THE INTEGRATION OF STATISTICAL AND AUTOMATIC PROCESS CONTROL IN THE CONTINUOUS PROCESSING INDUSTRIES

by

Richard A.W. Slocomb

A thesis submitted to the school of Graduate Studies
in partial fulfilment of the requirements for the degree of

Master of Applied Science

in the

Department of Chemical Engineering
University of Ottawa
Ottawa, Canada

March 15, 1994

ISBN 0-315-95978-9

ABSTRACT

One of the greatest problems in trying to integrate statistical process control (SPC) with automatic process control (APC) in the continuous processing industries (CPI) is dealing with high degrees of correlation in the measured data. The presence of serially correlated data is largely due to the fast sampling intervals and inertial elements common to the CPI. Traditional SPC charting techniques require independence of sampled data and therefore, in most CPI, these charts cannot be utilized in their original forms. In order to obtain process improvements using SPC techniques, modification of existing charts or implementation of new ones is required. Modification of existing charting procedures was shown to increase the detection time for assignable causes or reduce the in-control run length, ARL(0), as compared to data obeying the independence criterion.

A unique problem in the CPI, arising from integration of SPC with APC, is choosing the correct variable(s) for process monitoring. With the introduction of APC, one not only has the disturbance (equivalently the reconstructed output) and residuals to choose from, but also the manipulated variable(s). It was shown that the manipulated variable displayed superior process monitoring potential for first-order processes with moderate amounts of inertia, subject to an ARMA(1,1) disturbance when the autoregressive parameter, ϕ, is larger than the moving average parameter, θ. It was also shown for large amounts of process inertia that the reconstructed output (disturbance) was the most effective charting variable ($\phi > \theta$). However, when θ exceeds ϕ the residual chart performed the best.

In some very severe cases, process observations are so highly correlated that they display a wandering mean. Such nonstationary disturbances are extremely problematic in the CPI. These disturbances have typically been dealt with through data transformations, differencing and residual analysis yielding stationary, chartable data. However, these data transformations have traditionally produced less than acceptable ARL(Δ)s. The n^{th}-difference chart developed in this work, on the other hand, proved to be efficient at identifying the presence of assignable cause in first-order processes under Minimum Variance feedback control when subjected to IMA(1,1) disturbances displaying moderate degrees of nonstationarity ($\theta > 0.7$). Furthermore, it was shown that the performance of these charts is significantly affected by the presence of the autoregressive parameter (ie., when $\phi > 0.2$).

A case study involving a C_3 splitter provided the basis for development of a six-step procedure for the integration of SPC with APC. While carrying out integration on the C_3 splitter it was determined that the cause of disturbance nonstationarity must be sought out and removed if successful integration is to be achieved. For most nonstationary disturbances the amount of natural drift is often greater than or equal to the size of the step shifts that one is trying to detect. Thus, one is not able to differentiate between the common cause and assignable cause disturbances. More importantly, the nonstationarity of the disturbance indicates that the process is already under the influence of one or more assignable causes and thus should be further investigated to find and, if feasible, remove the assignable causes prior to continuation of the integration of SPC with APC.

ACKNOWLEDGEMENTS

I would like to thank Dr. David D. McLean for his patient and continual guidance throughout my graduate studies. I appreciated the opportunity to work in such a new and exciting area of research. I enjoyed, very much, working with Dr. McLean and wish him all the best in the years to come.

A very special thanks to my parents, Walt and Pat and my sister, Sandra, for their support throughout my University years. Not just monetary support, although that, too, was appreciated.

