5.0,6F11.6)
C   WRITE(9,4) TB,MMOL*(.1D4/(HFM/(.1D4*MMOL)))+4648202.89D0,CPFB,KFB
C 4  FORMAT(T2,1F6.1,1F10.3,2F12.2,1F10.4)
C   WRITE(9,4) TB,ROB,MUB
C   PEFB=PRFB*REFB
C   STFB=NUFB/PEFB
C   WRITE(8,4) TB,PRFB,REFB,PEFB,NUFB,STFB
C 4  FORMAT(T2,1F5.0,6E12.4)
C   WRITE(3,4) TB,(DMIX(I),I=1,6)
C   WRITE(2,4) TB,(LEFB(I),I=1,6)
C   WRITE(4,4) TB,(SC(I),I=1,6)
C   WRITE(5,4) TB,(SH(I),I=1,6)
C   WRITE(7,4) TB,(QP(I),I=1,4)
C   WRITE(8,4) TB,(MAS(I),I=1,4)
*
*****

```

## Appendix I

---

```

C   RETURN
    T1=TB+((QW*D)/(KFB*NUFB))
    DO 99 M=1,300
        CALL FRACTION(P,T1)
        DO 6 I=1,6
            YW(I) = Y(I)
6   CONTINUE
    TR=TBK/(T1+.27315D3)
*   Temperature correction factor for gas flow with large temperature
*   differences proposed by Gnielinski (1976)
    IF ((TR.LT..15D1).OR.(TR.GT..5D0)) THEN
        VP=TR**-.45D0
    ELSE
        PRINT*, ' Temperature RATIO out of range! '
        PRINT*, ' (0.5 < Tb/Tw < 1.5), Tb/Tw= ', TR
    END IF
*   Blowing correction factor for Sherwood number
*   Increase of mass transfer due to large composition difference
*   proposed by Keys-Crawford (1980)
    DO 7 L=1,6
        YWC=.1D0*MMOL/MM(L)
        IF (YW(L).GE.YWC) THEN
            DIF=(MMOL/MM(L))-YW(L)
            IF (DIF.NE.0.0D0) THEN
                BET(L)=(YW(L)-YB(L))/DIF
                BL(L)=DABS((DLOG(BET(L)+.1001D1))/BET(L))
                BL(L)=.1D1
            ELSE
                BL(L)=.1D1
            END IF
        ELSE
            BL(L)=.1D1
        END IF
    END IF
7   CONTINUE
    DT1=T1-TB
    NUJCR(1)=(MAS(1)*YW(1)-MAS(1)*YB(1))*VP*BL(1)/DT1
    SUM=NUJCR(1)
    NUCR(1)=SUM
    DO 9 J=2,4
        L=J+2

```

## Appendix I

```

      NUJCR(J)=(MAS(J)*YW(L)-MAS(J)*YB(L))*VP*BL(L)/DT1
      SUM=SUM+NUJCR(J)
      NUCR(J)=SUM
9      CONTINUE
      NUFBVP=NUFB*VP
      NUB=NUFBVP+SUM
      T2=TB+((QW*D)/(KFB*NUB))
      DT=T2-T1
      IF (ABS(DT).LE.E) THEN
* This block is only for plotting purpose *****
*
C      WRITE(7,10) TB,(BL(L),L=1,6)
      HTCFB=(NUFBVP*KFB/D)/1000.D0
      HTC1=HTCFB+(NUCR(1)*KFB/D)/1000.D0
      HTC4=HTCFB+(NUCR(2)*KFB/D)/1000.D0
      HTC5=HTCFB+(NUCR(3)*KFB/D)/1000.D0
      HTC6=HTCFB+(NUCR(4)*KFB/D)/1000.D0
C      WRITE(7,10) TB,HTCFB,HTC1,HTC4,HTC5,HTC6
10     FORMAT(T2,1F5.0,6E11.3)
      NU1=NUFBVP+NUCR(1)
      NU4=NUFBVP+NUCR(2)
      NU5=NUFBVP+NUCR(3)
      NU6=NUFBVP+NUCR(4)
C      WRITE(8,11) TB,NUFBVP,NU1,NU4,NU5,NU6
C      WRITE(9,11) TB,NUFBVP,(NUJCR(J),J=1,4)
C      WRITE(8,11) TB,VP
11     FORMAT(T2,1F5.0,6E11.4)
*
*****

      TW=T2
      HTC=QW/(TW - TB)
* Calculation of friction factor
C      IF (TW.LE.1000.D0) THEN
C          CALL IAPS(P,TW)
C      ELSE
C          CALL UODH2O(P,TW)
C      END IF
C      ROW=RHOL
C      MUW=UL
C      TR=(TW+.27315D3)/(TB+.27315D3)

```

## Appendix I

```

C      ROR=ROB/ROW
C      REWCO=(G*D/MUW*ROR)
C      IF ((REWCO.LT..14D5).OR.(REWCO.GT..1D7)) THEN
C          PRINT*, 'REYNOLDS NUMBER IS OUT OF RANGE !'
C          PRINT*, '(14 000 < REW* < 1 000 000), REW* =', REWCO
C      END IF
*      Friction factor proposed by Petukhov (19 )
C      XM=-.6D0+(56D1*(REWCO**(-.38D0)))
C      TX=TR**XM
C      F=FCP*TX
      RETURN
      ELSE
          T1=T2
      END IF
99 CONTINUE
      PRINT*, 'For VASICA M>300', M
      END
          SUBROUTINE NUKAKAC(N,PR,RE,NUCP,FCP)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 NUCP
      IF (N.EQ.1) THEN
          IF ((PR.LT..5D0).OR.(PR.GT..2D4)) THEN
              PRINT*, 'Prandtl number is OUT of range !'
              PRINT*, '(0.5 < Pr < 2000), Pr =', PR
          END IF
      ELSE IF (N.EQ.2) THEN
          IF ((PR.LT..5D0).OR.(PR.GT..2D4)) THEN
              PRINT*, 'Schmidt number is OUT of range !'
              PRINT*, '(0.5 < Sc < 2000), Sc =', PR
          END IF
      END IF
      IF ((RE.LT..23D4).OR.(RE.GT..5D7)) THEN
          PRINT*, 'Reynolds number is OUT of range !'
          PRINT*, '(2300 < Re < 5 000 000), Re =', RE
      END IF
*      Fanning friction factor by Bhatti-Shah (1986) recommended
*      in book by Kakac (1986)
      IF (RE.LT..21D4) THEN
          A=0.0D0
          B=.16D2

```



## Appendix I

---

```

      C=.1D1
    ELSE IF (RE.LE..4D4) THEN
      A=.54D-2
      B=.23D-7
      C=-.66666666666666667D0
    ELSE IF (RE.LT..1D7) THEN
      A=.128D-2
      B=.1143D0
      C=.32154D0
    ELSE
      PRINT,' Out of f range > 10 000 000 RelbG= ',RE
    END IF
    FCP=A+(B/(RE**C))
    FCP2=FCP*.5D0
* Nusselt number correlation by Gnielinski (1976) recommended in book
* by Kakac (1986)
    NUCP=((RE-.1D4)*PR*FCP2)/(.127D2 * DSQRT(FCP2) * ((PR**(2/3))
    I      -.1D1) + .1D1)
    RETURN
  END

      SUBROUTINE HEATEFF(J,QP)
    IMPLICIT REAL*8 (A-H,O-Z)
    INTEGER ACO,IJ
    REAL*8 FH(6),QP
    DIMENSION ACO(4,6)
    COMMON /AJI/ ACO
    CALL FRENTA(FH)
    QP=(0,0D0)
    DO 9 I=1,6
      QP=QP+(ACO(J,I)*FH(I))
9 CONTINUE
    RETURN
  END

      SUBROUTINE LEWIS(P,TB,KFB,ROB,CPFB)
    IMPLICIT REAL*8 (A-H,O-Z)
    REAL*8 P,TB,KFB,ROB,CPFB,Y(6),DBIN(6,6),DMIX(6),LEFB(6)
    COMMON /FRACT/ Y
    COMMON /BINDIF/ DBIN
    COMMON /DIFMIX/ DMIX
    COMMON /LEWNUM/ LEFB

```

## Appendix I

```

      CALL BINDCO(P,TB)
***** This part is only for plotting purpose *****
C    WRITE(11,1) TB,(DBIN(1,I),I=1,6)
      1 FORMAT (T2,1F5.0,6E10.3)
C    WRITE(12,2) TB,(DBIN(1,I),I=2,6),(DBIN(2,J),J=3,4)
      2 FORMAT (T2,1F5.0,7E10.3)
C    WRITE(13,3) (DBIN(2,J),J=5,6),(DBIN(3,K),K=4,6),(DBIN(4,L),L=5,6),
C    1DBIN(5,6)
      3 FORMAT (8E10.3)
*****
      DO 9 L=1,6
          CALL MIXDIFF(L,DMIXL)
          DMIX(L)=DMIXL
          LEFB(L)=KFB/(ROB*CPFB*DMIXL)
* Assumption that Lewis number is = 1
C    LEFB(L)=.1D1
      9 CONTINUE
      RETURN
      END

      SUBROUTINE BINDCO(P,TB)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 P,TB,TKB,DBIN(6,6),DBINLI
      I      .RM(6,6),SBIN(6,6),EPSB(6,6),RT(6,6),OMED(6,6),ZB(6,6),ZM
      COMMON /BINDIF/ DBIN
      COMMON /COMPR/ ZB,ZM
      TKB=TB+.27315D3
      CALL PARAMET(TKB)
      CALL COMPRE(P,TKB)
C    WRITE(16,1) TB,((ZB(1,J),J=1,6),J=1,6)
      1 FORMAT(T2,1F5.0,6E11.3/,6E12.3/,6E12.3/,6E12.3/,
      16E12.3)
C    DO 6 I=1,6
C      DO 5 J=1,6
C        ZB(I,J)=.1D1
      5 CONTINUE
      6 CONTINUE
C    WRITE(17,2) TB,ZM
      2 FORMAT (T2,1F5.0,1E11.3)
      DO 8 L=1,6
          DO 7 I=1,6

```

## Appendix I

---

```
      CALL REDMAS(L,I,RM(L,I))
      CALL SIGMABIN(L,I,SBIN(L,I))
      CALL EPSILBIN(L,I,EPSEB(L,I))
      RT(L,I)=TKB/EPSEB(L,I)
      CALL NEUFD(RT(L,I),OMED(L,I))
      CALL MASDIF(P,TKB,RM(L,I),ZB(L,I),SBIN(L,I),OMED(L,I),DBINLI)
      DBIN(L,I)=DBINLI
7     CONTINUE
8     CONTINUE
C     WRITE(12,4) TKB,DBIN(1,3),DBIN(2,3),DBIN(2,5),DBIN(3,6)
4     FORMAT (T2,1F9,1.4E12,5)
      RETURN
      END

      SUBROUTINE PARAMET(TK)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 TK,TT(19),EK(6,19),S(6,19),EPSK(6),SIG(6),BA(6,19),CA(6,19)
1     ,B(6),C(6),Y1,Y2,D1,D2,F1,F2,F3,F4,INSERT
      LOGICAL EQUAL
      COMMON /TEMP/ TT
      COMMON /EPSIL/ EK
      COMMON /SIGMA/ S
      COMMON /PARAM/ EPSK,SIG
      COMMON /VIRCO/ BA,CA
      COMMON /VCOEF/ B,C
      CALL SEARCH(TT,TK,19,J,EQUAL)
      DO 9 I=1,6
        IF (EQUAL.EQV..TRUE.) THEN
          EPSK(I)=EK(I,J)
          SIG(I)=S(I,J)
*     conversion virial coefficient units to m3/mol
          B(I)=BA(I,J)*.1D-5
*     conversion virial coefficient units to m6/mol2
          C(I)=CA(I,J)*.1D-11
        ELSE
          D1=TK-TT(J)
          D2=TT(J+1)-TK
          Y1=EK(I,J)
          Y2=EK(I,J+1)
          F1=INSERT(Y1,Y2,D1,D2)
          EPSK(I)=F1
```

## Appendix I

```

      Y1=S(I,J)
      Y2=S(I,J+1)
      F2=INSERT(Y1,Y2,D1,D2)
      SIG(I)=F2
      Y1=BA(I,J)
      Y2=BA(I,J+1)
      F3=INSERT(Y1,Y2,D1,D2)
*   conversion virial coefficient units to m3/mol
      B(I)=F3*.1D-5
      Y1=CA(I,J)
      Y2=CA(I,J+1)
      F4=INSERT(Y1,Y2,D1,D2)
*   conversion virial coefficient units to m6/mol2
      C(I)=F4*.1D-11
      END IF
9   CONTINUE
      RETURN
      END

      SUBROUTINE COMPRE(PMPA,TK)
*
*   This subroutine calculates compressibility factor for all binary
*   mixtures and mixture of all six components.
*   Results are stored in COMMON /COMPR/
*
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 PMPA,TK,Y(6),A(3),B(6),C(6),X(6),ZB(6,6),ZM,R
      COMMON /FRACT/ Y
      COMMON /VCOEF/ B,C
      COMMON /COMPR/ ZB,ZM
      DATA R/.831441D4/
      A(1)=(PMPA*.1D7)/(R*TK)
      A(2)=A(1)**.2D1
      A(3)=A(1)**.3D1
      DO 8 I=1,6
        DO 7 J=1,6
          IF (Y(I).EQ..1D1) THEN
            ZB(I,J)=.1D1
          ELSE
            X(I)=Y(I)/(Y(I)+Y(J))
            X(J)=Y(J)/(Y(I)+Y(J))

```

## Appendix I

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```

      Z1=X(I)*B(I)+X(J)*B(J)
      Z2=X(I)*((B(I)**2)-C(I))+X(J)*((B(I)**2)-C(J))
      Z3=X(I)*B(I)*C(I)+X(J)*B(J)*C(J)
      ZB(I,J)=.1D1+A(1)*Z1-(A(2)*Z2)-(.2D1*A(3)*Z3)
    END IF
7    CONTINUE
8    CONTINUE
      Z1=0.0D0
      Z2=0.0D0
      Z3=0.0D0
      DO 9 I=1,6
        Z1=Z1+(Y(I)*B(I))
        Z2=Z2+(Y(I)*((B(I)**2)-C(I)))
        Z3=Z3+(Y(I)*B(I)*C(I))
9    CONTINUE
      ZM=.1D1+A(1)*Z1-(A(2)*Z2)-(.2D1*A(3)*Z3)
      RETURN
      END

      SUBROUTINE REDMAS(L,I,RM)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 M(6),RM
      DATA M /.1801528D2, .201588D1, .319988D2, .1700734D2, .100794D1
1     , .1599940D2/
      RM=(.1D1/M(L))+(.1D1/M(I))
      RETURN
      END

      SUBROUTINE SIGMABIN(L,I,SBIN)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 SBIN,EPK(6),SIG(6)
      COMMON /PARAM/ EPK,SIG
      SBIN=.5D0*(SIG(L)+SIG(I))
      RETURN
      END

      SUBROUTINE EPSILBIN(L,I,EPKB)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 EPKB,EPK(6),SIG(6)
      COMMON /PARAM/ EPK,SIG
      EPKB=DSQRT(EPK(L)*EPK(I))
      RETURN
      END

```

## Appendix I

```

      SUBROUTINE NEUFD(RT,OMED)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 OMED,RT,A,B,C,D,E,F,G,H
      DATA A/,106036D1/,B/,156100D0/,C/,193000D0/,D/,476350D0/
1     E/,103587D1/,F/,152996D1/,G/,176474D1/,H/,389411D1/
      OMED=A*(RT)**(-B)+C*(DEXP(-D*RT))+E*(DEXP(-F*RT))+G*(DEXP(-H*RT))
      RETURN
      END

      SUBROUTINE MASDIF(P,TK,RM,ZBIN,SBIN,OME,DBIN)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 A,TK,P,RM,ZBIN,SBIN,OME,DBIN
      DATA A/,1882899D-9/
      DBIN=(A*DSQRT(RM)*(TK**.15D1)*ZBIN)/((SBIN**2)*OME*P)
      RETURN
      END

      SUBROUTINE MIXDIFF(L,DMIX)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 DMIX,Y(6),DBIN(6.6),SUM
      COMMON /FRACT/ Y
      COMMON /BINDIF/ DBIN
      IF (Y(1).LT..98D0) THEN
* For system in which all I components move with same velocity
        SUM=0.0D0
        DO 9 I=1,6
          IF (I.NE.L) SUM=SUM+(Y(I)/DBIN(L,I))
        9    CONTINUE
        DMIX=(.1D1-Y(L))/SUM
* For component 1 (H2O)
* when Y(1)~1 Diffusion coefficient is equal to the Self-diffusion
* when Y(1)~0.5 Diffusion coefficient is calculated as mixture of all
* components..
* for 0.5< Y(1) <1 Diffusion coefficient is calculated as proportional to
* above two cases (to make smooth transition)
        IF ((L.EQ.1).AND.(Y(1).GT..5D0)) THEN
          DMIX=DBIN(L,1)+(DMIX-DBIN(L,1))*(.1D1-Y(1))/(.1D1-.5D0)
          RETURN
        END IF
        RETURN
      ELSE
* For trace components I=2,6

```

## Appendix I

---

```

        DMIX=DBIN(L,I)
        RETURN
    END IF
END

        BLOCK DATASCO
* Stehiometric coefficients for choosen four chemical rections
    INTEGER I,ACO
    DIMENSION ACO(4,6)
    COMMON /AJI/ ACO
    DATA (ACO(I,I),I=1,6) /-2, 2, 1, 0, 0, 0/
    DATA (ACO(2,I),I=1,6) / 0,-1,-1, 2, 0, 0/
    DATA (ACO(3,I),I=1,6) / 0,-1, 0, 0, 2, 0/
    DATA (ACO(4,I),I=1,6) / 0, 0,-1, 0, 0, 2/
END

        BLOCK DATAES
    INTEGER I
    REAL*8 TT,EK(6,19),S(6,19),BA(6,19),CA(6,19)
    DIMENSION TT(19)
    COMMON /TEMP/ TT
    COMMON /EPSIL/ EK
    COMMON /SIGMA/ S
    COMMON /VIRCO/ BA,CA
*   TEMPERATURE K
    DATA (TT(I),I=1,19)/
*   0.10000D+04, 0.12000D+04, 0.14000D+04, 0.16000D+04, 0.18000D+04
*   0.20000D+04, 0.22000D+04, 0.24000D+04, 0.26000D+04, 0.28000D+04
*   0.30000D+04, 0.34000D+04, 0.36000D+04, 0.40000D+04, 0.44000D+04
*   0.48000D+04, 0.52000D+04, 0.56000D+04, 0.60000D+04/
*
*   Temperature dependant parameter for Lennard-Jones potential
*   function - Kesselman (1968)      K
*
    DATA (EK(1,I),I=1,19)/
*   0.52350D+03, 0.48110D+03, 0.45800D+03, 0.45350D+03, 0.45600D+03
*   0.46100D+03, 0.46740D+03, 0.47320D+03, 0.47820D+03, 0.48220D+03
*   0.48550D+03, 0.48990D+03, 0.49150D+03, 0.49400D+03, 0.49600D+03
*   0.49760D+03, 0.49860D+03, 0.49940D+03, 0.49980D+03/
    DATA (EK(2,I),I=1,19) /19*0.34100D+02/
    DATA (EK(3,I),I=1,19)/
*   0.11740D+03, 0.11750D+03, 0.11750D+03, 0.11750D+03, 0.11750D+03