I would also like to thank Wayne, Nancy, Jason and Michelle Dauphinee, for providing me with a home away from home and for putting up with me for so many years. And a big thanks to everyone at the University of Ottawa who made my stay in Ottawa both educational and fun.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

NOMENCLATURE

a_t	-	random variable, independent, identically distributed $N(0,\sigma_a^2)$.
B	-	backward shift operator, $Ba_t = a_{t-1}$
b	-	process delay.
D^{ss}	-	steady-state value of distillate flow, tonnes/day.
D_t	-	observed distillate flow, tonnes/day.
D^*_t	-	distillate flow deviation from steady-state, tonnes/day.
g	-	process gain constant.
g	-	minimum mean square error (MMSE) estimate of the process gain constant g.
G_p	-	process transfer function model.
H_0	-	null hypothesis.
H_1	-	alternate hypothesis.
k	-	slack or allowable variation in the mean value of the process variable.
Kc	-	process gain constant.
k_L	-	loss function model parameter.
L	-	Taguchi's loss function.
P_t	-	observed column pressure, kPa.
P^*_t	-	column pressure deviation from set-point, kPa.
Q^{ss}	-	steady-state value of reboiler duty, kW-hr/tonne/day.
Q_t	-	observed reboiler duty, kW-hr/tonne/day.
Q^*_t	-	reboiler duty deviation from steady-state, kW-hr/tonne/day.

$S_{h,t}$ - cumulative sum test statistic for identifying positive shifts in mean value of the process variable.

$S_{l,t}$ - cumulative sum test statistic for identifying negative shifts in mean value of the process variable.

T - process time constant.

w_t - reconstructed output, the value of the control variable if no APC is taken.

X_t - deviation of the manipulated variable from target value.

x_t - observed bottoms composition, ppm.

x^*_t - bottoms composition deviation from set-point, ppm.

y_{t+b} - output deviation from target at time t+b.

$y_{t/t-1}$ - forecasted value of output variable deviation from target at time t.

$\bar{Z}_t$ - smoothed value of the exponentially weighted moving average.

z_t - value of ARIMA(p,d,q) stochastic disturbance.

$z_{t+b+1/t}$ - conditional expectation of the stochastic disturbance.

Greek Letters

α - random variable, independent, identically distributed $N(0,\sigma_\alpha^2)$.

δ - process delay constant.

δ_{PD} - process inertia for the transfer function relating column pressure to distillate flow.

δ_{PQ} - process inertia for the transfer function relating column pressure to reboiler duty.

$\delta_{t0}[\Delta]$ - assignable cause entering a process as a step shift in the process mean, shift is measured in multiples of the process standard deviation.

δ_{xQ} - process inertia for the transfer function relating bottoms composition to reboiler duty.

Δ - size of step shift perturbing the disturbance.

$\Delta\sigma_y$ - magnitude of a step change in the value of the process mean.

$\varepsilon(t)$ - deviation of controlled variable from set-point at time, t.

η_t - process mean at time, t.

θ - moving average parameter for time series model.

θ - MMSE estimate of moving average parameter, θ.

λ - weighting constant given to past data when using the exponentially weighted moving average.

μ - process mean.

ζ_t - correlated noise, $\zeta_t = \phi\zeta_{t-1} + a_t$.

σ_a - standard deviation of random variable, a_t

σ_a - estimated standard deviation of random variable, a_t.

τ - nominal value of process mean.

τ_D - derivative time constant.

τ_I - integral time constant.

ϕ - autoregressive parameter for time series model.

ϕ - MMSE estimate of autoregressive parameter, ϕ.

ϕ_{1P} - autoregressive parameter for disturbance affecting the pressure in the Shell Canada distillation column.

ϕ_{1x} - autoregressive parameter for disturbance affecting bottoms composition in the Shell Canada distillation column.

ω_0 - process gain constant.

ω_{PD} - process gain constant for the transfer function relating column pressure to distillate flow, tonnes/(day kPa).

ω_{PQ} - process gain constant for the transfer function relating column pressure to reboiler duty, kW-hr/tonne/(day kPa).

ω_{xQ} - process gain constant for the transfer function relating bottoms composition to reboiler duty, kW-hr/tonne/(day ppm).

Mathematical Symbols

∇ - backward difference operator, $\nabla a_t \equiv (1\text{-}B)a_t = a_t - a_{t-1}$.