```

## Appendix I

```

* , 0.11750D+03, 0.11750D+03, 0.11750D+03, 0.11750D+03, 0.11750D+03
* , 0.11740D+03, 0.11740D+03, 0.11740D+03, 0.11740D+03, 0.11740D+03
* , 0.11740D+03, 0.11730D+03, 0.11730D+03, 0.11730D+03/
DATA (EK(4,I),I=1,19)/
*   0.10000D+03, 0.11200D+03, 0.12400D+03, 0.13200D+03, 0.14000D+03
* , 0.14750D+03, 0.15600D+03, 0.16250D+03, 0.16670D+03, 0.17280D+03
* , 0.17700D+03, 0.18440D+03, 0.18770D+03, 0.19400D+03, 0.19980D+03
* , 0.20490D+03, 0.20890D+03, 0.21220D+03, 0.21500D+03/
DATA (EK(5,I),I=1,19)/
*   0.35000D+03, 0.39000D+03, 0.43000D+03, 0.47000D+03, 0.50700D+03
* , 0.54780D+03, 0.58890D+03, 0.62780D+03, 0.66560D+03, 0.70170D+03
* , 0.73670D+03, 0.80340D+03, 0.83530D+03, 0.89690D+03, 0.95550D+03
* , 0.10118D+04, 0.10656D+04, 0.11169D+04, 0.11657D+04/
DATA (EK(6,I),I=1,19)/      5*0.11830D+03
* , 0.11830D+03, 0.11830D+03, 0.11830D+03, 0.11820D+03, 0.11810D+03
* , 0.11800D+03, 0.11770D+03, 0.11760D+03, 0.11730D+03, 0.11710D+03
* , 0.11680D+03, 0.11660D+03, 0.11640D+03, 0.11620D+03/
*
*   Temperature dependant parameter for Lennard-Jones potential
*   function - Kesselman (1968)      nm
*
DATA (S(1,I),I=1,19)/
*   0.28760D+00, 0.28600D+00, 0.28450D+00, 0.28340D+00, 0.28240D+00
* , 0.28150D+00, 0.28070D+00, 0.28000D+00, 0.27940D+00, 0.27880D+00
* , 0.27820D+00, 0.27720D+00, 0.27680D+00, 0.27600D+00, 0.27520D+00
* , 0.27490D+00, 0.27390D+00, 0.27330D+00, 0.27280D+00/
DATA (S(2,I),I=1,19)/
*   0.29380D+00, 0.29360D+00, 0.29350D+00, 0.29340D+00, 0.29340D+00
* , 0.29330D+00, 0.29330D+00, 0.29330D+00, 0.29320D+00, 0.29320D+00
* , 0.29320D+00, 0.29320D+00, 0.29320D+00, 0.29320D+00, 0.29320D+00
* , 0.29320D+00, 0.29320D+00, 0.29320D+00, 0.29320D+00/
DATA (S(3,I),I=1,19)/
*   0.34620D+00, 0.34620D+00, 0.34620D+00, 0.34620D+00, 0.34610D+00
* , 0.34610D+00, 0.34610D+00, 0.34610D+00, 0.34600D+00, 0.34600D+00
* , 0.34600D+00, 0.34600D+00, 0.34600D+00, 0.34590D+00, 0.34590D+00
* , 0.34580D+00, 0.34580D+00, 0.34570D+00, 0.34570D+00/
DATA (S(4,I),I=1,19)/
*   0.40500D+00, 0.40310D+00, 0.40120D+00, 0.39930D+00, 0.39740D+00
* , 0.39540D+00, 0.39330D+00, 0.39140D+00, 0.39000D+00, 0.38730D+00
* , 0.38570D+00, 0.38320D+00, 0.38180D+00, 0.37940D+00, 0.37730D+00

```



## Appendix I

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```
* 0.37540D+00, 0.37370D+00, 0.37210D+00, 0.37070D+00/
DATA (S(5,I),I=1,19)/
* 0.23700D+00, 0.23338D+00, 0.22976D+00, 0.22614D+00, 0.22252D+00
*, 0.21890D+00, 0.21610D+00, 0.21330D+00, 0.21070D+00, 0.20850D+00
*, 0.20630D+00, 0.20290D+00, 0.20140D+00, 0.19880D+00, 0.19650D+00
*, 0.19430D+00, 0.19230D+00, 0.19020D+00, 0.18820D+00/
DATA (S(6,I),I=1,19)/
* 0.29100D+00, 0.28920D+00, 0.28740D+00, 0.28560D+00, 0.28380D+00
*, 0.28200D+00, 0.28070D+00, 0.27950D+00, 0.27840D+00, 0.27740D+00
*, 0.27650D+00, 0.27480D+00, 0.27410D+00, 0.27280D+00, 0.27150D+00
*, 0.27040D+00, 0.26930D+00, 0.26840D+00, 0.26750D+00/
*
* Second virial coefficient - Kesselman (1968) cm3/mole
*
DATA (BA(1,I),I=1,19)/
* -0.21160D+02,-0.92900D+01,-0.28200D+01, 0.72000D+00, 0.30200D+01
*, 0.46800D+01, 0.59300D+01, 0.69300D+01, 0.77800D+01, 0.84900D+01
*, 0.90800D+01, 0.10030D+02, 0.10420D+02, 0.11010D+02, 0.11510D+02
*, 0.11870D+02, 0.12130D+02, 0.12330D+02, 0.12490D+02/
DATA (BA(2,I),I=1,19)/
* 0.16860D+02, 0.16700D+02, 0.16510D+02, 0.16300D+02, 0.16110D+02
*, 0.15900D+02, 0.15720D+02, 0.15540D+02, 0.15360D+02, 0.15200D+02
*, 0.15050D+02, 0.14760D+02, 0.14630D+02, 0.14370D+02, 0.14140D+02
*, 0.13930D+02, 0.13740D+02, 0.13560D+02, 0.13400D+02/
DATA (BA(3,I),I=1,19)/
* 0.22470D+02, 0.24410D+02, 0.25630D+02, 0.26400D+02, 0.26890D+02
*, 0.27210D+02, 0.27410D+02, 0.27520D+02, 0.27580D+02, 0.27600D+02
*, 0.27590D+02, 0.27530D+02, 0.27480D+02, 0.27370D+02, 0.27250D+02
*, 0.27000D+02, 0.26970D+02, 0.26770D+02, 0.26610D+02/
DATA (BA(4,I),I=1,19)/
* 0.50000D+02, 0.48000D+02, 0.46000D+02, 0.44000D+02, 0.42000D+02
*, 0.39350D+02, 0.39010D+02, 0.38670D+02, 0.38340D+02, 0.38010D+02
*, 0.37650D+02, 0.37060D+02, 0.36770D+02, 0.36230D+02, 0.35720D+02
*, 0.35220D+02, 0.34780D+02, 0.34340D+02, 0.33920D+02/
DATA (BA(5,I),I=1,19)/
* 0.60000D-10, 0.80000D-01, 0.10000D+00, 0.30000D+00, 0.50000D+00
*, 0.67000D+00, 0.87000D+00, 0.10400D+01, 0.11800D+01, 0.13000D+01
*, 0.14100D+01, 0.16000D+01, 0.16700D+01, 0.18100D+01, 0.19200D+01
*, 0.20100D+01, 0.20700D+01, 0.21200D+01, 0.21700D+01/
DATA (BA(6,I),I=1,19)/
```

## Appendix I

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```

*   0.14900D+02, 0.14840D+02, 0.14780D+02, 0.14720D+02, 0.14670D+02
*, 0.14620D+02, 0.14570D+02, 0.14480D+02, 0.14340D+02, 0.14210D+02
*, 0.14070D+02, 0.13800D+02, 0.13670D+02, 0.13420D+02, 0.13150D+02
*, 0.12910D+02, 0.12670D+02, 0.12450D+02, 0.12240D+02/

*
*   Third virial coefficient - Kesselman (1968)   cm6/mole2
*
DATA (CA(1,I),I=1,19)/
*   0.40790D+03, 0.33170D+03, 0.29570D+03, 0.27640D+03, 0.26390D+03
*, 0.25490D+03, 0.24750D+03, 0.24150D+03, 0.23590D+03, 0.23100D+03
*, 0.22660D+03, 0.21830D+03, 0.21480D+03, 0.20820D+03, 0.20200D+03
*, 0.19630D+03, 0.19060D+03, 0.18580D+03, 0.18150D+03/
DATA (CA(2,I),I=1,19)/
*   0.22600D+03, 0.21300D+03, 0.20200D+03, 0.19200D+03, 0.18400D+03
*, 0.17700D+03, 0.17100D+03, 0.16500D+03, 0.16000D+03, 0.15600D+03
*, 0.15200D+03, 0.14400D+03, 0.14100D+03, 0.13500D+03, 0.13000D+03
*, 0.12500D+03, 0.12100D+03, 0.11700D+03, 0.11400D+03/
DATA (CA(3,I),I=1,19)/
*   0.80540D+03, 0.78340D+03, 0.76240D+03, 0.74240D+03, 0.72290D+03
*, 0.70470D+03, 0.68750D+03, 0.67140D+03, 0.65630D+03, 0.64230D+03
*, 0.62920D+03, 0.60550D+03, 0.59450D+03, 0.57420D+03, 0.55770D+03
*, 0.53840D+03, 0.52760D+03, 0.51060D+03, 0.49800D+03/
DATA (CA(4,I),I=1,19)/ 19* 0.00000D+00/
DATA (CA(5,I),I=1,19)/ 19* 0.00000D+00/
DATA (CA(6,I),I=1,19)/ 19* 0.00000D+00/

*
***** END OF BLOCK DATA *
***** THIS IS THE END OF SUBROUTINES RELATED TO VASICA CODE *****
END

```

## PROGRAM IDENTIFICATION

\* Written by Aleksandar Vasic' /01/1988  
\* University of Ottawa

\*\*\*\*\*

\*\*\*\*\*

\*\*\*\*\* SUBROUTINE AND FUNCTION NAMES

\*\*\*\*\*

## BLOCK (0000) \*

269

## Appendix I

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```
PRINT*, 'EXECUTION of program HTCTW Started NOW.'
C PRINT*, 'd (m) = ? '
C READ*, D
C PRINT*, 'G (kg/m2 s) = ? '
C READ*, G
C PRINT*, 'P (MPa) = ? '
C READ*, P
C P=.101325D0
C PRINT*, 'QW (MW/m2) = ? '
C READ*, QWIN
QWIN=.1D1
C QW=QWIN*.1D7
C PRINT*, 'd= ', D, 'G= ', G, 'P= ', P, 'qw= ', QW
OPEN (UNIT=1, FILE='HTC.DAT')
C OPEN (UNIT=2, FILE='TW.DAT')
C OPEN (UNIT=2, FILE='LEDIS.DAT')
C OPEN (UNIT=3, FILE='DDIS.DAT')
C OPEN (UNIT=4, FILE='SCDIS.DAT')
C OPEN (UNIT=5, FILE='SHDIS.DAT')
C OPEN (UNIT=6, FILE='SCREAN.DAT')
C OPEN (UNIT=7, FILE='BL.DAT')
C OPEN (UNIT=7, FILE='BETA.DAT')
C OPEN (UNIT=7, FILE='HVDIS.DAT')
C OPEN (UNIT=7, FILE='HETEFF.DAT')
C OPEN (UNIT=8, FILE='MASS.DAT')
C OPEN (UNIT=8, FILE='NUNDIS.DAT')
C OPEN (UNIT=8, FILE='VP.DAT')
C OPEN (UNIT=8, FILE='NUMBER.DAT')
C OPEN (UNIT=9, FILE='YDIS.DAT')
C OPEN (UNIT=9, FILE='FROPRO.DAT')
C OPEN (UNIT=9, FILE='TERDIFF.DAT')
C OPEN (UNIT=9, FILE='NUJCR.DAT')
C OPEN (UNIT=9, FILE='PROPER.DAT')
C OPEN (UNIT=10, FILE='TWDIS.DAT')
C OPEN (UNIT=11, FILE='DIIDIS.DAT')
C OPEN (UNIT=12, FILE='DIJ1DIS.DAT')
C OPEN (UNIT=13, FILE='DIJ2DIS.DAT')
C OPEN (UNIT=14, FILE='LNQ.DAT')
C OPEN (UNIT=15, FILE='LNKP.DAT')
C OPEN (UNIT=16, FILE='ZB.DAT')
```

## Appendix I

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```

C  OPEN (UNIT=17,FILE='ZM.DAT')
C  WRITE(1,11) D,G,P,QWIN
C 11  FORMAT (T2,3HD= ,T5,F5.3,T10,1HM,T14,2HG=,T17,F5.0,T22,7HKG/M2 S,T
C 133.2HP=,T36,F7.3,T43,3HMPA,T49,3HQP=,T53,F7.3,T60,5HMW/M2)
C  P=0.01D0
C  DO 19 I=1,5
C  WRITE(9,111) P
C 111 FORMAT (/T20,4HP = ,1F6.2,3HMPa/)
C  DO 9 TB= 800.D0,4700.D0,100.D0
C  DO 99 TB= 800.D0,4700.D0,100.D0
C  PRINT*,TB
C  CALL VASICA (TB,G,D,P,QW,TW(6),HTC(6),F(6))
C 9  CONTINUE
C  P=P*10.D0
C 19  CONTINUE
*  Converting heat transfer coefficient units to kW/m2 K
C  DO 1 I=6,6
C  HTC(I)=HTC(I)/1000.D0
C 1  CONTINUE
C  WRITE (1,2) TB,HTC(1),HTC(2),HTC(3),HTC(4),HTC(5)
C 2  FORMAT (T2,1F9.1,5D10.4)
C  DO 3 I=1,5
C  DT(I)=TW(I)-TB
C 3  CONTINUE
C  WRITE (10,4) TB,(DT(I),I=1,5)
C 4  FORMAT (T2,1F9.1,5D12.6)
C  WRITE (1,5) TB,TW(1),TW(2),TW(3),TW(4),HTC(1),HTC(2),HTC(3),HTC(4)
C 5  FORMAT (T2,F5.0,T7,4F7.1,T36,4D 9.4)
C  WRITE (1,6) TB,TW(1),TW(2),TW(3),HTC(1),HTC(2),HTC(3)
C 6  FORMAT (T2,F9.1,T11,3F10.1,T41,3D10.5)
C  WRITE (1,7) TB,(HTC(I),I=6,6)
C 7  FORMAT (T2,F5.0,6E11.4)
C  WRITE (2,8) TB,(TW(I),I=6,6)
C 8  FORMAT (T2,F5.0,6F10.1)
C 99  CONTINUE

C  CLOSE (1)
C  CLOSE (2)
C  CLOSE (3)
C  CLOSE (4)

```

## Appendix I

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```
C  CLOSE (5)
C  CLOSE (6)
C  CLOSE (7)
C  CLOSE (8)
C  CLOSE (9)
C  CLOSE (10)
C  CLOSE (11)
C  CLOSE (12)
C  CLOSE (13)
C  CLOSE (14)
C  CLOSE (15)
C  CLOSE (16)
C  CLOSE (17)
  PRINT*, 'Execution of program HTCTW is FINISHED.'
*
***** END OF MAIN PROGRAM *
END
```

## **Appendix J**

### **Table of Dissociated Steam Composition at Pressure from 0.01 to 100.00 MPa and Temperature from 1000 to 3000°C**

This chapter includes a table of the mole fractions for six components which are formed by steam dissociation. The table is generated by the Fraction computer code listed in Appendix F.

# Appendix J

| t           | y <sub>i</sub>                                  |                |                |          |          |          |
|-------------|-------------------------------------------------|----------------|----------------|----------|----------|----------|
| °C          | mol <sub>i</sub> mol <sub>m</sub> <sup>-1</sup> |                |                |          |          |          |
| i           | 1                                               | 2              | 3              | 4        | 5        | 6        |
| Component   | H <sub>2</sub> O                                | H <sub>2</sub> | O <sub>2</sub> | HO       | H        | O        |
| P = 0.01MPa |                                                 |                |                |          |          |          |
| 1000.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1100.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1200.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1300.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1400.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1500.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1600.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1700.0      | 0.980370                                        | 0.010805       | 0.004525       | 0.003731 | 0.000454 | 0.000116 |
| 1800.0      | 0.966736                                        | 0.017658       | 0.007221       | 0.006942 | 0.001131 | 0.000311 |
| 1900.0      | 0.946460                                        | 0.027389       | 0.011014       | 0.011787 | 0.002588 | 0.000761 |
| 2000.0      | 0.917231                                        | 0.040560       | 0.016059       | 0.018946 | 0.005490 | 0.001714 |
| 2100.0      | 0.876673                                        | 0.057487       | 0.022435       | 0.028938 | 0.010879 | 0.003588 |
| 2200.0      | 0.822508                                        | 0.078060       | 0.030065       | 0.042080 | 0.020264 | 0.007023 |
| 2300.0      | 0.753029                                        | 0.101501       | 0.038628       | 0.058275 | 0.035640 | 0.012928 |
| 2400.0      | 0.667795                                        | 0.126139       | 0.047491       | 0.076761 | 0.059358 | 0.022456 |
| 2500.0      | 0.568469                                        | 0.149296       | 0.055675       | 0.095895 | 0.093779 | 0.036887 |
| 2600.0      | 0.459550                                        | 0.167460       | 0.061930       | 0.113111 | 0.140603 | 0.057345 |
| 2700.0      | 0.348560                                        | 0.176922       | 0.064957       | 0.125251 | 0.199952 | 0.084358 |
| 2800.0      | 0.245051                                        | 0.174943       | 0.063819       | 0.129407 | 0.269453 | 0.117328 |
| 2900.0      | 0.158157                                        | 0.161138       | 0.058411       | 0.124156 | 0.343934 | 0.154204 |
| 3000.0      | 0.093405                                        | 0.138197       | 0.049718       | 0.110525 | 0.416438 | 0.191718 |



# Appendix J

| t           | y <sub>i</sub>                                  |                |                |          |          |          |
|-------------|-------------------------------------------------|----------------|----------------|----------|----------|----------|
| °C          | mol <sub>i</sub> mol <sub>m</sub> <sup>-1</sup> |                |                |          |          |          |
| i           | 1                                               | 2              | 3              | 4        | 5        | 6        |
| Component   | H <sub>2</sub> O                                | H <sub>2</sub> | O <sub>2</sub> | HO       | H        | O        |
| P = 0.10MPa |                                                 |                |                |          |          |          |
| 1000.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1100.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1200.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1300.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1400.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1500.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1600.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1700.0      | 0.991184                                        | 0.005022       | 0.00214        | 0.001530 | 0.000098 | 0.000025 |
| 1800.0      | 0.984736                                        | 0.008321       | 0.003374       | 0.003256 | 0.000246 | 0.000067 |
| 1900.0      | 0.975501                                        | 0.013022       | 0.005176       | 0.005571 | 0.000564 | 0.000165 |
| 2000.0      | 0.962212                                        | 0.019535       | 0.007618       | 0.009056 | 0.001205 | 0.000373 |
| 2100.0      | 0.943734                                        | 0.028209       | 0.010798       | 0.014063 | 0.002410 | 0.000787 |
| 2200.0      | 0.918842                                        | 0.039324       | 0.014784       | 0.020944 | 0.004547 | 0.001557 |
| 2300.0      | 0.886300                                        | 0.053038       | 0.019598       | 0.030005 | 0.008140 | 0.002912 |
| 2400.0      | 0.844985                                        | 0.069306       | 0.025187       | 0.041437 | 0.013914 | 0.005171 |
| 2500.0      | 0.794053                                        | 0.087809       | 0.031402       | 0.055232 | 0.022743 | 0.008760 |
| 2600.0      | 0.733153                                        | 0.107876       | 0.037984       | 0.071099 | 0.035686 | 0.014202 |
| 2700.0      | 0.662669                                        | 0.128439       | 0.044548       | 0.088377 | 0.053875 | 0.022092 |
| 2800.0      | 0.583930                                        | 0.148046       | 0.050600       | 0.106001 | 0.078385 | 0.033037 |
| 2900.0      | 0.499356                                        | 0.164947       | 0.055571       | 0.122523 | 0.110040 | 0.047563 |
| 3000.0      | 0.412422                                        | 0.177300       | 0.058888       | 0.136247 | 0.149161 | 0.065981 |

# Appendix J

| t           | y <sub>i</sub>                                  |                |                |          |          |          |
|-------------|-------------------------------------------------|----------------|----------------|----------|----------|----------|
| °C          | mol <sub>i</sub> mol <sub>m</sub> <sup>-1</sup> |                |                |          |          |          |
| i           | 1                                               | 2              | 3              | 4        | 5        | 6        |
| Component   | H <sub>2</sub> O                                | H <sub>2</sub> | O <sub>2</sub> | HO       | H        | O        |
| P = 1.00MPa |                                                 |                |                |          |          |          |
| 1000.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1100.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1200.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1300.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1400.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1500.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1600.0      | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1700.0      | 0.996652                                        | 0.002215       | 0.001111       | 0.000000 | 0.000021 | 0.000006 |
| 1800.0      | 0.992953                                        | 0.003889       | 0.001571       | 0.001519 | 0.000053 | 0.000015 |
| 1900.0      | 0.988710                                        | 0.006109       | 0.002416       | 0.002607 | 0.000122 | 0.000036 |
| 2000.0      | 0.982614                                        | 0.009217       | 0.003569       | 0.004258 | 0.000262 | 0.000081 |
| 2100.0      | 0.974145                                        | 0.013413       | 0.005088       | 0.006657 | 0.000525 | 0.000171 |
| 2200.0      | 0.962727                                        | 0.018899       | 0.007027       | 0.010010 | 0.000997 | 0.000340 |
| 2300.0      | 0.947745                                        | 0.025859       | 0.009427       | 0.014531 | 0.001799 | 0.000639 |
| 2400.0      | 0.928570                                        | 0.034440       | 0.012317       | 0.020427 | 0.003102 | 0.001144 |
| 2500.0      | 0.904594                                        | 0.044735       | 0.015702       | 0.027877 | 0.005133 | 0.001959 |
| 2600.0      | 0.875273                                        | 0.056753       | 0.019560       | 0.037006 | 0.008185 | 0.003223 |
| 2700.0      | 0.840180                                        | 0.070402       | 0.023835       | 0.047860 | 0.012613 | 0.005110 |
| 2800.0      | 0.799066                                        | 0.085465       | 0.028432       | 0.060372 | 0.018833 | 0.007831 |
| 2900.0      | 0.751916                                        | 0.101585       | 0.033220       | 0.074342 | 0.027308 | 0.011629 |
| 3000.0      | 0.699012                                        | 0.118260       | 0.038024       | 0.089414 | 0.038523 | 0.016766 |

# Appendix J

| t            | y <sub>i</sub>                                  |                |                |          |          |          |
|--------------|-------------------------------------------------|----------------|----------------|----------|----------|----------|
| °C           | mol <sub>i</sub> mol <sub>m</sub> <sup>-1</sup> |                |                |          |          |          |
| i            | 1                                               | 2              | 3              | 4        | 5        | 6        |
| Component    | H <sub>2</sub> O                                | H <sub>2</sub> | O <sub>2</sub> | HO       | H        | O        |
| P = 10.00MPa |                                                 |                |                |          |          |          |
| 1000.0       | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1100.0       | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1200.0       | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1300.0       | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1400.0       | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1500.0       | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1600.0       | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1700.0       | 0.998824                                        | 0.000971       | 0.000581       | 0.000000 | 0.000004 | 0.000001 |
| 1800.0       | 0.996745                                        | 0.001809       | 0.000731       | 0.000700 | 0.000011 | 0.000003 |
| 1900.0       | 0.994778                                        | 0.002850       | 0.001124       | 0.001214 | 0.000026 | 0.000008 |
| 2000.0       | 0.991965                                        | 0.004310       | 0.001663       | 0.001988 | 0.000057 | 0.000017 |
| 2100.0       | 0.988061                                        | 0.006294       | 0.002378       | 0.003117 | 0.000114 | 0.000037 |
| 2200.0       | 0.982799                                        | 0.008909       | 0.003295       | 0.004706 | 0.000216 | 0.000074 |
| 2300.0       | 0.975891                                        | 0.012265       | 0.004443       | 0.006870 | 0.000392 | 0.000139 |
| 2400.0       | 0.967033                                        | 0.016465       | 0.005845       | 0.009729 | 0.000678 | 0.000249 |
| 2500.0       | 0.955916                                        | 0.021604       | 0.007518       | 0.013405 | 0.001128 | 0.000429 |
| 2600.0       | 0.942234                                        | 0.027759       | 0.009474       | 0.018013 | 0.001810 | 0.000709 |
| 2700.0       | 0.925699                                        | 0.034986       | 0.011716       | 0.023654 | 0.002812 | 0.001133 |
| 2800.0       | 0.906054                                        | 0.043309       | 0.014236       | 0.030410 | 0.004240 | 0.001752 |
| 2900.0       | 0.883088                                        | 0.052716       | 0.017015       | 0.038328 | 0.006221 | 0.002632 |
| 3000.0       | 0.856653                                        | 0.063155       | 0.020025       | 0.047418 | 0.008902 | 0.003848 |

# Appendix J

| t             | y <sub>i</sub>                                  |                |                |          |          |          |
|---------------|-------------------------------------------------|----------------|----------------|----------|----------|----------|
| °C            | mol <sub>i</sub> mol <sub>m</sub> <sup>-1</sup> |                |                |          |          |          |
| i             | 1                                               | 2              | 3              | 4        | 5        | 6        |
| Component     | H <sub>2</sub> O                                | H <sub>2</sub> | O <sub>2</sub> | HO       | H        | O        |
| P = 100.00MPa |                                                 |                |                |          |          |          |
| 1000.0        | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1100.0        | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1200.0        | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1300.0        | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1400.0        | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1500.0        | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1600.0        | 1.000000                                        | 0.000000       | 0.000000       | 0.000000 | 0.000000 | 0.000000 |
| 1700.0        | 0.999414                                        | 0.000457       | 0.000263       | 0.000135 | 0.000001 | 0.000000 |
| 1800.0        | 0.998488                                        | 0.000842       | 0.000339       | 0.000328 | 0.000002 | 0.000001 |
| 1900.0        | 0.997580                                        | 0.001326       | 0.000522       | 0.000565 | 0.000006 | 0.000002 |
| 2000.0        | 0.996278                                        | 0.002007       | 0.000774       | 0.000925 | 0.000012 | 0.000004 |
| 2100.0        | 0.994472                                        | 0.002936       | 0.001107       | 0.001453 | 0.000025 | 0.000008 |
| 2200.0        | 0.992039                                        | 0.004164       | 0.001537       | 0.002197 | 0.000047 | 0.000016 |
| 2300.0        | 0.988844                                        | 0.005749       | 0.002077       | 0.003216 | 0.000085 | 0.000030 |
| 2400.0        | 0.984747                                        | 0.007744       | 0.002740       | 0.004568 | 0.000147 | 0.000054 |
| 2500.0        | 0.979598                                        | 0.010206       | 0.003538       | 0.006320 | 0.000245 | 0.000093 |
| 2600.0        | 0.973248                                        | 0.013186       | 0.004480       | 0.008537 | 0.000395 | 0.000154 |
| 2700.0        | 0.965551                                        | 0.016730       | 0.005574       | 0.011283 | 0.000615 | 0.000247 |
| 2800.0        | 0.956363                                        | 0.020878       | 0.006825       | 0.014619 | 0.000931 | 0.000384 |
| 2900.0        | 0.945554                                        | 0.025660       | 0.008233       | 0.018601 | 0.001372 | 0.000579 |
| 3000.0        | 0.933006                                        | 0.031096       | 0.009798       | 0.023274 | 0.001975 | 0.000851 |

## Appendix K

### Table of Frozen Properties for Dissociated Steam at Pressure from 0.01 to 100.00 MPa and Temperature from 1000 to 3000°C\*

This chapter includes a table of three thermodynamic properties - molar mass, enthalpy and heat capacity, and one transport property - thermal conductivity\*\*. The table is generated by the Frozen Property computer code listed in Appendix G.

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\*

The zero value of enthalpy of water is set at triple point ( $t=0.01^{\circ}\text{C}$ ,  $P=611.73\text{Pa}$ )  $k_H=4.648202\text{MJ kg}_{\text{H}_2\text{O}}^{-1}$ .

\*\*

WARNING! The values of thermal conductivity are generated using data by Svehla (1964) which are lower than should be. Since, this are the only available data in literature for frozen thermal conductivity, they are adapted in this work. The estimated inaccuracy of the predictions is in order of -10%.

# Appendix K

| $t$                 | $\bar{M}_m$                       | $H_{fr}$             | $C_{pfr}$                                  | $k_{fr}$                                |
|---------------------|-----------------------------------|----------------------|--------------------------------------------|-----------------------------------------|
| $^{\circ}\text{C}$  | $\text{kg}_m \text{ kmol}_m^{-1}$ | $\text{J kg}_m^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{W m}^{-1} ^{\circ}\text{C}^{-1}$ |
| <b>P = 0.01 MPa</b> |                                   |                      |                                            |                                         |
| 1000.0              | 18.015                            | 4636875.0            | 2477.2                                     | 0.1504                                  |
| 1100.0              | 18.015                            | 4637125.9            | 2539.8                                     | 0.1655                                  |
| 1200.0              | 18.015                            | 4637382.8            | 2598.4                                     | 0.1809                                  |
| 1300.0              | 18.015                            | 4637645.4            | 2652.8                                     | 0.1961                                  |
| 1400.0              | 18.015                            | 4637913.2            | 2703.1                                     | 0.2112                                  |
| 1500.0              | 18.015                            | 4638185.9            | 2749.3                                     | 0.2262                                  |
| 1600.0              | 18.015                            | 4638463.0            | 2791.8                                     | 0.2416                                  |
| 1700.0              | 17.894                            | 4638940.5            | 2832.0                                     | 0.2571                                  |
| 1800.0              | 17.807                            | 4639368.9            | 2869.0                                     | 0.2735                                  |
| 1900.0              | 17.674                            | 4639878.9            | 2903.3                                     | 0.2906                                  |
| 2000.0              | 17.475                            | 4640506.3            | 2935.3                                     | 0.3090                                  |
| 2100.0              | 17.188                            | 4641298.0            | 2965.6                                     | 0.3294                                  |
| 2200.0              | 16.786                            | 4642316.2            | 2994.7                                     | 0.3519                                  |
| 2300.0              | 16.241                            | 4643643.2            | 3023.3                                     | 0.3777                                  |
| 2400.0              | 15.529                            | 4645384.3            | 3052.1                                     | 0.4073                                  |
| 2500.0              | 14.639                            | 4647669.5            | 3082.1                                     | 0.4413                                  |
| 2600.0              | 13.581                            | 4650647.2            | 3114.6                                     | 0.4796                                  |
| 2700.0              | 12.396                            | 4654459.1            | 3150.7                                     | 0.5217                                  |
| 2800.0              | 11.159                            | 4659182.0            | 3191.1                                     | 0.5654                                  |
| 2900.0              | 9.969                             | 4664731.3            | 3235.8                                     | 0.6071                                  |
| 3000.0              | 8.919                             | 4670776.3            | 3282.6                                     | 0.6426                                  |

# Appendix K

| $t$                    | $\bar{M}_m$                       | $H_{fr}$             | $C_{pfr}$                                  | $k_{fr}$                                |
|------------------------|-----------------------------------|----------------------|--------------------------------------------|-----------------------------------------|
| $^{\circ}\text{C}$     | $\text{kg}_m \text{ kmol}_m^{-1}$ | $\text{J kg}_m^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{W m}^{-1} ^{\circ}\text{C}^{-1}$ |
| $P = 0.10 \text{ MPa}$ |                                   |                      |                                            |                                         |
| 1000.0                 | 18.015                            | 4636875.0            | 2477.2                                     | 0.1504                                  |
| 1100.0                 | 18.015                            | 4637125.9            | 2539.8                                     | 0.1655                                  |
| 1200.0                 | 18.015                            | 4637382.8            | 2598.4                                     | 0.1806                                  |
| 1300.0                 | 18.015                            | 4637645.4            | 2652.8                                     | 0.1957                                  |
| 1400.0                 | 18.015                            | 4637913.2            | 2703.1                                     | 0.2107                                  |
| 1500.0                 | 18.015                            | 4638185.9            | 2749.3                                     | 0.2258                                  |
| 1600.0                 | 18.015                            | 4638463.0            | 2791.8                                     | 0.2406                                  |
| 1700.0                 | 17.962                            | 4638830.6            | 2831.2                                     | 0.2555                                  |
| 1800.0                 | 17.922                            | 4639181.3            | 2867.8                                     | 0.2706                                  |
| 1900.0                 | 17.864                            | 4639565.3            | 2901.5                                     | 0.2860                                  |
| 2000.0                 | 17.779                            | 4639998.1            | 2932.6                                     | 0.3018                                  |
| 2100.0                 | 17.658                            | 4640495.5            | 2961.5                                     | 0.3183                                  |
| 2200.0                 | 17.491                            | 4641077.4            | 2988.5                                     | 0.3357                                  |
| 2300.0                 | 17.266                            | 4641768.5            | 3013.8                                     | 0.3542                                  |