GLOSSARY OF ABBREVIATIONS

			Page
ACF	-	Autocorrelation function.	87
APC	-	Automatic process control.	1
AR	-	Autoregressive.	31
ARL(0)	-	In-control average run length.	31
ARL	-	Average run length.	52
ARMA	-	Autoregressive moving average disturbance.	4
ARMAX	-	Autoregressive moving average with exogenous inputs.	113
ARIMA	-	Autoregressive integrated moving average.	4
ASPC	-	Algorithmic statistical process control.	35
CL	-	Control limits.	45
CPI	-	Continuous processing industry.	3
CUSUM	-	Cumulative sum.	15
CV	-	Control variable.	57
EWMA	-	Exponentially weighted moving average.	16
FOPDT	-	First-order plus dead-time.	12
iid	-	Independently, identically distributed.	3
IMA	-	Integrated moving average.	26
LCL	-	Lower control limit.	45
MA	-	Moving average.	59

MRL	-	Median run length.	70
MSE	-	Mean squared error.	38
MV	-	Minimum variance.	23
PACF	-	Partial autocorrelation function.	87
PG	-	Pure gain.	12
PID	-	Proportional plus integral plus derivative.	22
PRBS	-	Pseudo-random binary sequence.	95
PQV	-	Product quality variable.	4
SPC	-	Statistical process control.	2
UCL	-	Upper control limit.	45

Chapter 1

INTRODUCTION

Since the early 1980's there has been a significant shift in focus by industry, from producing quantity to producing quality. This shift, to a large extent, has been due to the success of the Japanese at implementing the principles of quality control and quality management. To keep their market share in today's highly competitive market, North American companies have begun to realize they need to improve their product quality and productivity. One way in which these goals can be achieved is through implementation of better methods of process control.

There are two widely accepted means of controlling industrial processes - automatic process control (APC) and statistical process control (SPC). Automatic process control makes use of algorithms relating process inputs to process outputs to automatically compensate for process perturbations by manipulating selected input variables. This makes APC a useful tool in the continuous processing industry (CPI) where process data is collected at high rates using on-line computers. APC is a very effective method of regulating a process about its mean (target) value, since it continuously implements control action after new observations become available. However, APC has been criticized for compensating for disturbances, rather than removing their cause. On the other hand, SPC utilizes various statistical techniques to determine the need for process adjustment, the adjustment being removal of the cause of the upset. SPC assumes that a process is in control as long as the measurements of the product quality variable (PQV) randomly fluctuate about a fixed mean value, μ, with constant variance, σ^2. Thus, as long as PQV data fall within specified control limits, the process is said to be following its *common cause model*, and is in a state of control. Any deviation from this common cause model is indicative of a process shift, or *assignable cause*. An assignable cause is indicated by an observation falling outside the control limits. When an assignable cause is indicated, control action is taken to set the process back on target until the cause for the shift is located and removed. This continuous process of identification and subsequent removal of assignable cause results in a greater understanding of the process and yields a higher quality product by eliminating causes rather than compensating for them. However, SPC has been criticized for not being able to effectively regulate a process.

It has long been thought that these two methods of process control were only effective in their respective industries, discrete item manufacturing for SPC and continuous processing for APC. This naive assumption is largely due to the fact that SPC and APC were generally employed by distinctly different professions, statisticians and engineers, respectively. Recently, with the overlap occurring between these two professions, due to the increasing industrial focus on product quality and productivity, advocates of these two methods of control have come together and have begun to realize that their methods are not contradictory, but rather complimentary. Each approach's shortcomings can potentially be compensated for through integration of both methods.

Integration yields a process that effectively regulates the process to target using APC while providing effective process monitoring and removal of assignable cause using SPC.

Despite the potential gains available to the continuous processing industries (CPI) via integration, very little has been published on how one gets started. Many authors have indicated the need for an integrated method of process control and some have even carried out integration on their own processes (Vander Wiel *et al.*, 1992; MacGregor, 1988; Palm, 1990; Box and Kramer, 1992; Hoerl and Palm, 1992; Wardrop and Garcia, 1992). However, at the time of carrying out this work no one had rigorously outlined a procedure for setting up an integrated system. Such a procedure is needed to highlight disturbance and process modelling, the choice of automatic process control algorithms and which process variables are the most effective for process monitoring. The four step procedure recently developed by Vander Wiel *et al.* (1993) is a significant move towards identifying such a procedure. However, many of the major questions about integration have still not been thoroughly addressed in the literature. These include:

> Can SPC charts be used *effectively* when the data is not independent and identically distributed (i.i.d.)?
>
> Can APC system variables be used effectively as process monitoring variables?
>
> What procedure should be used to set up an effective integrated control scheme?