| 2400.0                 | 16.970                            | 4642599.4            | 3037.8                                     | 0.3743                                  |
| 2500.0                 | 16.589                            | 4643606.8            | 3060.8                                     | 0.3961                                  |
| 2600.0                 | 16.113                            | 4644834.5            | 3083.3                                     | 0.4201                                  |
| 2700.0                 | 15.533                            | 4646333.8            | 3105.5                                     | 0.4470                                  |
| 2800.0                 | 14.848                            | 4648162.2            | 3128.1                                     | 0.4769                                  |
| 2900.0                 | 14.062                            | 4650380.9            | 3151.4                                     | 0.5096                                  |
| 3000.0                 | 13.195                            | 4653047.9            | 3176.0                                     | 0.5453                                  |

# Appendix K

| t                  | $\tilde{M}_m$                     | $H_{fr}$             | $C_{p_{fr}}$                               | $k_{fr}$                                |
|--------------------|-----------------------------------|----------------------|--------------------------------------------|-----------------------------------------|
| $^{\circ}\text{C}$ | $\text{kg}_m \text{ kmol}_m^{-1}$ | $\text{J kg}_m^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{W m}^{-1} ^{\circ}\text{C}^{-1}$ |
| P = 1.00 MPa       |                                   |                      |                                            |                                         |
| 1000.0             | 18.015                            | 4636875.0            | 2477.2                                     | 0.1504                                  |
| 1100.0             | 18.015                            | 4637125.9            | 2539.8                                     | 0.1655                                  |
| 1200.0             | 18.015                            | 4637382.8            | 2598.4                                     | 0.1806                                  |
| 1300.0             | 18.015                            | 4637645.4            | 2652.8                                     | 0.1957                                  |
| 1400.0             | 18.015                            | 4637913.2            | 2703.1                                     | 0.2107                                  |
| 1500.0             | 18.015                            | 4638185.9            | 2749.3                                     | 0.2255                                  |
| 1600.0             | 18.015                            | 4638463.0            | 2791.8                                     | 0.2402                                  |
| 1700.0             | 17.995                            | 4638775.5            | 2830.9                                     | 0.2548                                  |
| 1800.0             | 17.973                            | 4639098.5            | 2867.4                                     | 0.2695                                  |
| 1900.0             | 17.947                            | 4639429.7            | 2900.9                                     | 0.2841                                  |
| 2000.0             | 17.909                            | 4639783.7            | 2931.6                                     | 0.2988                                  |
| 2100.0             | 17.856                            | 4640166.4            | 2960.1                                     | 0.3134                                  |
| 2200.0             | 17.783                            | 4640585.1            | 2986.5                                     | 0.3284                                  |
| 2300.0             | 17.687                            | 4641048.2            | 3011.0                                     | 0.3441                                  |
| 2400.0             | 17.561                            | 4641566.0            | 3033.8                                     | 0.3600                                  |
| 2500.0             | 17.400                            | 4642149.9            | 3055.2                                     | 0.3769                                  |
| 2600.0             | 17.198                            | 4642813.3            | 3075.3                                     | 0.3943                                  |
| 2700.0             | 16.949                            | 4643571.2            | 3094.4                                     | 0.4129                                  |
| 2800.0             | 16.649                            | 4644440.5            | 3112.5                                     | 0.4330                                  |
| 2900.0             | 16.292                            | 4645439.9            | 3130.1                                     | 0.4541                                  |
| 3000.0             | 15.876                            | 4646589.6            | 3147.2                                     | 0.4770                                  |



# Appendix K

| t                    | $\bar{M}_m$                                     | $H_{fr}$                        | $C_{p_{fr}}$                                     | $k_{fr}$                           |
|----------------------|-------------------------------------------------|---------------------------------|--------------------------------------------------|------------------------------------|
| °C                   | kg <sub>m</sub> kmol <sub>m</sub> <sup>-1</sup> | J kg <sub>m</sub> <sup>-1</sup> | J kg <sub>m</sub> <sup>-1</sup> °C <sup>-1</sup> | W m <sup>-1</sup> °C <sup>-1</sup> |
| <b>P = 10.00 MPa</b> |                                                 |                                 |                                                  |                                    |
| 1000.0               | 18.015                                          | 4636875.0                       | 2477.2                                           | 0.1504                             |
| 1100.0               | 18.015                                          | 4637125.9                       | 2539.8                                           | 0.1655                             |
| 1200.0               | 18.015                                          | 4637382.8                       | 2598.4                                           | 0.1806                             |
| 1300.0               | 18.015                                          | 4637645.4                       | 2652.8                                           | 0.1957                             |
| 1400.0               | 18.015                                          | 4637913.2                       | 2703.1                                           | 0.2107                             |
| 1500.0               | 18.015                                          | 4638185.9                       | 2749.3                                           | 0.2255                             |
| 1600.0               | 18.015                                          | 4638463.0                       | 2791.8                                           | 0.2402                             |
| 1700.0               | 18.008                                          | 4638754.4                       | 2830.8                                           | 0.2545                             |
| 1800.0               | 17.996                                          | 4639061.0                       | 2867.2                                           | 0.2687                             |
| 1900.0               | 17.984                                          | 4639369.0                       | 2900.6                                           | 0.2830                             |
| 2000.0               | 17.967                                          | 4639688.8                       | 2931.2                                           | 0.2972                             |
| 2100.0               | 17.943                                          | 4640023.0                       | 2959.6                                           | 0.3111                             |
| 2200.0               | 17.910                                          | 4640374.3                       | 2985.8                                           | 0.3253                             |
| 2300.0               | 17.867                                          | 4640746.0                       | 3010.0                                           | 0.3395                             |
| 2400.0               | 17.812                                          | 4641141.7                       | 3032.5                                           | 0.3537                             |
| 2500.0               | 17.741                                          | 4641565.8                       | 3053.4                                           | 0.3683                             |
| 2600.0               | 17.653                                          | 4642022.6                       | 3073.0                                           | 0.3830                             |
| 2700.0               | 17.545                                          | 4642517.3                       | 3091.3                                           | 0.3979                             |
| 2800.0               | 17.415                                          | 4643055.3                       | 3108.4                                           | 0.4136                             |
| 2900.0               | 17.260                                          | 4643642.3                       | 3124.7                                           | 0.4298                             |
| 3000.0               | 17.078                                          | 4644284.5                       | 3140.0                                           | 0.4465                             |

# Appendix K

| t                     | $\tilde{M}_m$                     | $H_{fr}$             | $C_{p_{fr}}$                               | $k_{fr}$                                |
|-----------------------|-----------------------------------|----------------------|--------------------------------------------|-----------------------------------------|
| $^{\circ}\text{C}$    | $\text{kg}_m \text{ kmol}_m^{-1}$ | $\text{J kg}_m^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{W m}^{-1} ^{\circ}\text{C}^{-1}$ |
| <b>P = 100.00 MPa</b> |                                   |                      |                                            |                                         |
| 1000.0                | 18.015                            | 4636875.0            | 2477.2                                     | 0.1504                                  |
| 1100.0                | 18.015                            | 4637125.9            | 2539.8                                     | 0.1655                                  |
| 1200.0                | 18.015                            | 4637382.8            | 2598.4                                     | 0.1806                                  |
| 1300.0                | 18.015                            | 4637645.4            | 2652.8                                     | 0.1957                                  |
| 1400.0                | 18.015                            | 4637913.2            | 2703.1                                     | 0.2107                                  |
| 1500.0                | 18.015                            | 4638185.9            | 2749.3                                     | 0.2255                                  |
| 1600.0                | 18.015                            | 4638463.0            | 2791.8                                     | 0.2398                                  |
| 1700.0                | 18.012                            | 4638749.3            | 2830.7                                     | 0.2544                                  |
| 1800.0                | 18.006                            | 4639043.9            | 2867.1                                     | 0.2684                                  |
| 1900.0                | 18.001                            | 4639341.3            | 2900.4                                     | 0.2826                                  |
| 2000.0                | 17.993                            | 4639645.8            | 2931.1                                     | 0.2965                                  |
| 2100.0                | 17.982                            | 4639958.5            | 2959.3                                     | 0.3103                                  |
| 2200.0                | 17.967                            | 4640280.3            | 2985.5                                     | 0.3238                                  |
| 2300.0                | 17.948                            | 4640612.6            | 3009.6                                     | 0.3375                                  |
| 2400.0                | 17.922                            | 4640956.8            | 3032.0                                     | 0.3510                                  |
| 2500.0                | 17.891                            | 4641314.4            | 3052.8                                     | 0.3644                                  |
| 2600.0                | 17.851                            | 4641687.3            | 3072.2                                     | 0.3778                                  |
| 2700.0                | 17.803                            | 4642077.3            | 3090.3                                     | 0.3915                                  |
| 2800.0                | 17.745                            | 4642486.2            | 3107.2                                     | 0.4051                                  |
| 2900.0                | 17.677                            | 4642916.1            | 3123.1                                     | 0.4191                                  |
| 3000.0                | 17.596                            | 4643369.1            | 3138.0                                     | 0.4330                                  |

## Appendix L

### Table of Effective Properties for Dissociated Steam at Pressure from 0.01 to 100.00 MPa and Temperature from 1000 to 3000°C\*

This chapter includes table of four thermodynamic properties - specific volume, entropy, enthalpy and heat capacity, and two transport properties - viscosity and thermal conductivity. This table is generated by the UODH<sub>2</sub>O (University of Ottawa Dissociated H<sub>2</sub>O) computer code listed in Appendix H.

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The zero value of the enthalpy is set at triple point of water ( $t=0.01^{\circ}\text{C}$ ,  $P=611.73\text{Pa}$ )  $h_{ii}=15.25\text{MJ kg}_{ii}^{-1}$ .

# Appendix L

| t                  | v                           | S                                          | H                    | Cp                                         | $\mu$                            | k                                       |
|--------------------|-----------------------------|--------------------------------------------|----------------------|--------------------------------------------|----------------------------------|-----------------------------------------|
| $^{\circ}\text{C}$ | $\text{m}^3 \text{kg}^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{J kg}_m^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{kg m}^{-1} \text{s}^{-1}$ | $\text{W m}^{-1} ^{\circ}\text{C}^{-1}$ |
| P = 0.01 MPa       |                             |                                            |                      |                                            |                                  |                                         |
| 1000.0             | 58.7595                     | 14562.4                                    | 4637412.0            | 2502.0                                     | 0.0000473                        | 0.1607                                  |
| 1100.0             | 63.3795                     | 14753.3                                    | 4891264.0            | 2593.5                                     | 0.0000504                        | 0.1822                                  |
| 1200.0             | 67.9995                     | 14937.1                                    | 5152384.5            | 2712.6                                     | 0.0000531                        | 0.2023                                  |
| 1300.0             | 72.6342                     | 15115.5                                    | 5424162.5            | 2879.4                                     | 0.0000556                        | 0.2218                                  |
| 1400.0             | 77.2961                     | 15291.0                                    | 5709403.5            | 3121.8                                     | 0.0000581                        | 0.2504                                  |
| 1500.0             | 82.0027                     | 15467.5                                    | 6013765.0            | 3474.6                                     | 0.0000605                        | 0.2824                                  |
| 1600.0             | 86.7885                     | 15650.3                                    | 6346441.5            | 3979.6                                     | 0.0000628                        | 0.3393                                  |
| 1700.0             | 91.7009                     | 15844.1                                    | 6719627.5            | 4685.1                                     | 0.0000651                        | 0.4053                                  |
| 1800.0             | 96.9691                     | 16068.9                                    | 7184361.0            | 5769.6                                     | 0.0000672                        | 0.5283                                  |
| 1900.0             | 102.3541                    | 16303.9                                    | 7678361.0            | 6972.1                                     | 0.0000692                        | 0.6723                                  |
| 2000.0             | 108.5182                    | 16606.6                                    | 8364013.9            | 8774.5                                     | 0.0000710                        | 0.9374                                  |
| 2100.0             | 114.9682                    | 16934.1                                    | 9120013.9            | 10797.0                                    | 0.0000727                        | 1.2469                                  |
| 2200.0             | 122.8080                    | 17386.7                                    | 10237009.0           | 13644.2                                    | 0.0000739                        | 1.7908                                  |
| 2300.0             | 131.1580                    | 17885.2                                    | 11486509.0           | 16794.2                                    | 0.0000749                        | 2.4208                                  |
| 2400.0             | 143.6776                    | 18594.7                                    | 12770755.0           | 21059.8                                    | 0.0000753                        | 3.3288                                  |
| 2500.0             | 157.7276                    | 19381.7                                    | 14067755.0           | 25734.8                                    | 0.0000754                        | 4.3388                                  |
| 2600.0             | 177.5564                    | 20484.0                                    | 17616312.0           | 31861.8                                    | 0.0000755                        | 5.6487                                  |
| 2700.0             | 199.5064                    | 21702.0                                    | 21991312.0           | 38521.8                                    | 0.0000756                        | 7.0687                                  |
| 2800.0             | 229.8687                    | 23259.4                                    | 26984795.0           | 45880.4                                    | 0.0000759                        | 8.1559                                  |
| 2900.0             | 263.3187                    | 24941.4                                    | 32205295.0           | 53495.4                                    | 0.0000762                        | 9.1209                                  |
| 3000.0             | 302.5475                    | 26706.0                                    | 37937114.0           | 56981.1                                    | 0.0000775                        | 9.0472                                  |

# Appendix L

| t            | v                               | S                                                | H                               | Cp                                               | μ                                  | k                                  |
|--------------|---------------------------------|--------------------------------------------------|---------------------------------|--------------------------------------------------|------------------------------------|------------------------------------|
| °C           | m <sup>3</sup> kg <sup>-1</sup> | J kg <sub>m</sub> <sup>-1</sup> °C <sup>-1</sup> | J kg <sub>m</sub> <sup>-1</sup> | J kg <sub>m</sub> <sup>-1</sup> °C <sup>-1</sup> | kg m <sup>-1</sup> s <sup>-1</sup> | W m <sup>-1</sup> °C <sup>-1</sup> |
| P = 0.10 MPa |                                 |                                                  |                                 |                                                  |                                    |                                    |
| 1000.0       | 5.8755                          | 13499.4                                          | 4636875.0                       | 2493.7                                           | 0.0000473                          | 0.1604                             |
| 1100.0       | 6.3370                          | 13689.5                                          | 4889801.0                       | 2570.1                                           | 0.0000504                          | 0.1814                             |
| 1200.0       | 6.7990                          | 13872.4                                          | 5149653.0                       | 2657.6                                           | 0.0000531                          | 0.1987                             |
| 1300.0       | 7.2617                          | 14047.5                                          | 5416773.5                       | 2764.7                                           | 0.0000556                          | 0.2147                             |
| 1400.0       | 7.7254                          | 14218.4                                          | 5693088.5                       | 2905.5                                           | 0.0000581                          | 0.2351                             |
| 1500.0       | 8.1909                          | 14385.4                                          | 5981598.0                       | 3093.8                                           | 0.0000605                          | 0.2571                             |
| 1600.0       | 8.6605                          | 14552.2                                          | 6285302.0                       | 3348.4                                           | 0.0000629                          | 0.2886                             |
| 1700.0       | 9.1352                          | 14713.3                                          | 6609395.0                       | 3688.3                                           | 0.0000653                          | 0.3236                             |
| 1800.0       | 9.6240                          | 14891.7                                          | 6975238.5                       | 4183.9                                           | 0.0000675                          | 0.3791                             |
| 1900.0       | 10.1175                         | 15077.2                                          | 7354238.5                       | 4727.9                                           | 0.0000697                          | 0.4421                             |
| 2000.0       | 10.6414                         | 15281.3                                          | 7811509.0                       | 5504.2                                           | 0.0000717                          | 0.5435                             |
| 2100.0       | 11.1764                         | 15492.3                                          | 8297509.0                       | 6365.7                                           | 0.0000737                          | 0.6590                             |
| 2200.0       | 11.7772                         | 15743.9                                          | 8916642.0                       | 7527.8                                           | 0.0000754                          | 0.8436                             |
| 2300.0       | 12.4022                         | 16010.4                                          | 9584642.0                       | 8800.3                                           | 0.0000771                          | 1.0536                             |
| 2400.0       | 13.1369                         | 16342.4                                          | 10468435.0                      | 10439.7                                          | 0.0000783                          | 1.3697                             |
| 2500.0       | 13.9119                         | 16698.4                                          | 11431435.0                      | 12213.7                                          | 0.0000795                          | 1.7247                             |
| 2600.0       | 14.8808                         | 17151.7                                          | 12728730.0                      | 14423.7                                          | 0.0000802                          | 2.2296                             |
| 2700.0       | 15.9208                         | 17640.7                                          | 14148730.0                      | 16793.7                                          | 0.0000808                          | 2.7896                             |
| 2800.0       | 17.2753                         | 18263.6                                          | 16057006.0                      | 19679.4                                          | 0.0000811                          | 3.5087                             |
| 2900.0       | 18.7453                         | 18935.6                                          | 18144506.0                      | 22754.4                                          | 0.0000813                          | 4.2862                             |
| 3000.0       | 20.6725                         | 19772.5                                          | 20873897.0                      | 26396.3                                          | 0.0000815                          | 5.1424                             |

# Appendix L

| t            | v                               | S                                                | H                               | Cp                                               | μ                                  | k                                  |
|--------------|---------------------------------|--------------------------------------------------|---------------------------------|--------------------------------------------------|------------------------------------|------------------------------------|
| °C           | m <sup>3</sup> kg <sup>-1</sup> | J kg <sub>m</sub> <sup>-1</sup> °C <sup>-1</sup> | J kg <sub>m</sub> <sup>-1</sup> | J kg <sub>m</sub> <sup>-1</sup> °C <sup>-1</sup> | kg m <sup>-1</sup> s <sup>-1</sup> | W m <sup>-1</sup> °C <sup>-1</sup> |
| P = 1.00 MPa |                                 |                                                  |                                 |                                                  |                                    |                                    |
| 1000.0       | 0.5872                          | 12434.4                                          | 4633875.0                       | 2495.7                                           | 0.0000473                          | 0.1600                             |
| 1100.0       | 0.6336                          | 12625.3                                          | 4887532.5                       | 2563.7                                           | 0.0000504                          | 0.1805                             |
| 1200.0       | 0.6799                          | 12807.7                                          | 5146921.5                       | 2635.4                                           | 0.0000531                          | 0.1970                             |
| 1300.0       | 0.7262                          | 12981.8                                          | 5412310.5                       | 2715.0                                           | 0.0000556                          | 0.2120                             |
| 1400.0       | 0.7725                          | 13150.2                                          | 5685162.5                       | 2808.0                                           | 0.0000581                          | 0.2288                             |
| 1500.0       | 0.8188                          | 13313.5                                          | 5966014.5                       | 2924.7                                           | 0.0000605                          | 0.2463                             |
| 1600.0       | 0.8654                          | 13472.6                                          | 6256329.5                       | 3064.1                                           | 0.0000630                          | 0.2675                             |
| 1700.0       | 0.9122                          | 13629.8                                          | 6558839.0                       | 3241.3                                           | 0.0000654                          | 0.2900                             |
| 1800.0       | 0.9596                          | 13787.2                                          | 6882760.7                       | 3485.8                                           | 0.0000676                          | 0.2989                             |
| 1900.0       | 1.0072                          | 13944.7                                          | 7213260.7                       | 3750.8                                           | 0.0000699                          | 0.3029                             |
| 2000.0       | 1.0562                          | 14107.7                                          | 7580335.7                       | 4110.9                                           | 0.0000721                          | 0.3643                             |
| 2100.0       | 1.1057                          | 14272.7                                          | 7960835.7                       | 4505.9                                           | 0.0000742                          | 0.4468                             |
| 2200.0       | 1.1578                          | 14450.9                                          | 8397295.5                       | 5018.7                                           | 0.0000763                          | 0.5301                             |
| 2300.0       | 1.2108                          | 14633.9                                          | 8854295.5                       | 5574.7                                           | 0.0000783                          | 0.6136                             |
| 2400.0       | 1.2678                          | 14837.7                                          | 9395052.2                       | 6266.4                                           | 0.0000800                          | 0.7311                             |
| 2500.0       | 1.3263                          | 15049.2                                          | 9966552.2                       | 7007.9                                           | 0.0000816                          | 0.8611                             |
| 2600.0       | 1.3917                          | 15291.1                                          | 10658018.0                      | 7897.5                                           | 0.0000830                          | 1.0383                             |
| 2700.0       | 1.4597                          | 15544.1                                          | 11393518.0                      | 8841.5                                           | 0.0000843                          | 1.2328                             |
| 2800.0       | 1.5380                          | 15838.8                                          | 12295069.0                      | 9941.7                                           | 0.0000853                          | 1.4898                             |
| 2900.0       | 1.6200                          | 16148.8                                          | 13257569.0                      | 11099.2                                          | 0.0000863                          | 1.7698                             |
| 3000.0       | 1.7173                          | 16512.2                                          | 14440250.0                      | 12404.8                                          | 0.0000870                          | 2.1211                             |

# Appendix L

| t                    | v                           | S                                          | H                    | Cp                                         | $\mu$                            | k                                       |
|----------------------|-----------------------------|--------------------------------------------|----------------------|--------------------------------------------|----------------------------------|-----------------------------------------|
| $^{\circ}\text{C}$   | $\text{m}^3 \text{kg}^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{J kg}_m^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{kg m}^{-1} \text{s}^{-1}$ | $\text{W m}^{-1} ^{\circ}\text{C}^{-1}$ |
| <b>P = 10.00 MPa</b> |                             |                                            |                      |                                            |                                  |                                         |
| 1000.0               | 0.0584                      | 11354.8                                    | 4608727.0            | 2551.4                                     | 0.0000473                        | 0.1600                                  |
| 1100.0               | 0.0632                      | 11549.4                                    | 4868190.0            | 2605.8                                     | 0.0000504                        | 0.1805                                  |
| 1200.0               | 0.0679                      | 11734.9                                    | 5131116.0            | 2660.2                                     | 0.0000531                        | 0.1962                                  |
| 1300.0               | 0.0726                      | 11911.3                                    | 5399505.0            | 2718.2                                     | 0.0000556                        | 0.2102                                  |
| 1400.0               | 0.0773                      | 12079.4                                    | 5673162.5            | 2782.3                                     | 0.0000581                        | 0.2253                                  |
| 1500.0               | 0.0820                      | 12241.8                                    | 5952551.5            | 2856.3                                     | 0.0000605                        | 0.2408                                  |
| 1600.0               | 0.0867                      | 12398.4                                    | 6237940.5            | 2943.6                                     | 0.0000630                        | 0.2578                                  |
| 1700.0               | 0.0914                      | 12551.2                                    | 6531524.0            | 3046.3                                     | 0.0000654                        | 0.2753                                  |
| 1800.0               | 0.0961                      | 12699.9                                    | 6837399.2            | 3177.8                                     | 0.0000677                        | 0.2961                                  |
| 1900.0               | 0.1008                      | 12847.4                                    | 7146899.2            | 3318.3                                     | 0.0000700                        | 0.3181                                  |
| 2000.0               | 0.1056                      | 12993.8                                    | 7475784.0            | 3498.3                                     | 0.0000722                        | 0.3456                                  |
| 2100.0               | 0.1104                      | 13139.8                                    | 7811784.0            | 3692.8                                     | 0.0000744                        | 0.3751                                  |
| 2200.0               | 0.1153                      | 13287.6                                    | 8173752.2            | 3935.9                                     | 0.0000765                        | 0.4130                                  |
| 2300.0               | 0.1202                      | 13436.1                                    | 8545252.2            | 4196.9                                     | 0.0000786                        | 0.4540                                  |
| 2400.0               | 0.1253                      | 13590.5                                    | 8954058.7            | 4511.0                                     | 0.0000806                        | 0.5067                                  |
| 2500.0               | 0.1305                      | 13747.0                                    | 9376558.7            | 4844.5                                     | 0.0000826                        | 0.5637                                  |
| 2600.0               | 0.1360                      | 13913.4                                    | 9848435.0            | 5234.6                                     | 0.0000843                        | 0.6419                                  |
| 2700.0               | 0.1415                      | 14083.4                                    | 10338435.0           | 5645.6                                     | 0.0000860                        | 0.7279                                  |
| 2800.0               | 0.1474                      | 14264.3                                    | 10892441.0           | 6112.2                                     | 0.0000876                        | 0.8231                                  |
| 2900.0               | 0.1535                      | 14449.3                                    | 11469941.0           | 6599.2                                     | 0.0000892                        | 0.9216                                  |
| 3000.0               | 0.1601                      | 14651.9                                    | 12129004.0           | 7139.6                                     | 0.0000905                        | 1.0493                                  |

# Appendix L

| t                     | v                           | S                                          | H                    | Cp                                         | $\mu$                            | k                                       |
|-----------------------|-----------------------------|--------------------------------------------|----------------------|--------------------------------------------|----------------------------------|-----------------------------------------|
| $^{\circ}\text{C}$    | $\text{m}^3 \text{kg}^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{J kg}_m^{-1}$ | $\text{J kg}_m^{-1} ^{\circ}\text{C}^{-1}$ | $\text{kg m}^{-1} \text{s}^{-1}$ | $\text{W m}^{-1} ^{\circ}\text{C}^{-1}$ |
| <b>P = 100.00 MPa</b> |                             |                                            |                      |                                            |                                  |                                         |
| 1000.0                | 0.0057                      | 10115.6                                    | 4369784.0            | 3126.7                                     | 0.0000473                        | 0.1541                                  |
| 1100.0                | 0.0063                      | 10361.1                                    | 4693348.5            | 3069.5                                     | 0.0000504                        | 0.1666                                  |
| 1200.0                | 0.0069                      | 10579.3                                    | 5001376.0            | 3011.0                                     | 0.0000531                        | 0.1766                                  |
| 1300.0                | 0.0074                      | 10776.4                                    | 5300255.5            | 2974.1                                     | 0.0000556                        | 0.1856                                  |
| 1400.0                | 0.0079                      | 10958.9                                    | 5595061.0            | 2963.1                                     | 0.0000581                        | 0.1957                                  |
| 1500.0                | 0.0084                      | 11130.6                                    | 5888329.5            | 2974.4                                     | 0.0000605                        | 0.2062                                  |
| 1600.0                | 0.0089                      | 11292.3                                    | 6198154.0            | 3005.3                                     | 0.0000630                        | 0.2244                                  |
| 1700.0                | 0.0094                      | 11447.7                                    | 6487088.5            | 3052.3                                     | 0.0000655                        | 0.2454                                  |
| 1800.0                | 0.0099                      | 11577.5                                    | 6785839.0            | 3118.7                                     | 0.0000679                        | 0.2664                                  |
| 1900.0                | 0.0104                      | 11698.5                                    | 7091839.0            | 3190.7                                     | 0.0000702                        | 0.2874                                  |
| 2000.0                | 0.0109                      | 11851.0                                    | 7408080.0            | 3282.4                                     | 0.0000724                        | 0.3084                                  |
| 2100.0                | 0.0114                      | 12015.0                                    | 7728080.0            | 3381.4                                     | 0.0000746                        | 0.3294                                  |
| 2200.0                | 0.0119                      | 12158.1                                    | 8060881.2            | 3503.1                                     | 0.0000767                        | 0.3657                                  |
| 2300.0                | 0.0124                      | 12293.6                                    | 8398381.2            | 3633.1                                     | 0.0000788                        | 0.4077                                  |
| 2400.0                | 0.0129                      | 12428.0                                    | 8753437.2            | 3781.0                                     | 0.0000809                        | 0.4417                                  |
| 2500.0                | 0.0134                      | 12562.0                                    | 9114937.2            | 3935.5                                     | 0.0000829                        | 0.4727                                  |
| 2600.0                | 0.0139                      | 12696.8                                    | 9498748.0            | 4113.8                                     | 0.0000847                        | 0.5194                                  |
| 2700.0                | 0.0144                      | 12831.8                                    | 9890748.0            | 4300.8                                     | 0.0000865                        | 0.5719                                  |
| 2800.0                | 0.0159                      | 12969.7                                    | 10310179.0           | 4509.7                                     | 0.0000885                        | 0.6167                                  |
| 2900.0                | 0.0155                      | 13108.7                                    | 10739679.0           | 4726.7                                     | 0.0000905                        | 0.6587                                  |
| 3000.0                | 0.0161                      | 13251.0                                    | 11202828.0           | 4963.5                                     | 0.0000920                        | 0.7234                                  |

Note: The values for  $\mu$  and k at pressure of 100MPa were extrapolated by the author.



## Appendix M

### **Look-up Table of Convective Heat Transfer Coefficients for High Temperature Dissociated Steam in Tube Flow at Pressure from 0.01 to 100.00MPa and Temperature from 1000 to 3000°C\***

This chapter includes a look-up table for heat transfer coefficients generated by the High Temperature Steam Heat Transfer code (VASICA). The values of the heat flux, 0.1 and 0.5MW m<sup>-2</sup>, tube diameter 0.01 and 0.05m, and mass velocity from 100 to 7500 kg m<sup>-2</sup> s<sup>-1</sup>, are in the range of values applicable in industry.

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\*

In this work the heat transferred by radiation is not considered.

# Appendix M

|                                    |      | Constant Heat Flux at the Wall      |        |        |       |        |        |       |       |
|------------------------------------|------|-------------------------------------|--------|--------|-------|--------|--------|-------|-------|
|                                    |      | MW m <sup>2</sup>                   |        |        |       |        |        |       |       |
|                                    |      | 0.1                                 |        |        |       |        |        |       |       |
|                                    |      | Tube Diameter                       |        |        |       |        |        |       |       |
|                                    |      | m                                   |        |        |       |        |        |       |       |
|                                    |      | 0.01                                |        |        |       | 0.05   |        |       |       |
|                                    |      | Absolute Pressure                   |        |        |       |        |        |       |       |
|                                    |      | MPa                                 |        |        |       |        |        |       |       |
|                                    |      | 0.1                                 | 1.0    | 10.0   | 100.0 | 0.1    | 1.0    | 10.0  | 100.0 |
| G                                  | t    | Heat Transfer Coefficients          |        |        |       |        |        |       |       |