One of the most difficult problems to overcome using SPC charting procedures in the continuous processing industries is how to chart data that is not independent (i.e., correlated data). Correlation results from the short sampling intervals and inertial elements (i.e., those having capacity to store mass or energy such as mixing tanks and reactors). Traditionally, SPC charts were developed to examine product quality data that were independently and identically Normally distributed with fixed mean, μ, and constant variance, σ^2. Thus, as long as the data (i.e., observed values of the PQV, y_t) followed the traditional SPC model,

$$y_t = \mu + a_t \tag{1}$$

where the a_t's are iid random 'shocks' driving the process, the process was considered "in-control" from a statistical point of view. However, in the CPI, process disturbances are correlated and even nonstationary. More complex model forms such as autoregressive integrated moving average models, ARIMA(p,d,q) (Box and Jenkins, 1970), given by

$$\nabla^d y_t = \frac{(1-\theta_1 B-\theta_2 B^2-...-\theta_q B^q)}{(1-\phi_1 B-\phi_2 B^2-...-\phi_p B^p)} a_t \tag{2}$$

are used, where the θ_i are moving average parameters ($-1<\theta_i<1$), the ϕ_i are autoregressive parameters ($-1<\phi_i<1$), B is the backward shift operator ($Ba_t \equiv a_{t-1}$) and ∇ is the backward difference operator ($\nabla a_t \equiv (1-B)a_t \equiv a_t - a_{t-1}$). As already mentioned equation 2 can be use to describe the class of ARIMA models, however it can also be used to describe ARMA(p,q) disturbances by setting d=0 (i.e., removing the ∇^d operator).

A more explicit form of equation 2 is obtained by writing the equation in expanded form, thus for an ARIMA(1,1,1) model,

$$y_t = (1+\phi_1)y_{t-1} - \phi_1 y_{t-2} + a_t - \theta_1 a_{t-1}. \tag{3}$$

Therefore, it becomes evident that the PQV is dependent upon previous values of the PQV and previous values of the white noise. Thus a new definition of an "in-control" process was needed. Box and Kramer (1992) stated that when a *stable common cause model* explains the process variation, the system is said to be in a state of control and temporary deviations from the model, signalled by outliers, is an indication of *assignable cause*. Thus, as long as the process variability is described by equation 2, with d=0, then the process is considered to be in a state of control (see Figure 1). For non-zero values of d, the common cause model is not *stable*, that is, the process disturbance does not have a fixed mean and thus has an undefined variance (see Figure 2). Consequently, non-stationary data cannot be meaningfully plotted on traditional control charts.