| Mg m <sup>-2</sup> s <sup>-1</sup> | °C   | kW m <sup>-2</sup> °C <sup>-1</sup> |        |        |       |        |        |       |       |
| 0.10                               | 1000 | 0.666                               | 0.666  | 0.667  | 0.689 | 0.464  | 0.464  | 0.464 | 0.481 |
|                                    | 1500 | 0.790                               | 0.790  | 0.790  | 0.790 | 0.632  | 0.596  | 0.584 | 0.576 |
|                                    | 2000 | 1.713                               | 1.259  | 1.055  | 0.961 | 1.245  | 0.910  | 0.758 | 0.687 |
|                                    | 2500 | 4.453                               | 2.418  | 1.596  | 1.241 | 3.220  | 1.754  | 1.157 | 0.896 |
|                                    | 3000 | 9.897                               | 4.838  | 2.628  | 1.715 | 7.124  | 3.502  | 1.909 | 1.246 |
| 0.25                               | 1000 | 1.408                               | 1.409  | 1.411  | 1.460 | 0.998  | 0.998  | 1.000 | 1.032 |
|                                    | 1500 | 1.661                               | 1.661  | 1.661  | 1.661 | 1.177  | 1.177  | 1.177 | 1.177 |
|                                    | 2000 | 3.493                               | 2.585  | 2.185  | 2.004 | 2.502  | 1.847  | 1.556 | 1.423 |
|                                    | 2500 | 9.210                               | 4.993  | 3.303  | 2.581 | 6.564  | 3.561  | 2.354 | 1.836 |
|                                    | 3000 | 20.650                              | 10.090 | 5.476  | 3.582 | 14.670 | 7.172  | 3.897 | 2.547 |
| 0.50                               | 1000 | 2.454                               | 2.454  | 2.458  | 2.541 | 1.780  | 1.780  | 1.782 | 1.834 |
|                                    | 1500 | 2.881                               | 2.881  | 2.881  | 2.881 | 2.078  | 2.078  | 2.078 | 2.078 |
|                                    | 2000 | 5.974                               | 4.434  | 3.761  | 3.459 | 4.322  | 3.203  | 2.711 | 2.490 |
|                                    | 2500 | 15.820                              | 8.569  | 5.674  | 4.443 | 11.390 | 6.169  | 4.082 | 3.193 |
|                                    | 3000 | 35.580                              | 17.360 | 9.420  | 6.165 | 25.560 | 12.460 | 6.759 | 4.420 |
| 0.75                               | 1000 | 3.397                               | 3.397  | 3.403  | 3.513 | 2.501  | 2.501  | 2.504 | 2.572 |
|                                    | 1500 | 3.976                               | 3.976  | 3.976  | 3.976 | 2.908  | 2.908  | 2.908 | 2.908 |
|                                    | 2000 | 8.198                               | 6.091  | 5.174  | 4.762 | 5.992  | 4.447  | 3.772 | 3.468 |
|                                    | 2500 | 21.740                              | 11.770 | 7.794  | 6.108 | 15.820 | 8.558  | 5.665 | 4.435 |
|                                    | 3000 | 48.940                              | 23.860 | 12.940 | 8.471 | 35.540 | 17.300 | 9.378 | 6.133 |

# Appendix M

|                                    |      | Constant Heat Flux at the Wall      |         |        |        |         |         |        |        |
|------------------------------------|------|-------------------------------------|---------|--------|--------|---------|---------|--------|--------|
|                                    |      | MW m <sup>-2</sup>                  |         |        |        |         |         |        |        |
|                                    |      | 0.1                                 |         |        |        |         |         |        |        |
|                                    |      | Tube Diameter                       |         |        |        |         |         |        |        |
|                                    |      | m                                   |         |        |        |         |         |        |        |
|                                    |      | 0.01                                |         |        |        | 0.05    |         |        |        |
|                                    |      | Absolute Pressure                   |         |        |        |         |         |        |        |
|                                    |      | MPa                                 |         |        |        |         |         |        |        |
|                                    |      | 0.1                                 | 1.0     | 10.0   | 100.0  | 0.1     | 1.0     | 10.0   | 100.0  |
| G                                  | t    | Heat Transfer Coefficients          |         |        |        |         |         |        |        |
| Mg m <sup>-2</sup> s <sup>-1</sup> | °C   | kW m <sup>-2</sup> °C <sup>-1</sup> |         |        |        |         |         |        |        |
| 1.0                                | 1000 | 4.283                               | 4.283   | 4.290  | 4.425  | 3.188   | 3.188   | 3.193  | 3.275  |
|                                    | 1500 | 5.003                               | 5.003   | 5.003  | 5.003  | 3.696   | 3.696   | 3.696  | 3.696  |
|                                    | 2000 | 10.280                              | 7.642   | 6.495  | 5.981  | 7.579   | 5.629   | 4.779  | 4.398  |
|                                    | 2500 | 27.270                              | 14.750  | 9.775  | 7.663  | 20.010  | 10.820  | 7.166  | 5.614  |
|                                    | 3000 | 61.420                              | 29.930  | 16.230 | 10.620 | 45.000  | 21.890  | 11.860 | 7.756  |
| 2.5                                | 1000 | 9.037                               | 9.038   | 9.051  | 9.308  | 6.981   | 6.982   | 6.989  | 7.144  |
|                                    | 1500 | 10.490                              | 10.490  | 10.490 | 10.490 | 8.032   | 8.032   | 8.032  | 8.032  |
|                                    | 2000 | 21.370                              | 15.900  | 13.540 | 12.480 | 16.270  | 12.110  | 10.300 | 9.490  |
|                                    | 2500 | 56.680                              | 30.640  | 20.300 | 15.930 | 42.980  | 23.220  | 15.370 | 12.060 |
|                                    | 3000 | 127.800                             | 62.160  | 33.670 | 22.040 | 96.760  | 46.960  | 25.400 | 16.610 |
| 5.0                                | 1000 | 16.080                              | 16.080  | 16.100 | 16.520 | 12.780  | 12.780  | 12.790 | 13.040 |
|                                    | 1500 | 18.580                              | 18.580  | 18.580 | 18.580 | 14.630  | 14.630  | 14.630 | 14.630 |
|                                    | 2000 | 37.650                              | 28.040  | 23.880 | 22.020 | 29.460  | 21.930  | 18.670 | 17.210 |
|                                    | 2500 | 99.800                              | 53.920  | 35.720 | 28.040 | 77.750  | 41.970  | 27.790 | 21.810 |
|                                    | 3000 | 225.000                             | 109.300 | 59.170 | 38.710 | 175.100 | 84.850  | 45.860 | 29.980 |
| 7.5                                | 1000 | 22.640                              | 22.650  | 22.670 | 23.220 | 18.290  | 18.290  | 18.310 | 18.630 |
|                                    | 1500 | 26.100                              | 26.100  | 26.100 | 26.100 | 20.880  | 20.880  | 20.880 | 20.880 |
|                                    | 2000 | 52.740                              | 39.280  | 33.460 | 30.860 | 41.940  | 31.230  | 26.590 | 24.520 |
|                                    | 2500 | 139.700                             | 75.440  | 49.980 | 39.230 | 110.600 | 59.680  | 39.520 | 31.010 |
|                                    | 3000 | 314.900                             | 152.900 | 82.720 | 54.110 | 249.100 | 120.600 | 65.160 | 42.590 |

# Appendix M

|                                    |      | Constant Heat Flux at the Wall      |        |        |       |        |        |       |       |
|------------------------------------|------|-------------------------------------|--------|--------|-------|--------|--------|-------|-------|
|                                    |      | MW m <sup>-2</sup>                  |        |        |       |        |        |       |       |
|                                    |      | 0.5                                 |        |        |       |        |        |       |       |
|                                    |      | Tube Diameter                       |        |        |       |        |        |       |       |
|                                    |      | m                                   |        |        |       |        |        |       |       |
|                                    |      | 0.01                                |        |        |       | 0.05   |        |       |       |
|                                    |      | MPa                                 |        |        |       |        |        |       |       |
|                                    |      | 0.1                                 | 1.0    | 10.0   | 100.0 | 0.1    | 1.0    | 10.0  | 100.0 |
| G                                  | t    | Heat Transfer Coefficients          |        |        |       |        |        |       |       |
| Mg m <sup>-2</sup> s <sup>-1</sup> | °C   | kW m <sup>-2</sup> °C <sup>-1</sup> |        |        |       |        |        |       |       |
| 0.10                               | 1000 | 0.625                               | 0.591  | 0.571  | 0.581 | 0.479  | 0.433  | 0.401 | 0.395 |
|                                    | 1500 | 1.024                               | 0.875  | 0.791  | 0.745 | 0.789  | 0.658  | 0.576 | 0.527 |
|                                    | 2000 | 1.974                               | 1.406  | 1.115  | 0.962 | 1.507  | 1.066  | 0.830 | 0.700 |
|                                    | 2500 | 4.716                               | 2.616  | 1.713  | 1.289 | 3.477  | 1.950  | 1.276 | 0.949 |
|                                    | 3000 | 9.924                               | 4.978  | 2.747  | 1.784 | 7.145  | 3.638  | 2.026 | 1.315 |
| 0.25                               | 1000 | 1.279                               | 1.280  | 1.282  | 1.330 | 0.874  | 0.874  | 0.875 | 0.907 |
|                                    | 1500 | 1.989                               | 1.768  | 1.661  | 1.610 | 1.437  | 1.261  | 1.170 | 1.125 |
|                                    | 2000 | 3.748                               | 2.714  | 2.225  | 1.988 | 2.760  | 1.983  | 1.603 | 1.414 |
|                                    | 2500 | 9.482                               | 5.194  | 3.416  | 2.622 | 6.833  | 3.761  | 2.469 | 1.880 |
|                                    | 3000 | 20.680                              | 10.230 | 5.598  | 3.649 | 14.700 | 7.316  | 4.018 | 2.615 |
| 0.50                               | 1000 | 2.320                               | 2.320  | 2.324  | 2.406 | 1.648  | 1.648  | 1.651 | 1.702 |
|                                    | 1500 | 3.164                               | 2.984  | 2.923  | 2.884 | 2.475  | 2.217  | 2.091 | 2.030 |
|                                    | 2000 | 6.224                               | 4.554  | 3.791  | 3.436 | 4.575  | 3.327  | 2.747 | 2.471 |
|                                    | 2500 | 16.100                              | 8.771  | 5.785  | 4.480 | 11.670 | 6.371  | 4.194 | 3.231 |
|                                    | 3000 | 35.620                              | 17.510 | 9.543  | 6.232 | 25.600 | 12.610 | 6.882 | 4.488 |
| 0.75                               | 1000 | 3.261                               | 3.261  | 3.267  | 3.377 | 2.366  | 2.367  | 2.370 | 2.438 |
|                                    | 1500 | 3.877                               | 3.877  | 3.877  | 3.877 | 3.217  | 3.031  | 2.965 | 2.919 |
|                                    | 2000 | 8.446                               | 6.208  | 5.200  | 4.737 | 6.243  | 4.567  | 3.802 | 3.446 |
|                                    | 2500 | 22.020                              | 11.970 | 7.904  | 6.143 | 16.090 | 8.760  | 5.775 | 4.472 |
|                                    | 3000 | 48.980                              | 24.010 | 13.070 | 8.537 | 35.580 | 17.450 | 9.501 | 6.200 |

# Appendix M

|                                    |      | Constant Heat Flux at the Wall      |         |        |        |         |         |        |        |
|------------------------------------|------|-------------------------------------|---------|--------|--------|---------|---------|--------|--------|
|                                    |      | MW m <sup>-2</sup>                  |         |        |        |         |         |        |        |
|                                    |      | 0.5                                 |         |        |        |         |         |        |        |
|                                    |      | Tube Diameter                       |         |        |        |         |         |        |        |
|                                    |      | m                                   |         |        |        |         |         |        |        |
|                                    |      | 0.01                                |         |        |        | 0.05    |         |        |        |
|                                    |      | MPa                                 |         |        |        |         |         |        |        |
|                                    |      | 0.1                                 | 1.0     | 10.0   | 100.0  | 0.1     | 1.0     | 10.0   | 100.0  |
| G                                  | t    | Heat Transfer Coefficients          |         |        |        |         |         |        |        |
| Mg m <sup>-2</sup> s <sup>-1</sup> | °C   | kW m <sup>-2</sup> °C <sup>-1</sup> |         |        |        |         |         |        |        |
| 1.0                                | 1000 | 4.145                               | 4.146   | 4.153  | 4.288  | 3.052   | 3.053   | 3.057  | 3.139  |
|                                    | 1500 | 4.904                               | 4.904   | 4.904  | 4.904  | 3.597   | 3.597   | 3.597  | 3.597  |
|                                    | 2000 | 10.530                              | 7.756   | 6.520  | 5.955  | 7.828   | 5.746   | 4.807  | 4.373  |
|                                    | 2500 | 27.550                              | 14.960  | 9.884  | 7.698  | 20.290  | 11.030  | 7.276  | 5.649  |
|                                    | 3000 | 61.460                              | 30.080  | 16.350 | 10.690 | 45.040  | 22.040  | 11.980 | 7.822  |
| 2.5                                | 1000 | 8.898                               | 8.899   | 8.912  | 9.168  | 6.842   | 6.843   | 6.851  | 7.005  |
|                                    | 1500 | 10.390                              | 10.390  | 10.390 | 10.390 | 7.931   | 7.931   | 7.931  | 7.931  |
|                                    | 2000 | 21.610                              | 16.010  | 13.560 | 12.450 | 16.520  | 12.220  | 10.320 | 9.462  |
|                                    | 2500 | 56.960                              | 30.840  | 20.410 | 15.960 | 43.260  | 23.420  | 15.480 | 12.090 |
|                                    | 3000 | 127.800                             | 62.310  | 33.800 | 22.100 | 96.800  | 47.110  | 25.530 | 16.680 |
| 5.0                                | 1000 | 15.940                              | 15.940  | 15.960 | 16.380 | 12.640  | 12.640  | 12.650 | 12.900 |
|                                    | 1500 | 18.480                              | 18.480  | 18.480 | 18.480 | 14.530  | 14.530  | 14.530 | 14.530 |
|                                    | 2000 | 37.890                              | 28.150  | 23.900 | 21.990 | 29.710  | 22.040  | 18.690 | 17.180 |
|                                    | 2500 | 100.100                             | 54.120  | 35.830 | 28.070 | 78.030  | 42.170  | 27.900 | 21.840 |
|                                    | 3000 | 225.000                             | 109.500 | 59.300 | 38.780 | 175.100 | 85.000  | 45.990 | 30.040 |
| 7.5                                | 1000 | 22.500                              | 22.500  | 22.530 | 23.080 | 18.150  | 18.150  | 18.170 | 18.490 |
|                                    | 1500 | 26.000                              | 26.000  | 26.000 | 26.000 | 20.780  | 20.780  | 20.780 | 20.780 |
|                                    | 2000 | 52.980                              | 39.390  | 33.480 | 30.830 | 42.190  | 31.340  | 26.610 | 24.490 |
|                                    | 2500 | 140.000                             | 75.650  | 50.090 | 39.260 | 110.900 | 59.880  | 39.630 | 31.040 |
|                                    | 3000 | 314.900                             | 153.000 | 82.840 | 54.180 | 249.100 | 120.800 | 65.290 | 42.650 |

## Appendix N

# Conversion of Units and Fundamental Constants

### Conversion of Units

Conversion of reported values from the references to SI units

|                      |                                                                                                                           |
|----------------------|---------------------------------------------------------------------------------------------------------------------------|
| pressure             | $1 \text{ atm} = 101.325 \text{ kN m}^{-2}$                                                                               |
| specific volume      | $1 \text{ cm}^3 \text{ g}^{-1} = 10^{-3} \text{ m}^3 \text{ kg}^{-1}$                                                     |
| heat capacity        | $1 \text{ cal mol}^{-1} \text{ K}^{-1} = 4.1868 (\text{molar mass})^{-1} \text{ kJ kg}^{-1} \text{ K}^{-1}$               |
|                      | $1 \text{ cal g}^{-1} \text{ K}^{-1} = 4.1869 \text{ kJ kg}^{-1} \text{ K}^{-1}$                                          |
| enthalpy             | $1 \text{ kcal mol}^{-1} = 4.1868 (\text{molar mass})^{-1} \text{ kJ kg}^{-1}$                                            |
|                      | $1 \text{ cal g}^{-1} = 4.1868 \text{ kJ kg}^{-1}$                                                                        |
| entropy              | $1 \text{ cal mol}^{-1} \text{ K}^{-1} = 4.1868 \cdot 10^{-3} (\text{molar mass})^{-1} \text{ kJ kg}^{-1} \text{ K}^{-1}$ |
|                      | $1 \text{ cal g}^{-1} \text{ K}^{-1} = 4.1868 \text{ kJ kg}^{-1} \text{ K}^{-1}$                                          |
| thermal conductivity | $1 \text{ cal cm}^{-1} \text{ s}^{-1} \text{ K}^{-1} = 4.1868 \cdot 10^{-2} \text{ W m}^{-1} \text{ K}^{-1}$              |
| viscosity            | $1 \text{ poise} = 10^{-1} \text{ N s m}^{-2}$                                                                            |

## Appendix N

dipole moment                      1 Debye =  $10^{-18}$  esu (electrostatic units)

molecular distance              1 Å =  $10^{-10}$  m = 0.1 nm

### Fundamental Constants

| <u>Quantity</u>                                                      | <u>Symbol</u>     | <u>Value</u>               | <u>Units</u>                           |
|----------------------------------------------------------------------|-------------------|----------------------------|----------------------------------------|
| Avogadro Constant                                                    | $N_A$             | $6.022045 \times 10^{23}$  | $\text{mol}^{-1}$                      |
| Molar Gas Constant                                                   | $\tilde{R}$       | 8.31441                    | $\text{J mol}^{-1} \text{K}^{-1}$      |
| Molar Volume, Ideal Gas<br>$T_o = 273.15\text{K}, p_o = 1\text{atm}$ | $V_m = R T_o/p_o$ | $22.41383 \times 10^{-3}$  | $\text{m}^3 \text{mol}^{-1}$           |
| Boltzmann Constant                                                   | $k_B = R/N_A$     | $1.380662 \times 10^{-23}$ | $\text{J K}^{-1} \text{molecule}^{-1}$ |
| Planck's Constant                                                    | $h$               | $6.626176 \times 10^{-34}$ | $\text{J s}$                           |
| pi number                                                            | $\pi$             | 3.141592653                | dimensionless                          |
| Stefan-Boltzmann Constant                                            | $\sigma$          | $5.67032 \times 10^{-8}$   | $\text{W m}^{-2} \text{K}^{-4}$        |

### Defined Constants

|                     |     |                       |                   |
|---------------------|-----|-----------------------|-------------------|
| Standard gravity    | $g$ | 9.80665               | $\text{m s}^{-1}$ |
| Standard atmosphere | atm | $1.01325 \times 10^5$ | $\text{N m}^{-2}$ |
| Velocity of light   | $c$ | $2.998 \times 10^8$   | $\text{m s}^{-1}$ |

Note: Values of the fundamental constants are from  
"Handbook of Chemistry and Physics", 56th edition, CRC Press, Inc.

# Appendix O

## Glossary

**CHF** Critical Heat Flux.

**dissociation** Reversible decomposition of the molecules of a compound under particular conditions.

**effective properties** Properties of the multi-component gas mixture which include effects of chemical reactions among components.

**equilibrium (chemical)** The state of a system in which there is balance between concentration of reactants and products of the chemical reaction under specific conditions.

**equilibrium (mechanical)** The state of a system in which there is no pressure difference among its components.

**equilibrium (phase)** The state of a system in which there is balance between concentration of components in two separate phases (solid-liquid, solid-vapour or liquid-vapour).

**equilibrium (thermal)** The state of a system in which there is no temperature difference among its components.

**frozen properties** Properties of the multi-component gas mixture which is frozen state.

**frozen state** State of the multi-component gas mixture with infinite time required that chemical reaction among components to occur (state of chemically non-reacting gases).

**high temperature** Temperatures higher than 1000K.



## Appendix O

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**HTC** Heat Transfer Coefficient.

**ideal gas mixture** Ideal mixture of ideal gases is ideal gas mixture.

**ideal mixture** Mixture which does not show enthalpy change due to mixing is ideal mixture. The total thermodynamic property of an ideal mixture is the sum of the total properties of the individual species.

**ideal solution** Solution which show no enthalpy change due to mixing and no attractive forces between components is ideal solution.

**JANAF tables** Joint-Army-Navy-Air-Force thermochemical tables.

**LOCA** Loss-Of-Coolant-Accident.

**mixture** The product of mixing where components are not in a fixed proportion to each other.

**moderate temperature** Temperatures up to 1000K.

**non-equilibrium** Transition state (time dependant state) between two equilibrium states.

**solution** A single, homogeneous liquid, solid, or gas phase that is a mixture in which the components are uniformly distributed throughout the mixture.

## **Appendix P**

**Manuscript of the paper, "A comparison of predictions of high-temperature steam properties" by Vasić et al. (1992).**

### A comparison of predictions of high-temperature steam properties

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Recent literature pertaining to high temperature steam properties has been assessed. After careful assessment of available sets of property tables and equations for high temperature (including dissociated) steam, a set of high temperature steam properties was selected, based heavily on Vargaftik steam tables. A computer code, UODH<sub>2</sub>O (University of Ottawa Dissociated H<sub>2</sub>O code) is constructed to compute high-temperature steam properties using a lookup table and interpretation technique. The code, which required input values of pressure (0.01-100.MPa) and temperature (1000-5726.85°C), can predict four thermodynamic properties - specific volume, entropy, enthalpy and heat capacity, and two transport properties - viscosity and thermal conductivity.

#### 1. Introduction

The properties of steam have been extensively investigated and well documented at low and moderate temperatures up to 1000°C. However, studies in combustion, space rocket propulsion, nuclear reactors, solar furnace and arc plasma require knowledge of steam properties at much higher temperatures. Extrapolation of steam-property equations to temperatures well beyond the range of their intended applications or the use of ideal gas laws to predict steam properties at high temperature is often a common practice. This approach produces large inaccuracies, and becomes completely unacceptable in the temperature range when dissociation occurs. The effect of such steam property extrapolation on the heat transfer coefficient is shown in fig. 1. Both temperature scales in °C and K are given in all figures. When comparing the predictions based on the extrapolation of ASME property equations by Meyer [2], or NBS/NRC equations by Haar [4] with those based on dissociated steam tables from Vargaftik [5] (with the prediction method developed by Kesselman [6]), differences of up to an order of magnitude can be encountered.

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## Appendix P

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To predict the thermodynamic properties of steam at high temperature, steam may be postulated as either a non-dissociated or dissociated gas. For a non-dissociated gas, it may be treated as an ideal or real gas, while for a dissociated gas, it may be treated as an ideal mixture of ideal gases (ideal gas mixture) or ideal mixture of real gases (ideal solution), or a non-ideal (real) mixture of real gases (non-ideal solution). Depending on the postulate, several analyses of studies can be found.

The thermodynamic properties of non-dissociated steam as an ideal gas were tabulated in the JANAF tables by Chase [7]-page 1274, and for a real gas by Chase [7]-pp. 1275-1279 and Haar [4]. The thermodynamic properties of dissociated steam as a ideal gas mixture were reported by Straub [8], Ihara [9], Svehla [10]-(frozen<sup>\*\*</sup> and equilibrium<sup>\*\*\*</sup> state), Rybakov [11] and Burnhorn [12], and for an ideal solution by Artym [13] and Kmonicek [14]. Finally, Vargaftik [5], Geftter [15] and Kesselman [6] presented a non-ideal solution. Transport properties predictions were published by Haar [4], Matsunaga [16], Kesselman [17] and [18], Svehla [19], for non-dissociated steam, and Baronnet [20], Vargaftik [5], Kesselman [6] and Svehla [10]-(frozen and equilibrium state) for dissociated steam.

Most of aforementioned analyses are based on the following assumptions and theory:

- i. Ideal gas or real gas assumption for prediction properties for individual pure components;
- ii. Non-dissociated or dissociated gas assumption; the latter including the effect of chemical reactions in equilibrium state;
- iii. Ideal mixing or real mixing assumption in the mixing process; the latter includes the interactions of all components; and
- iv. Statistical thermodynamics.

### 2. Comparison

All available data sets and equations for high temperature steam properties have been

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<sup>\*\*</sup> The state of a multi-component gas mixture requires infinite time for chemical reactions between components to occur (mixture of chemically non-reacting gases).

<sup>\*\*\*</sup> The state of a system in which balance between concentration of reactants and products of the chemical reactions (under specific conditions) is reached.

## Appendix P

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extracted from the literature, converted to the same units (SI), changed to the same reference state\* and analyzed. Figs. 2 to 9 present predictions of steam properties from various sources for temperatures ranging from 300 to 3000 °C at a pressure of 0.1MPa. In fig. 2, Haar [4] shows the specific volume of non-dissociating steam being almost a linear function of temperature, whereas, for dissociated steam it is an exponential function of temperature at high temperatures. Predicted values published for the latter case include Kmonicek [14], Gefter [15] and Vargaftik [5]; they are all in good agreement.

Fig. 3. presents entropy of steam as a function of temperature. Extrapolation from ASME property equations by Meyer [2] shows an incorrect downward trend at high temperatures. When steam was considered as a non-dissociated real gas (Chase [7] and Haar [4]), a similar rate of increase of entropy with temperature at all temperatures was found. For dissociated steam, Svehla [10], Kmonicek [14], Gefter [15], Ihara [9] and Vargaftik [5] show the entropy increasing exponentially at higher temperatures. Rybakov [11] predicts a more linear rise of entropy with temperature at higher temperatures; it is suspected that the selection of constants in his prediction method may involve some uncertainties.

All the observations made on the entropy are equally applicable to enthalpy as illustrated in fig. 4. With the exception that, for dissociated steam Rybakov's [11] results now follow the exponential relation with temperature at high temperatures as the other sources (Svehla, Kmonicek, Gefter, Ihara, Vargaftik) including Straub's [8] data.

Fig. 5. presents the heat capacity (at constant pressure) as a function of temperature. Again, it is possible to recognize three types of predictions. In the first type, the prediction of heat capacity using extrapolation of ASME [2] property equations results in heat capacity approaching zero at 2600 °C (impossible since thermal dissociation is an endothermic reaction; thus, the heat capacity can not be zero). For the second type, by considering steam as a non-dissociated gas (Chase [7], Haar [4] and Svehla [10]), the heat capacity was found to increase almost linearly with temperature. Finally, for dissociating steam, Svehla [10], Gefter [15], Ihara [9], Vargaftik [5] and Straub [8] found the heat capacity increasing exponentially with temperature at high temperatures due to the endothermic reaction.

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\* The zero value of entropy and enthalpy of water at triple point ( $t = 0.01$  °C,  $P = 611.73$  Pa).

## Appendix P

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Heat capacity is defined as the partial derivative of enthalpy with respect to temperature at constant pressure. Due to various methods of calculating partial derivatives, different results can be obtained, even though all sources have similar values of enthalpy (see fig. 4.). Data presented by Vargaftik [5] are calculated by summing the derivatives of gas mixture components' enthalpy, while those by Straub [8] are calculated by taking the derivative of enthalpy of the mixture as a whole. This may account for a significant difference in predicting heat capacity from the two sources.

Properties predicted by Artym [13] are in very high temperature range from 5000 K to 20000 K and pressure from 1 to 1000 bar. It is of interest to compare his results with other predictions. Table 1. shows very good agreement with other sources.

Viscosity for steam as a function of temperature is depicted in fig. 6. Extrapolation from ASME [2] property equations show a linear relation of temperature; it predicts the highest value of viscosity at high temperatures among all sources (non-dissociated real gas by Haar [4], Svehla [19], Kesselman [17] and Matsunaga [16], and dissociated gas by Svehla [10], Vargaftik [5] and Baronnet [20]). On the other hand, Vargaftik [5] gives the lowest value of viscosity at high temperatures. To be able to judge which is correct, it is necessary to analyze figs 7 and 8. The viscosity of hydrogen and oxygen (products of steam dissociation) and the viscosity of dissociated steam are plotted in fig. 7. These predicted values of viscosity are from Tsedeberg [21] for hydrogen, Vargaftik [22] for dissociated hydrogen, Vasserman [23] for oxygen, Tsitelauri [24] for dissociated oxygen, ASME [2] property equation extrapolation for steam, Svehla [10] for dissociated steam and Vargaftik [5] also for dissociated steam. In general, oxygen has the highest value of viscosity, steam falls in the middle and hydrogen gives the lowest. Fig. 8. illustrates the molar fractions of components from dissociated steam. Steam dissociation starts around 1600 °C and is completed around 4400 °C with final decomposition products being atomic hydrogen and atomic oxygen. Therefore, the viscosity of dissociated steam should depend on the value of individual component viscosity and the percentage of that component in the mixture as well. Based on the above argument, the results presented by Vargaftik [5] and Svehla [10] seem reasonable. However, according to Matsunaga [16], Svehla's results were calculated using erroneous reference viscosity experimental data from Bonilla [25], thus, viscosity values presented by Vargaftik [5] are recommended.

Fig. 9. presents thermal conductivity of steam as a function of temperature from all

available sources. The data presented by Svehla [10], Vargaftik [5] and Baronet [20] all considering dissociation, look reasonable. Since the prediction of thermal conductivity involves the viscosity data for components in the mixture, the results of Vargaftik [5] are again recommended.

At temperatures higher than 1600 °C the values of properties predicted based on non-dissociated and dissociated steam differ considerably; hence, the properties must be evaluated based on dissociated steam. As stated by Kesselman [6], dissociated steam behaves as an ideal solution at all temperatures and pressures up to 10 MPa. For higher pressures, the assumption of ideal mixture behaviour is slightly erroneous. Some typical high pressure property values are shown in figs. 10 and 11.

### 3. Conclusions and Discussion

The dissociated steam properties presented by Vargaftik [5] using the prediction method of Kesselman [6] are most accurate and hence adopted in our property code. The most recent publication by Patel [26] also recommends the tables by Vargaftik [5] for prediction of thermodynamic properties in the temperature range from 1250 to 6000 K. No experimental data at high temperatures are available at present for verification. A computer code, UODH2O, has been constructed using a lookup table and interpretation technique to compute high temperature steam properties\*. Most of the entries of the lookup table come directly from Vargaftik's [5] data. Additional entries are added to expand the parametric range of the code. The property code is valid for temperature ranging from 1000 to 5726.85 °C and pressure from 0.01 to 100.00 MPa. Table 2. presents a sample of the high temperature steam properties table for temperatures from 1000 to 3000 °C and 1300 to 3300 K, and pressures 0.1, 0.5, and 1.0 MPa, generated by the UODH2O code.

The property code is simple, accurate and easy to use. The program size of the code requires 67k memory. It can be used alone or as a subroutine of other program. The property code can easily be updated when more accurate predicted values of properties or experimental data become available. The complete study of present topic including property tables and computer program listing can be found in ref. [27].

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\* The computer code is available from the authors.

## Appendix P

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### Nomenclature

|                |                                    |                                     |
|----------------|------------------------------------|-------------------------------------|
| C <sub>p</sub> | Heat capacity at constant pressure | J kg <sup>-1</sup> °C <sup>-1</sup> |
| d <sub>i</sub> | Internal diameter of pipe          | m                                   |
| G              | Mass flux                          | kg m <sup>-2</sup> s <sup>-1</sup>  |
| H              | Enthalpy                           | J kg <sup>-1</sup>                  |
| k              | Thermal conductivity               | W m <sup>-1</sup> °C <sup>-1</sup>  |
| P              | Absolute pressure                  | MPa                                 |
| S              | Entropy                            | J kg <sup>-1</sup> °C <sup>-1</sup> |
| t              | Temperature                        | °C                                  |
| T              | Absolute temperature               | K                                   |
| v              | Specific volume                    | m <sup>3</sup> kg <sup>-1</sup>     |
| μ              | Viscosity                          | kg m <sup>-1</sup> s <sup>-1</sup>  |

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Table 1. Comparison of data by Artym [13] with other works at  $T = 5000 \text{ K}$   $P = 0.1 \text{ MPa}$

|               | $v$                          | $S$                                            | $H$                | $C_p$                                          |
|---------------|------------------------------|------------------------------------------------|--------------------|------------------------------------------------|
|               | $\text{m}^3 \text{ kg}^{-1}$ | $\text{J kg}^{-1} \text{ }^\circ\text{C}^{-1}$ | $\text{J kg}^{-1}$ | $\text{J kg}^{-1} \text{ }^\circ\text{C}^{-1}$ |
| Artym [13]    | 67.535                       | 28499                                          | 68461000           | 7853                                           |
| Ihara [9]     | -                            | 28565                                          | 68806000           | 6937                                           |
| Gefter [15]   | 67.705                       | 28541                                          | 68706000           | 7230                                           |
| Kesselman [6] | 67.71                        | 28536                                          | 68638000           | 7660                                           |
| Kmonicek [14] | 67.704                       | 28537                                          | 68650000           | -                                              |

## Appendix P

Table 2. The Dissociated steam properties table for temperatures from 1000 to 3000 °C and 1300 to 3300 K, and pressures 0.1, 0.5 and 1.0 MPa

| t           | v                               | S                                   | H                  | Cp                                  | $\mu$                              | k                                  |
|-------------|---------------------------------|-------------------------------------|--------------------|-------------------------------------|------------------------------------|------------------------------------|
| °C          | m <sup>3</sup> kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | J kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | kg m <sup>-1</sup> s <sup>-1</sup> | W m <sup>-1</sup> °C <sup>-1</sup> |
| P = 0.1 MPa |                                 |                                     |                    |                                     |                                    |                                    |
| 1000        | 5.875                           | 13499                               | 4636875            | 2494                                | 0.000047                           | 0.1604                             |
| 1100        | 6.337                           | 13690                               | 4889801            | 2570                                | 0.000050                           | 0.1814                             |
| 1200        | 6.799                           | 13872                               | 5149653            | 2658                                | 0.000053                           | 0.1987                             |
| 1300        | 7.262                           | 14048                               | 5416773            | 2765                                | 0.000056                           | 0.2147                             |
| 1400        | 7.725                           | 14218                               | 5693088            | 2905                                | 0.000058                           | 0.2351                             |
| 1500        | 8.191                           | 14385                               | 5981598            | 3094                                | 0.000061                           | 0.2571                             |
| 1600        | 8.661                           | 14552                               | 6285302            | 3348                                | 0.000063                           | 0.2886                             |
| 1700        | 9.135                           | 14713                               | 6609395            | 3688                                | 0.000065                           | 0.3236                             |
| 1800        | 9.624                           | 14892                               | 6975238            | 4184                                | 0.000068                           | 0.3791                             |
| 1900        | 10.117                          | 15077                               | 7354238            | 4728                                | 0.000070                           | 0.4421                             |
| 2000        | 10.641                          | 15281                               | 7811509            | 5504                                | 0.000072                           | 0.5435                             |
| 2100        | 11.176                          | 15492                               | 8297509            | 6366                                | 0.000074                           | 0.6590                             |
| 2200        | 11.777                          | 15744                               | 8916641            | 7528                                | 0.000075                           | 0.8436                             |
| 2300        | 12.402                          | 16010                               | 9584641            | 8800                                | 0.000077                           | 1.0536                             |
| 2400        | 13.137                          | 16342                               | 10468434           | 10440                               | 0.000078                           | 1.3697                             |
| 2500        | 13.912                          | 16698                               | 11431434           | 12214                               | 0.000080                           | 1.7247                             |
| 2600        | 14.881                          | 17152                               | 12728729           | 14424                               | 0.000080                           | 2.2296                             |
| 2700        | 15.921                          | 17641                               | 14148729           | 16794                               | 0.000081                           | 2.7896                             |
| 2800        | 17.275                          | 18264                               | 16057005           | 19679                               | 0.000081                           | 3.5087                             |
| 2900        | 18.745                          | 18936                               | 18144505           | 22754                               | 0.000081                           | 4.2862                             |
| 3000        | 20.672                          | 19773                               | 20873896           | 26396                               | 0.000082                           | 5.1424                             |

# Appendix P

| t           | v                               | S                                   | H                  | Cp                                  | μ                                  | k                                  |
|-------------|---------------------------------|-------------------------------------|--------------------|-------------------------------------|------------------------------------|------------------------------------|
| °C          | m <sup>3</sup> kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | J kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | kg m <sup>-1</sup> s <sup>-1</sup> | W m <sup>-1</sup> °C <sup>-1</sup> |
| P = 0.5 MPa |                                 |                                     |                    |                                     |                                    |                                    |
| 1000        | 1.175                           | 12755                               | 4635875            | 2493                                | 0.000047                           | 0.1604                             |
| 1100        | 1.267                           | 12946                               | 4888801            | 2564                                | 0.000050                           | 0.1814                             |
| 1200        | 1.360                           | 13128                               | 5147921            | 2639                                | 0.000053                           | 0.1980                             |
| 1300        | 1.452                           | 13303                               | 5414042            | 2725                                | 0.000056                           | 0.2130                             |
| 1400        | 1.545                           | 13472                               | 5687162            | 2829                                | 0.000058                           | 0.2302                             |
| 1500        | 1.638                           | 13636                               | 5969477            | 2959                                | 0.000061                           | 0.2482                             |
| 1600        | 1.731                           | 13797                               | 6263255            | 3126                                | 0.000063                           | 0.2717                             |
| 1700        | 1.825                           | 13956                               | 6570496            | 3341                                | 0.000065                           | 0.2972                             |
| 1800        | 1.920                           | 14118                               | 6903441            | 3641                                | 0.000068                           | 0.3333                             |
| 1900        | 2.016                           | 14280                               | 7244441            | 3967                                | 0.000070                           | 0.3733                             |
| 2000        | 2.116                           | 14452                               | 7630794            | 4417                                | 0.000072                           | 0.4319                             |
| 2100        | 2.217                           | 14627                               | 8033794            | 4913                                | 0.000074                           | 0.4974                             |
| 2200        | 2.324                           | 14821                               | 8508847            | 5564                                | 0.000076                           | 0.5936                             |
| 2300        | 2.434                           | 15021                               | 9010347            | 6272                                | 0.000078                           | 0.7011                             |
| 2400        | 2.554                           | 15251                               | 9621206            | 7161                                | 0.000080                           | 0.8452                             |
| 2500        | 2.679                           | 15492                               | 10272206           | 8116                                | 0.000081                           | 1.0027                             |
| 2600        | 2.823                           | 15776                               | 13322888           | 9275                                | 0.000082                           | 1.2498                             |
| 2700        | 2.973                           | 16076                               | 17254388           | 10509                               | 0.000084                           | 1.5298                             |