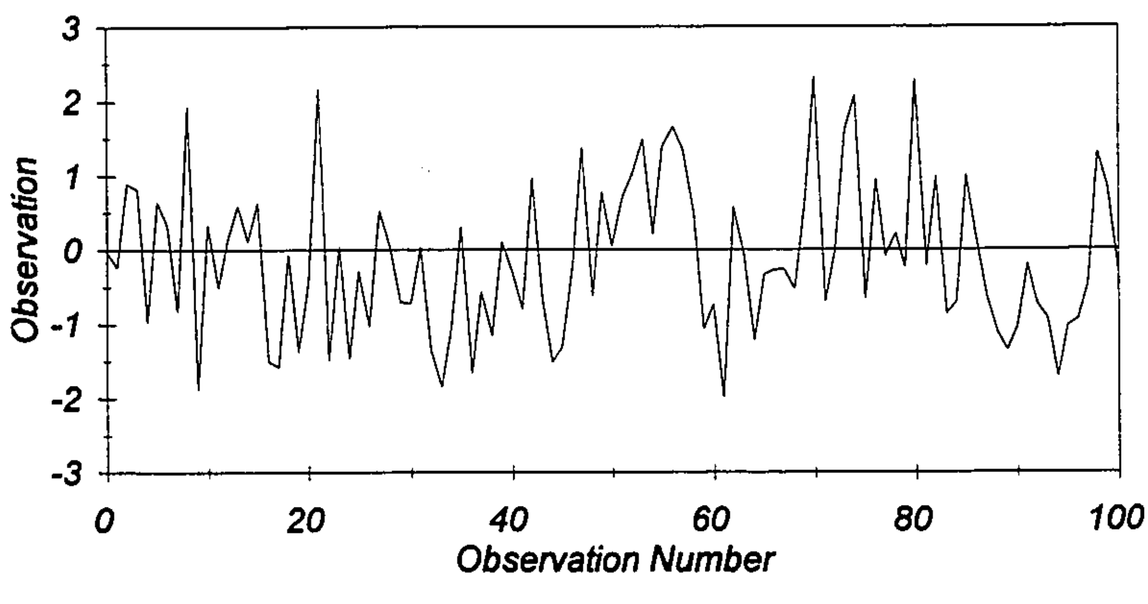


Figure 1: Representative data for a stable common cause model, ARMA(1,1) with θ_1=0.4 and ϕ_1=0.6.

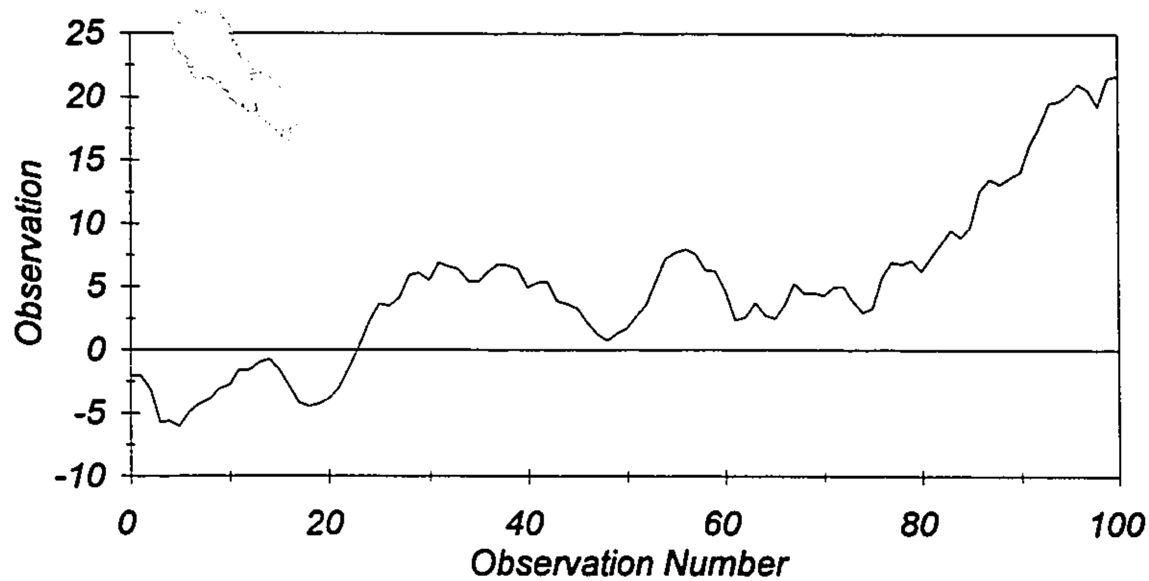


Figure 2: Representative data for an unstable common cause model, ARIMA(1,1,1) with $\theta_1=0.4$ and $\phi_1=0.6$.

Methods are available for transforming nonstationary data to yield stationary, chartable data. These methods include plotting the difference between successive observations, and plotting residuals, the difference between the actual value of the process variable and its predicted value. Although these transformations allow plotting on a SPC chart, their application is seriously questioned since the lack of stationarity itself may be an indication that the process is not in a state of control.