| 2800        | 3.151                           | 16435                               | 17446100           | 11963                               | 0.000084                           | 1.8866                             |
| 2900        | 3.340                           | 16816                               | 16265100           | 13498                               | 0.000085                           | 2.2716                             |
| 3000        | 3.572                           | 17272                               | 16606349           | 15274                               | 0.000086                           | 2.7444                             |

## Appendix P

| t                  | v                           | S                                        | H                  | Cp                                       | $\mu$                            | k                                       |
|--------------------|-----------------------------|------------------------------------------|--------------------|------------------------------------------|----------------------------------|-----------------------------------------|
| $^{\circ}\text{C}$ | $\text{m}^3 \text{kg}^{-1}$ | $\text{J kg}^{-1} ^{\circ}\text{C}^{-1}$ | $\text{J kg}^{-1}$ | $\text{J kg}^{-1} ^{\circ}\text{C}^{-1}$ | $\text{kg m}^{-1} \text{s}^{-1}$ | $\text{W m}^{-1} ^{\circ}\text{C}^{-1}$ |
| P = 1.0 MPa        |                             |                                          |                    |                                          |                                  |                                         |
| 1000               | 0.587                       | 12434                                    | 4633875            | 2496                                     | 0.000047                         | 0.1600                                  |
| 1100               | 0.634                       | 12625                                    | 4887532            | 2564                                     | 0.000050                         | 0.1805                                  |
| 1200               | 0.680                       | 12808                                    | 5146921            | 2635                                     | 0.000053                         | 0.1970                                  |
| 1300               | 0.726                       | 12982                                    | 5412310            | 2715                                     | 0.000056                         | 0.2120                                  |
| 1400               | 0.772                       | 13150                                    | 5685162            | 2808                                     | 0.000058                         | 0.2288                                  |
| 1500               | 0.819                       | 13314                                    | 5966014            | 2925                                     | 0.000061                         | 0.2463                                  |
| 1600               | 0.865                       | 13473                                    | 6256329            | 3064                                     | 0.000063                         | 0.2675                                  |
| 1700               | 0.912                       | 13630                                    | 6558839            | 3241                                     | 0.000065                         | 0.2900                                  |
| 1800               | 0.960                       | 13787                                    | 6882760            | 3486                                     | 0.000068                         | 0.2989                                  |
| 1900               | 1.007                       | 13945                                    | 7213260            | 3751                                     | 0.000070                         | 0.3029                                  |
| 2000               | 1.056                       | 14108                                    | 7580335            | 4111                                     | 0.000072                         | 0.3643                                  |
| 2100               | 1.106                       | 14273                                    | 7960835            | 4506                                     | 0.000074                         | 0.4468                                  |
| 2200               | 1.158                       | 14451                                    | 8397295            | 5019                                     | 0.000076                         | 0.5301                                  |
| 2300               | 1.211                       | 14634                                    | 8854295            | 5575                                     | 0.000078                         | 0.6136                                  |
| 2400               | 1.268                       | 14838                                    | 9395052            | 6266                                     | 0.000080                         | 0.7311                                  |
| 2500               | 1.326                       | 15049                                    | 9966552            | 7008                                     | 0.000082                         | 0.8611                                  |
| 2600               | 1.392                       | 15291                                    | 10658018           | 7898                                     | 0.000083                         | 1.0383                                  |
| 2700               | 1.460                       | 15544                                    | 11393518           | 8842                                     | 0.000084                         | 1.2328                                  |
| 2800               | 1.538                       | 15839                                    | 12295068           | 9942                                     | 0.000085                         | 1.4898                                  |
| 2900               | 1.620                       | 16149                                    | 13257568           | 11099                                    | 0.000086                         | 1.7698                                  |
| 3000               | 1.717                       | 16512                                    | 14440249           | 12405                                    | 0.000087                         | 2.1211                                  |

## Appendix P

| T           | v                               | S                                   | H                  | Cp                                  | $\mu$                              | k                                  |
|-------------|---------------------------------|-------------------------------------|--------------------|-------------------------------------|------------------------------------|------------------------------------|
| K           | m <sup>3</sup> kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | J kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | kg m <sup>-1</sup> s <sup>-1</sup> | W m <sup>-1</sup> °C <sup>-1</sup> |
| P = 0.1 MPa |                                 |                                     |                    |                                     |                                    |                                    |
| 1300        | 5.999                           | 13552                               | 4704000            | 2513                                | 0.000048                           | 0.1660                             |
| 1400        | 6.461                           | 13740                               | 4958000            | 2591                                | 0.000051                           | 0.1870                             |
| 1500        | 6.923                           | 13921                               | 5220000            | 2682                                | 0.000054                           | 0.2030                             |
| 1600        | 7.386                           | 14094                               | 5489000            | 2795                                | 0.000056                           | 0.2190                             |
| 1700        | 7.850                           | 14264                               | 5768000            | 2946                                | 0.000059                           | 0.2410                             |
| 1800        | 8.316                           | 14430                               | 6060000            | 3148                                | 0.000061                           | 0.2630                             |
| 1900        | 8.787                           | 14597                               | 6368000            | 3422                                | 0.000064                           | 0.2980                             |
| 2000        | 9.263                           | 14756                               | 6698000            | 3786                                | 0.000066                           | 0.3330                             |
| 2100        | 9.757                           | 14941                               | 7077000            | 4330                                | 0.000068                           | 0.3960                             |
| 2200        | 10.250                          | 15127                               | 7456000            | 4874                                | 0.000070                           | 0.4590                             |
| 2300        | 10.785                          | 15338                               | 7942000            | 5735                                | 0.000072                           | 0.5745                             |
| 2400        | 11.320                          | 15549                               | 8428000            | 6597                                | 0.000074                           | 0.6900                             |
| 2500        | 11.945                          | 15815                               | 9095999            | 7869                                | 0.000076                           | 0.9000                             |
| 2600        | 12.570                          | 16082                               | 9763999            | 9142                                | 0.000078                           | 1.1100                             |
| 2700        | 13.345                          | 16438                               | 10726999           | 10916                               | 0.000079                           | 1.4650                             |
| 2800        | 14.120                          | 16794                               | 11689999           | 12690                               | 0.000080                           | 1.8200                             |
| 2900        | 15.160                          | 17283                               | 13109999           | 15060                               | 0.000080                           | 2.3800                             |
| 3000        | 16.200                          | 17772                               | 14529999           | 17430                               | 0.000081                           | 2.9400                             |
| 3100        | 17.670                          | 18444                               | 16617499           | 20505                               | 0.000081                           | 3.7175                             |
| 3200        | 19.140                          | 19116                               | 18704999           | 23580                               | 0.000081                           | 4.4950                             |
| 3300        | 21.235                          | 20013                               | 21669998           | 27430                               | 0.000082                           | 5.3800                             |

## Appendix P

| T           | v                               | S                                   | H                  | Cp                                  | $\mu$                              | k                                  |
|-------------|---------------------------------|-------------------------------------|--------------------|-------------------------------------|------------------------------------|------------------------------------|
| K           | m <sup>3</sup> kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | J kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | kg m <sup>-1</sup> s <sup>-1</sup> | W m <sup>-1</sup> °C <sup>-1</sup> |
| P = 0.5 MPa |                                 |                                     |                    |                                     |                                    |                                    |
| 1300        | 1.200                           | 12808                               | 4703000            | 2512                                | 0.000048                           | 0.1660                             |
| 1400        | 1.292                           | 12996                               | 4957000            | 2583                                | 0.000051                           | 0.1870                             |
| 1500        | 1.385                           | 13176                               | 5218000            | 2660                                | 0.000054                           | 0.2020                             |
| 1600        | 1.477                           | 13349                               | 5486000            | 2749                                | 0.000056                           | 0.2170                             |
| 1700        | 1.570                           | 13517                               | 5761000            | 2858                                | 0.000059                           | 0.2350                             |
| 1800        | 1.663                           | 13679                               | 6046000            | 2996                                | 0.000061                           | 0.2530                             |
| 1900        | 1.756                           | 13840                               | 6343000            | 3174                                | 0.000064                           | 0.2785                             |
| 2000        | 1.850                           | 13999                               | 6654000            | 3402                                | 0.000066                           | 0.3040                             |
| 2100        | 1.946                           | 14161                               | 6995000            | 3728                                | 0.000068                           | 0.3440                             |
| 2200        | 2.042                           | 14324                               | 7336000            | 4055                                | 0.000070                           | 0.3840                             |
| 2300        | 2.143                           | 14499                               | 7739000            | 4550                                | 0.000073                           | 0.4495                             |
| 2400        | 2.244                           | 14674                               | 8142000            | 5046                                | 0.000075                           | 0.5150                             |
| 2500        | 2.354                           | 14874                               | 8643500            | 5754                                | 0.000077                           | 0.6225                             |
| 2600        | 2.463                           | 15075                               | 9145000            | 6462                                | 0.000078                           | 0.7300                             |
| 2700        | 2.588                           | 15316                               | 9795999            | 7417                                | 0.000080                           | 0.8875                             |
| 2800        | 2.713                           | 15557                               | 10446999           | 8373                                | 0.000082                           | 1.0450                             |
| 2900        | 2.863                           | 15857                               | 14378496           | 9606                                | 0.000083                           | 1.3250                             |
| 3000        | 3.013                           | 16157                               | 18309996           | 10840                               | 0.000084                           | 1.6050                             |
| 3100        | 3.202                           | 16537                               | 17129001           | 12375                               | 0.000085                           | 1.9900                             |
| 3200        | 3.391                           | 16918                               | 15948001           | 13910                               | 0.000085                           | 2.3750                             |
| 3300        | 3.638                           | 17401                               | 16847999           | 15775                               | 0.000086                           | 2.8800                             |



## Appendix P

| T           | v                               | u                                   | H                  | C <sub>p</sub>                      | μ                                  | k                                  |
|-------------|---------------------------------|-------------------------------------|--------------------|-------------------------------------|------------------------------------|------------------------------------|
| K           | m <sup>3</sup> kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | J kg <sup>-1</sup> | J kg <sup>-1</sup> °C <sup>-1</sup> | kg m <sup>-1</sup> s <sup>-1</sup> | W m <sup>-1</sup> °C <sup>-1</sup> |
| P = 1.0 MPa |                                 |                                     |                    |                                     |                                    |                                    |
| 1300        | 0.600                           | 12487                               | 4701000            | 2514                                | 0.000048                           | 0.1655                             |
| 1400        | 0.646                           | 12676                               | 4956000            | 2582                                | 0.000051                           | 0.1860                             |
| 1500        | 0.692                           | 12856                               | 5217000            | 2655                                | 0.000054                           | 0.2010                             |
| 1600        | 0.739                           | 13028                               | 5484000            | 2737                                | 0.000056                           | 0.2160                             |
| 1700        | 0.785                           | 13195                               | 5759000            | 2834                                | 0.000059                           | 0.2335                             |
| 1800        | 0.831                           | 13357                               | 6042000            | 2958                                | 0.000061                           | 0.2510                             |
| 1900        | 0.878                           | 13515                               | 6335000            | 3103                                | 0.000064                           | 0.2735                             |
| 2000        | 0.925                           | 13672                               | 6641000            | 3292                                | 0.000066                           | 0.2960                             |
| 2100        | 0.972                           | 13829                               | 6971500            | 3557                                | 0.000068                           | 0.3000                             |
| 2200        | 1.020                           | 13987                               | 7302000            | 3822                                | 0.000071                           | 0.3040                             |
| 2300        | 1.070                           | 14152                               | 7682500            | 4217                                | 0.000073                           | 0.3865                             |
| 2400        | 1.119                           | 14317                               | 8063000            | 4612                                | 0.000075                           | 0.4690                             |
| 2500        | 1.172                           | 14500                               | 8520000            | 5168                                | 0.000077                           | 0.5525                             |
| 2600        | 1.225                           | 14683                               | 8977000            | 5724                                | 0.000079                           | 0.6360                             |
| 2700        | 1.284                           | 14894                               | 9548499            | 6465                                | 0.000080                           | 0.7660                             |
| 2800        | 1.342                           | 15106                               | 10119999           | 7207                                | 0.000082                           | 0.8960                             |
| 2900        | 1.410                           | 15359                               | 10855499           | 8151                                | 0.000083                           | 1.0905                             |
| 3000        | 1.478                           | 15612                               | 11590999           | 9095                                | 0.000085                           | 1.2850                             |
| 3100        | 1.560                           | 15922                               | 12553499           | 10252                               | 0.000086                           | 1.5650                             |
| 3200        | 1.642                           | 16232                               | 13515999           | 11410                               | 0.000087                           | 1.8450                             |
| 3300        | 1.745                           | 16615                               | 14779499           | 12770                               | 0.000087                           | 2.2225                             |

## Appendix P

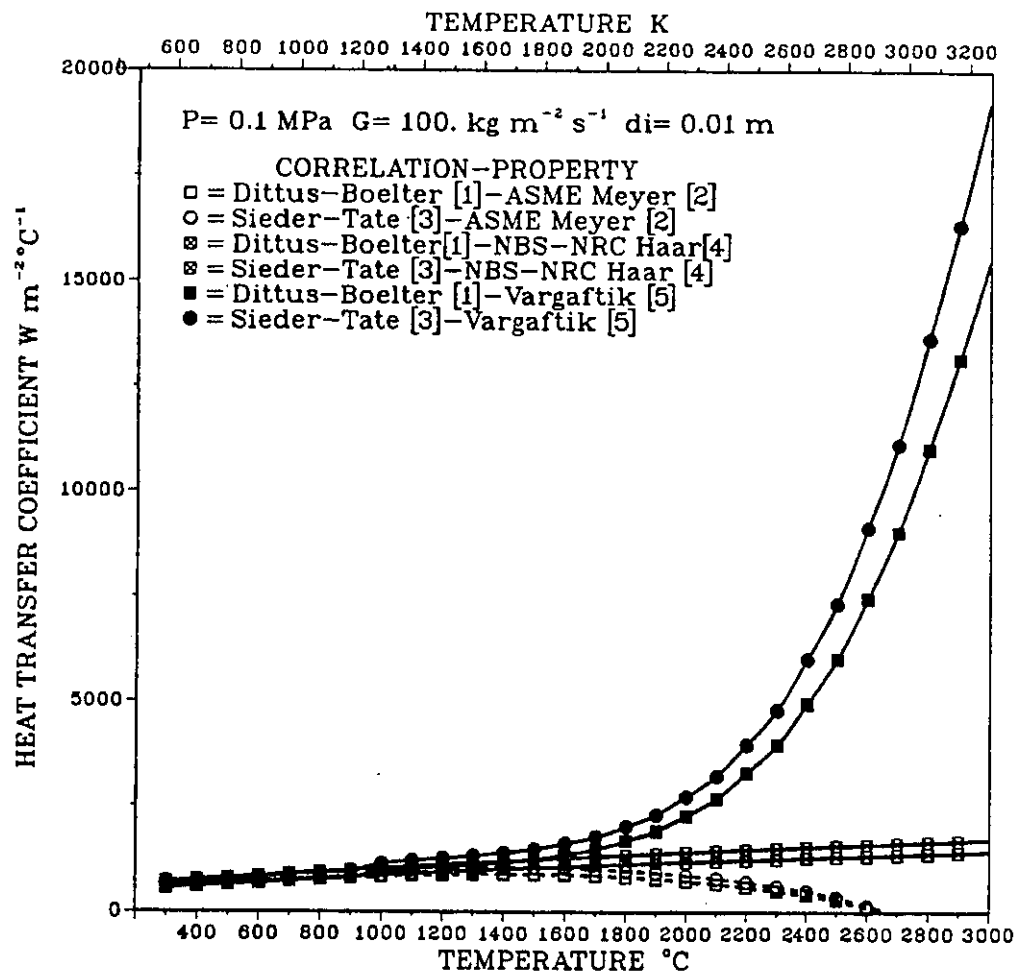


Fig. 1. Heat transfer coefficient in turbulent pipe flow as a function of temperature.

## Appendix P

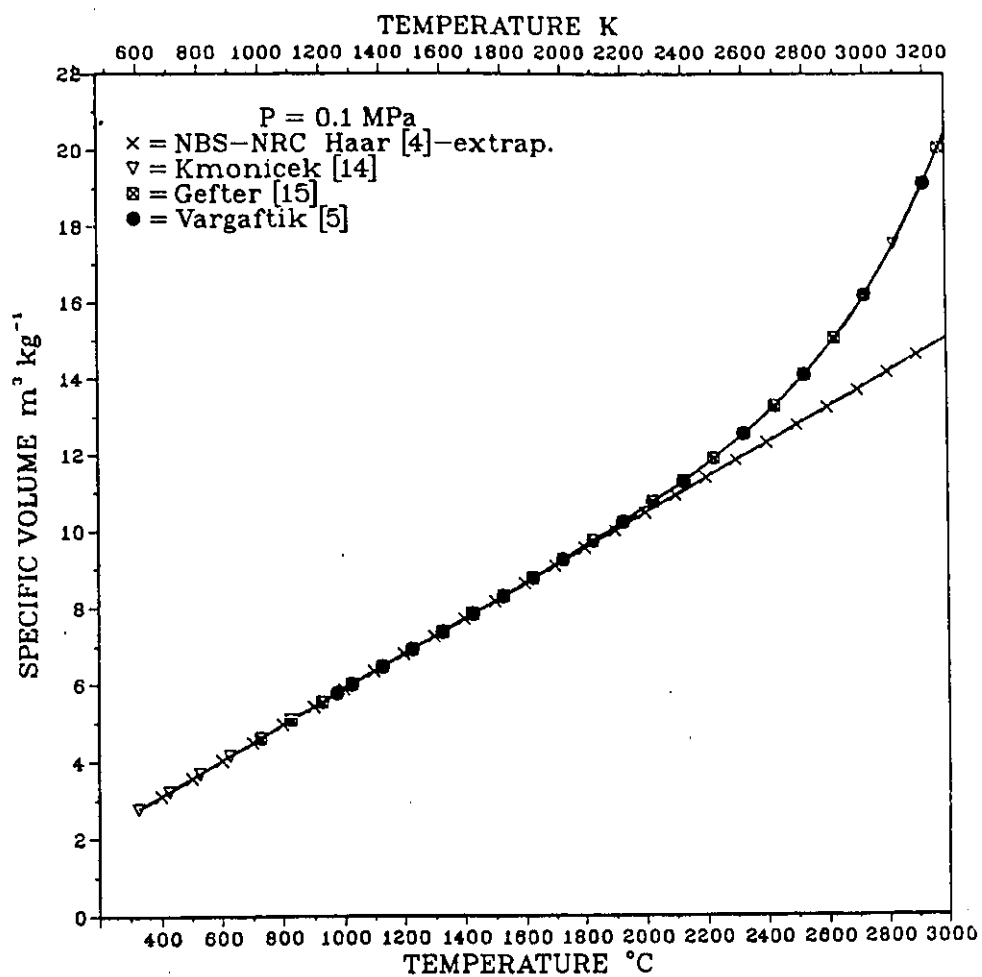


Fig. 2. Specific volume of steam as a function of temperature.

## Appendix P

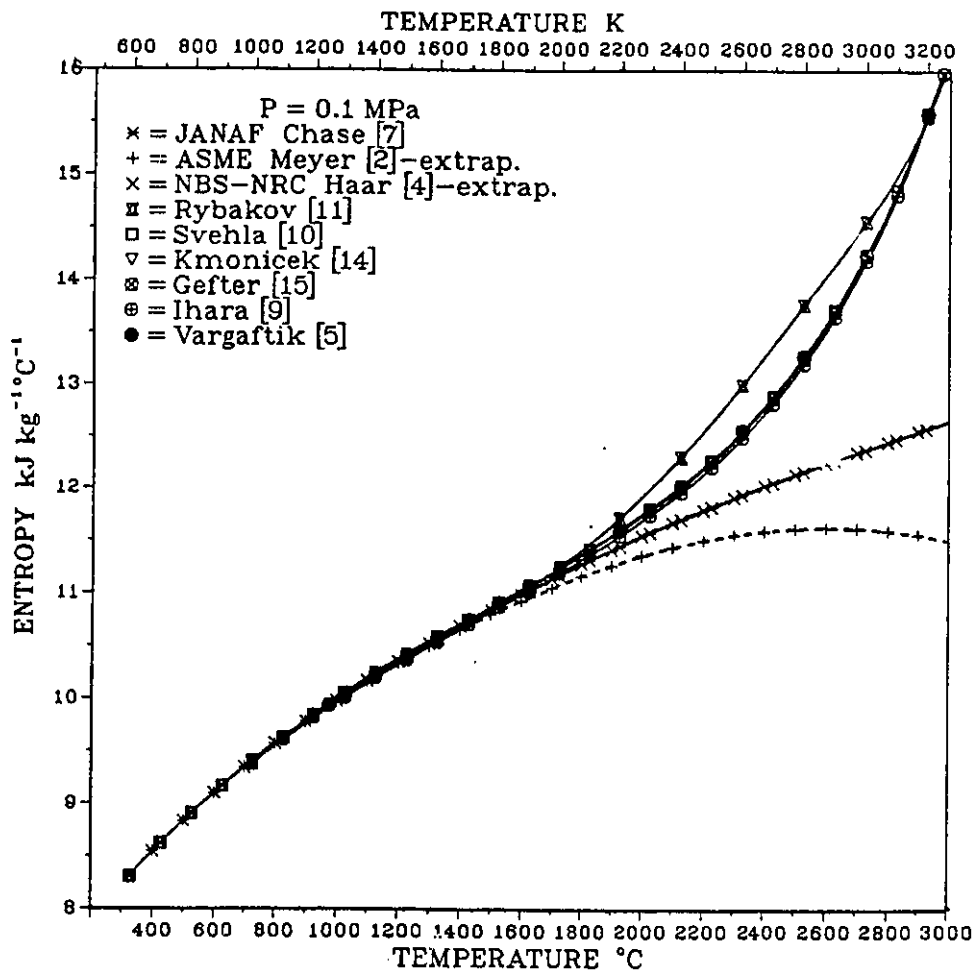


Fig. 3. Entropy of steam as a function of temperature.

## Appendix P

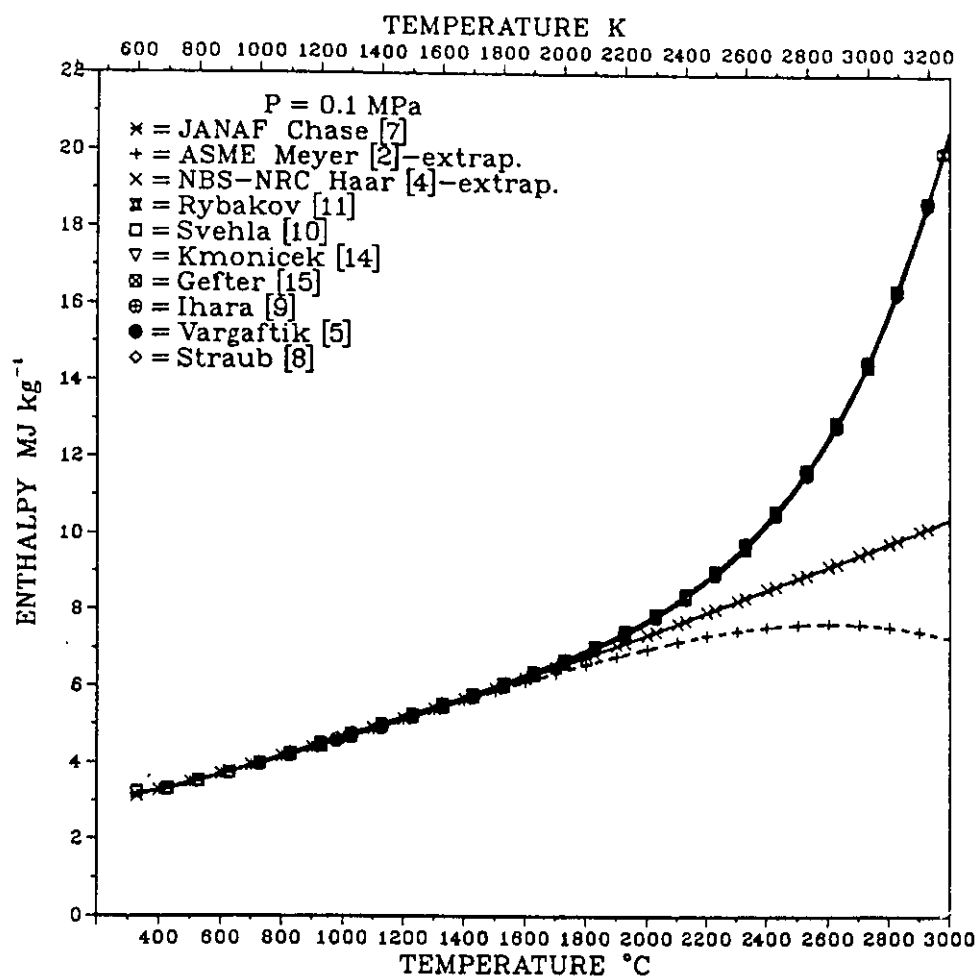


Fig. 4. Enthalpy of steam as a function of temperature.

## Appendix P

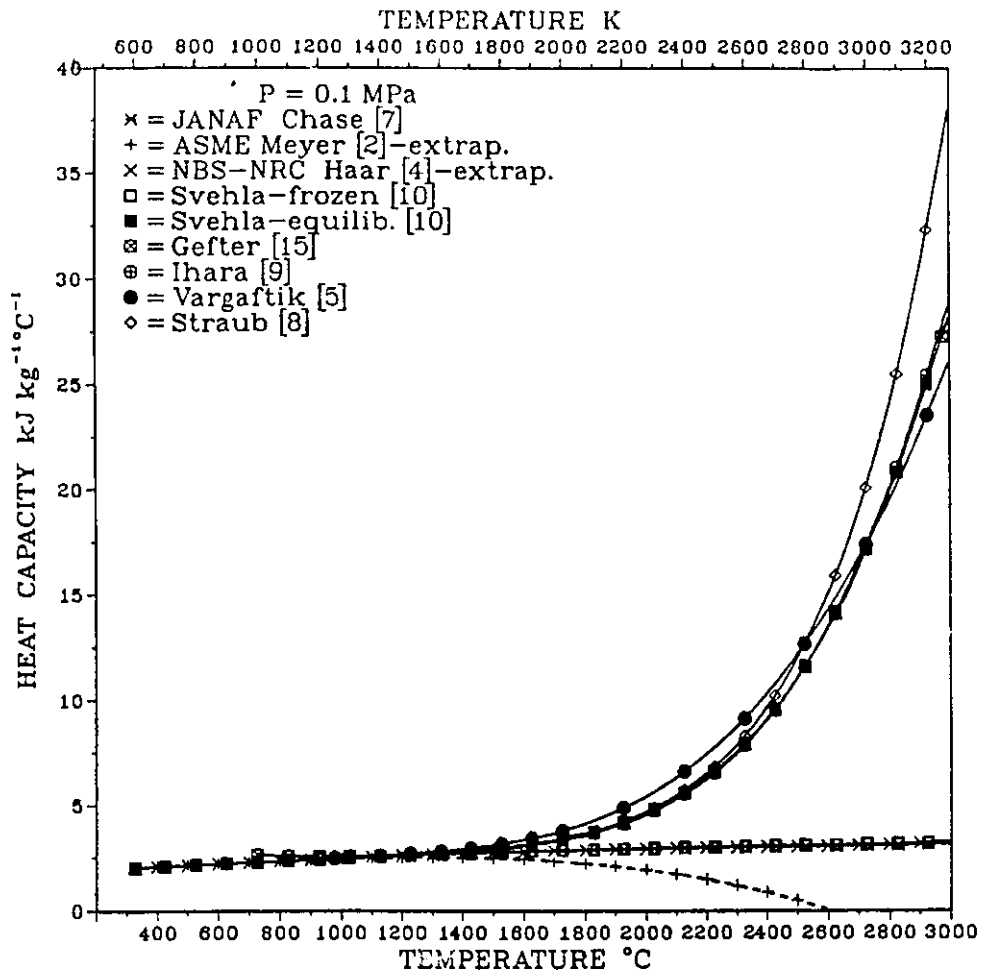


Fig. 5. Heat capacity of steam as a function of temperature.

## Appendix P

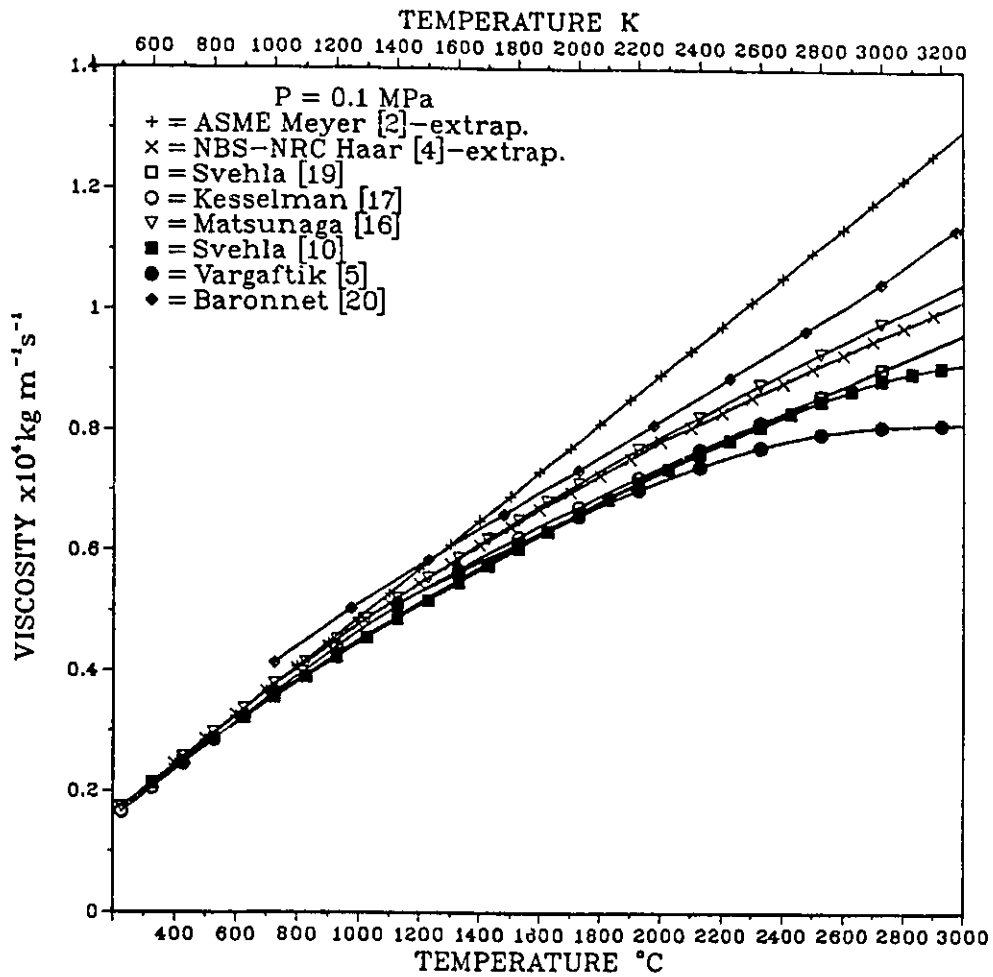


Fig. 6. Viscosity of steam as a function of temperature.

## Appendix P

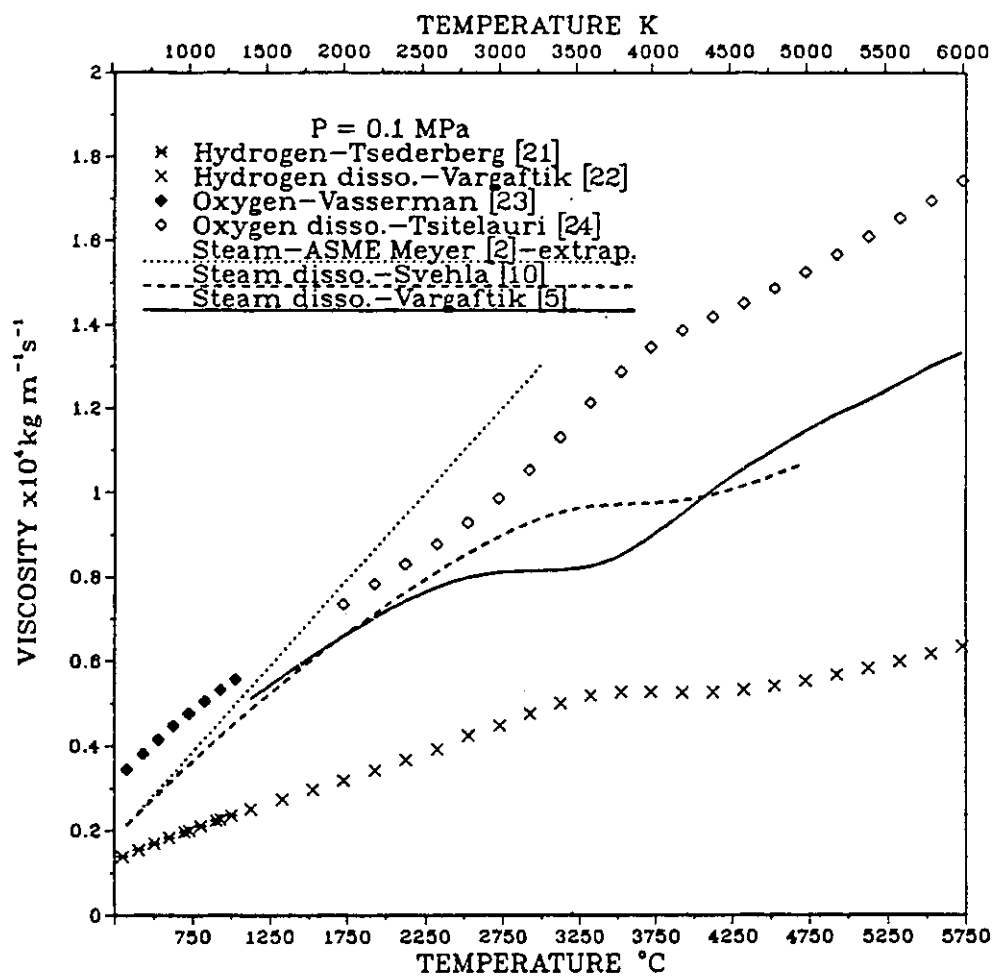


Fig. 7. Viscosity of hydrogen, oxygen and steam as a function of temperature.



## Appendix P

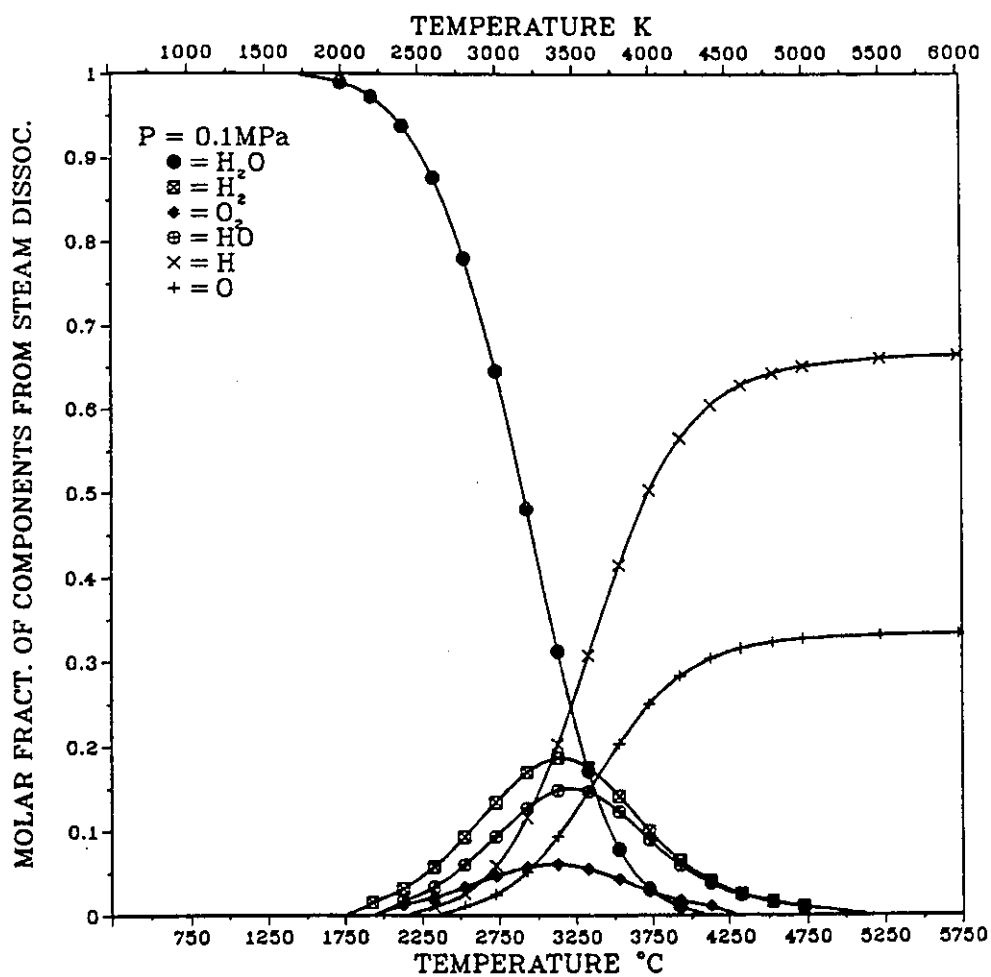


Fig. 8. Molar fraction of components from dissociated steam as a function of temperature at pressure 0.1 MPa.

## Appendix P

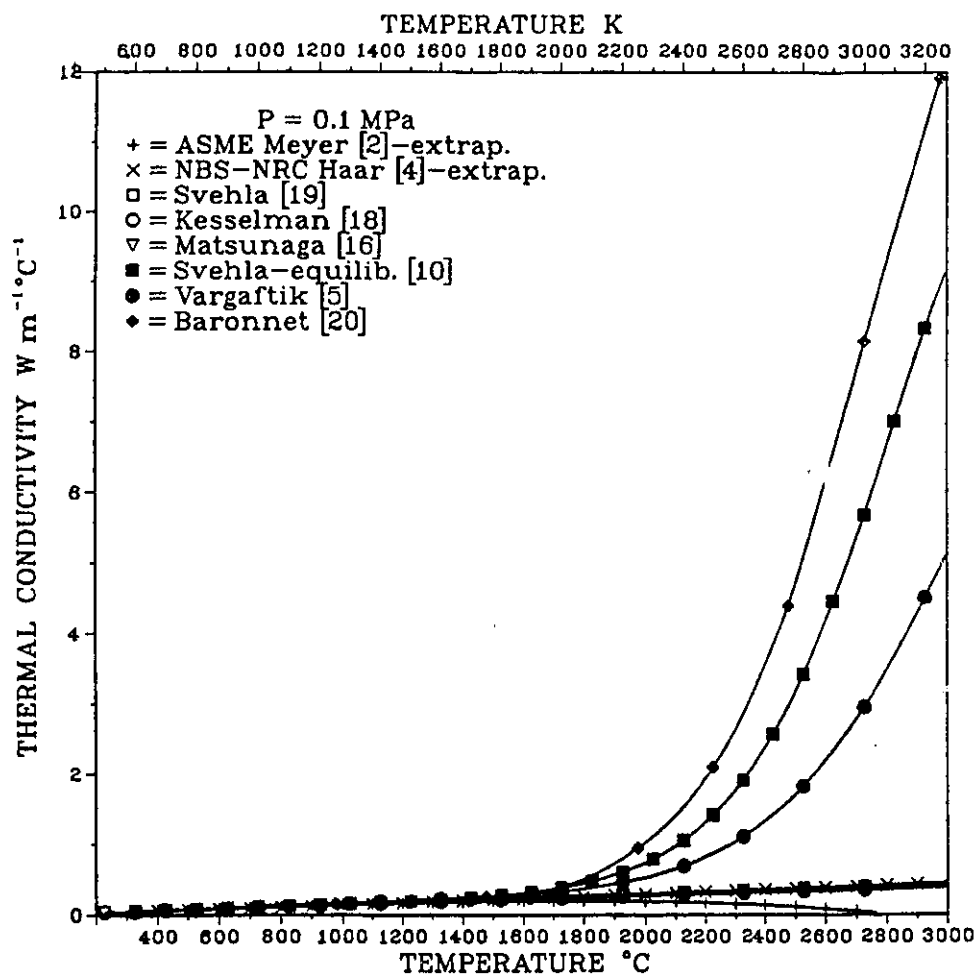


Fig. 9. Thermal conductivity of dissociated steam as a function of temperature.

## Appendix P

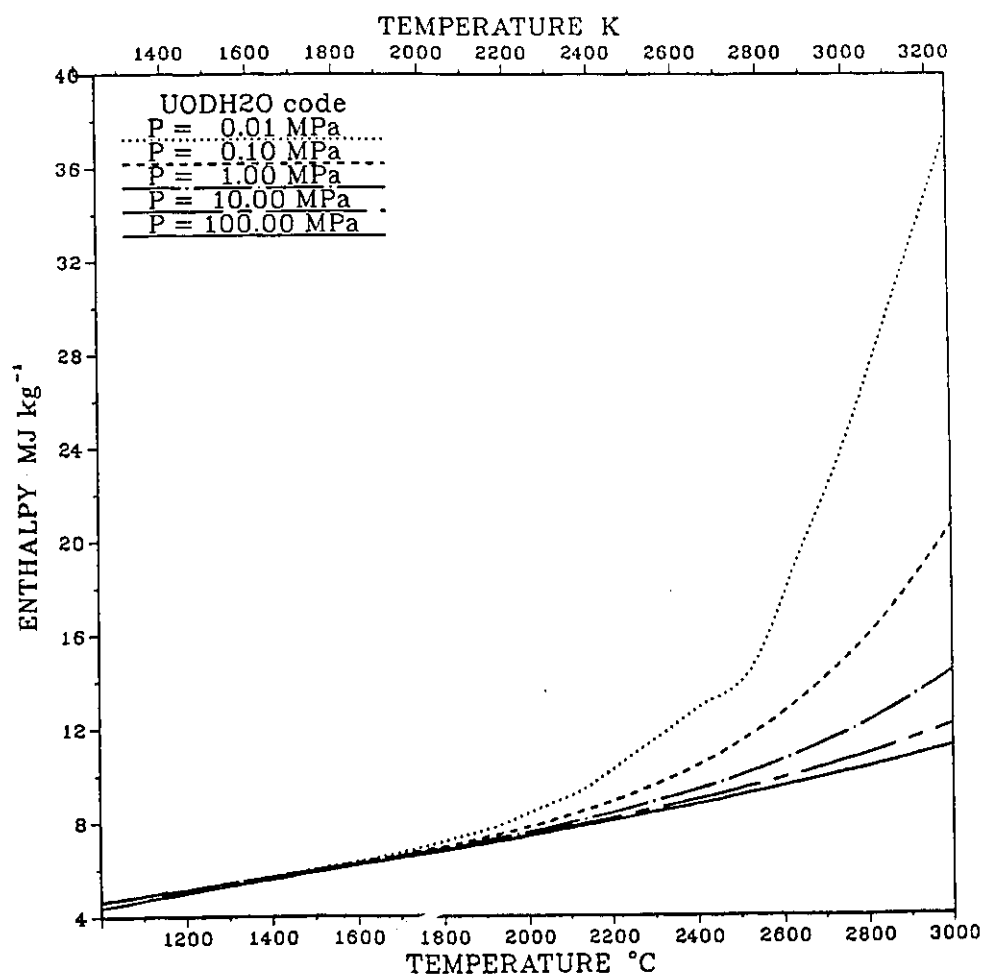


Fig. 10. Enthalpy of dissociated steam as a function of temperature and pressure.

## Appendix P

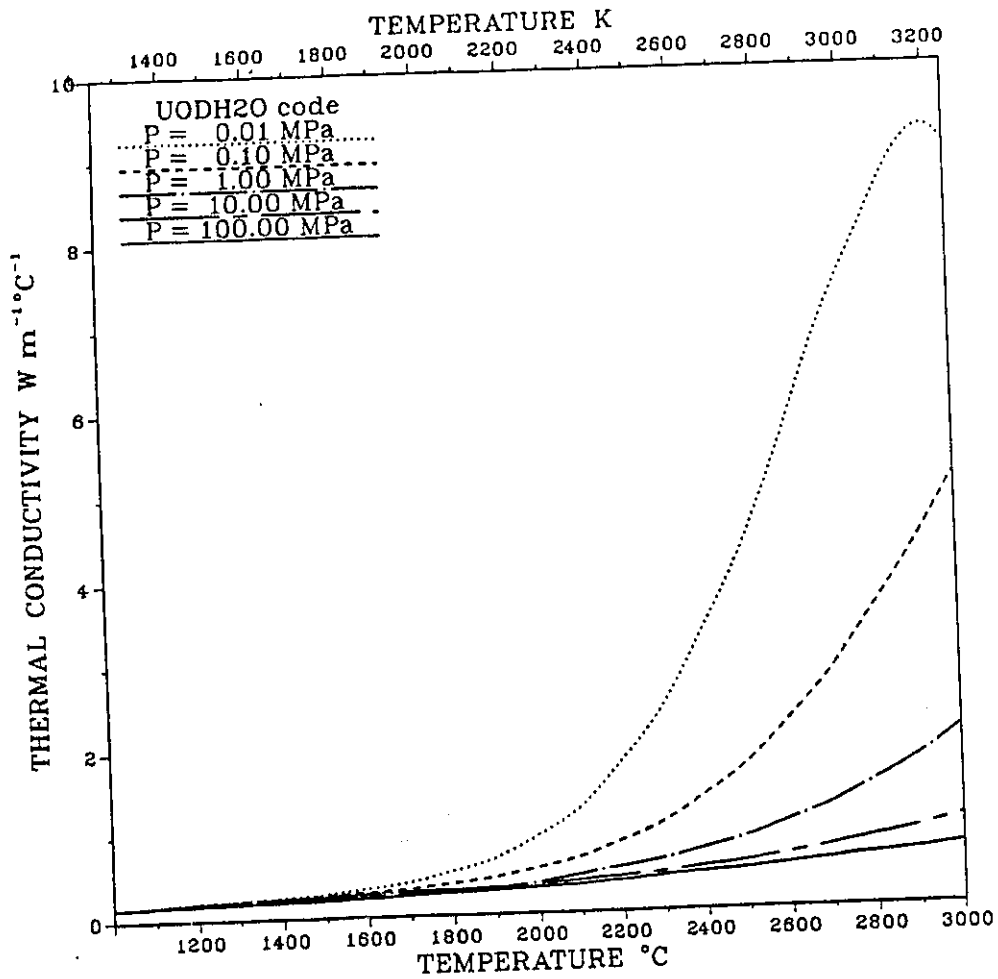


Fig. 11. Thermal conductivity of dissociated steam as a function of temperature and pressure.