Several approaches have been suggested for the integration of SPC with APC (Kramer and Box, 1990; MacGregor, 1988, 1991; English and Case, 1990). These methods include plotting the manipulated variable, disturbance, residuals or forecast errors, reconstructed process outputs and output deviations from target on traditional SPC charts. However, an extensive comparison of these potential charting variables has not been carried out in terms of their effectiveness for identification of assignable cause.

Additionally, most of the work that has been done in the area of SPC charting for the continuous processing industry has dealt with autoregressive disturbances (English *et al.*, 1990; Harris and Ross, 1990) and ARMA disturbances (Vander Wiel *et al.*, 1992). Although these are very important disturbances in the CPI it has also been suggested that nonstationary disturbances, from the class of autoregressive integrated moving average models (ARIMA(p,d,q)), are commonly encountered (MacGregor, 1988; Cott, 1993). From a strict SPC viewpoint, it can be argued that a process that is nonstationary is not in a state of statistical control and therefore should not be charted until the cause of the nonstationarity is identified and removed. On the other hand, from an APC standpoint, stationarity can be induced through the use of APC and one could then use the deviation from target of the controlled variable as a charting variable. It may not always be feasible to remove the cause of the nonstationarity and therefore one would like to explore the possibilities for monitoring a nonstationary process. Thus, a major part of this work will deal with the identification of assignable cause in nonstationary disturbances, for an integrated system.

The specific objectives of this thesis are:

(i) to evaluate the sensitivity of potential charting variables by examining how a step change in the mean value of the disturbance propagates through the process to the various charting variables for both ARMA and ARIMA disturbance models,

(ii) to evaluate the effectiveness of Shewhart charts and a new charting procedure, n^{th}-difference charts at detecting assignable cause in nonstationary processes and

(iii) to demonstrate the steps involved in setting up an integrated system using an industrial example (Cott, 1992) .

The first objective will allow us, given a specific process and disturbance model, to highlight which process variables should be used for process monitoring. Evaluation of the effectiveness of Shewhart and n^{th}-difference charting procedures will indicate some of the problems unique to charting data generated by a continuous process and will identify the suitability of each approach. The last objective allows us to simultaneously, through example, address all of the major issues of integration that have, to date, not been adequately dealt with, including the choice of process variable(s) for charting, derivation of generalized minimum variance (MV) feedback controllers and dealing with nonstationary processes.

In the chapter that follows we will present background outlining process modelling, SPC charting, APC and a critical survey of the literature pertinent to the area of integration. Chapter 3 will contain the theory and methodology for work done on selection of charting variables, the n^{th}-difference charting procedure, a generalized derivation of two minimum variance controllers as well as the simulation software. Chapter 4 will provide the results and discussion on the effectiveness of the n^{th}-difference charts and the selection of charting variables. A case study, based on Shell Canada's C_3 splitter, will be presented, as a six-step strategy for integration, in Chapter 5. The final two chapters contain conclusions, recommendations and references.

Chapter 2

BACKGROUND AND LITERATURE SURVEY

This chapter focusses on the specifics of APC and SPC in terms of what each method consists of, their philosophies and traditional uses. The criticisms of each method are addressed such that the need for integration of SPC with APC is more clearly understood. Time series modelling is discussed since it provides the foundation for integration. Once sufficient background information on the two methods of control has been provided a critical assessment of articles dealing with their integration and related topics, such as the charting of correlated observations, is given. Evaluation of the strengths and limitations of the methods suggested for integration is provided and finally summarized.

2.1 Time Series Approach to Modelling

Before being able to integrate SPC with APC, one must first develop appropriate models to describe the system being investigated. Figure 3 shows an open-loop block diagram for a typical process which indicates the need for models describing the process dynamics, G_p, the process disturbance, z_t, and the amount of adjustment of the manipulated variable, X_{t-1}, required to keep the process output close to the set-point. The transfer function model with added disturbance is given by

$$y_t = G_p\, X_{t-1} + z_t \tag{4}$$

where y_t is the output deviation from target of the controlled variable. One of the most effective methods of modelling data when it is available at discrete, equispaced, time intervals is the use of time-series analysis (Box and Jenkins, 1970). The models are expressed mathematically by linear difference equations, the discrete time equivalent of linear differential equations.

Classical methods for estimating transfer function models describing the process, based on deterministic perturbations of the input, have not always been successful. This is because the response of the system is often masked by uncontrollable disturbances called noise (Box and Jenkins, 1970). Time series modelling allows us to make allowances for such disturbances. In addition, these models are computationally easy to employ in computer algorithms.

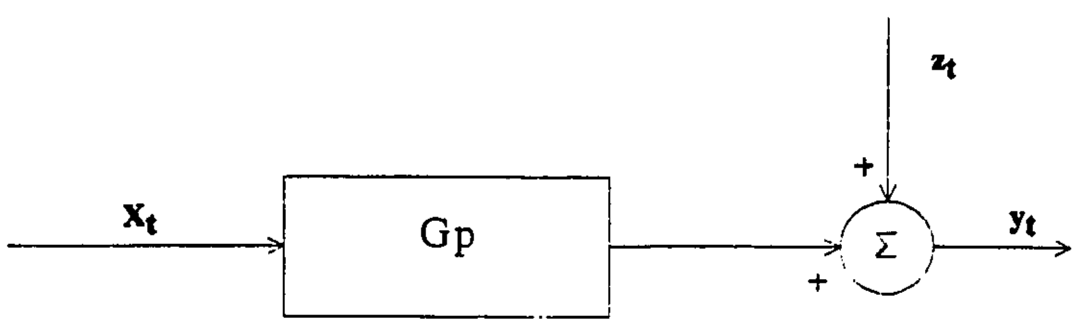


Figure 3: Open-loop block diagram.

2.1.1 Disturbance Models. The simplest stochastic disturbance model is the stationary white noise model which assumes that the disturbance, z_t, fluctuates randomly about a fixed mean, μ, and has a constant variance, σ_a^2. This model can be expressed mathematically as

$$z_t = \mu + a_t \tag{5}$$

where the a_t's are independent identically distributed random 'shocks' with mean zero and constant variance, σ_a^2. This model is sometimes referred to as the SPC model, since this is the model form used as the basis for the traditional SPC charting procedures. This is also the model form typically encountered in the discrete item manufacturing industry where process measurements are typically independent of one another. However, in the continuous processing industry (CPI), where process measurements are taken over short sampling intervals, data are dependent on previous disturbances. These data are referred to as being autocorrelated.

There are two main classes of stochastic disturbance models used to describe autocorrelated data, the autoregressive moving average, ARMA(p,q), and the autoregressive integrated moving average models, ARIMA(p,d,q). The general form of both of these models is shown in equation 2, where setting d=0 yields the ARMA model. Often, commonly encountered disturbances in the CPI can be adequately described by these models with values of p and q ≤ 2 and values of d = 0 or 1, yielding models of the form

$$z_t = \frac{(1-\theta B)}{\nabla^d (1-\phi B)} a_t \tag{6}$$

where B is the backward shift operator ($Ba_t = a_{t-1}$) and $\nabla^d \equiv (1-B)^d$ is the backward difference operator.

2.1.2 Process Models. Two important types of process models that are encountered in the CPI, are the pure-gain (PG) and the first-order plus dead-time (FOPDT) models. A pure-gain model is representative of the transfer function typically found in the discrete item manufacturing industry, that is the change in the input variable is wholly transferred to the output variable within one sampling interval. The form of the PG transfer function is:

$$y_t = gX_{t-1} + z_t \tag{7}$$

where y_t is the output deviation from target, g is the process gain, X_{t-1} is the manipulated variable expressed as a deviation variable and z_t is the process disturbance. A FOPDT model is expressed mathematically as,

$$y_t = \frac{\omega_0}{(1-\delta B)} X_{t-b-1} + z_t \tag{8}$$

where $\omega_0 \equiv g(1-\delta)$ is the process gain constant, $\delta \equiv e^{-1/T}$ $(0 < \delta < 1)$ is the process inertia, T is the process time constant and b is the dead time. The quantity $(1-\delta)$ represents the fraction of the change in the input variable felt in the output variable after one sampling interval. A FOPDT process model is very useful in the CPI because it can also be used to approximate the dynamics of second and higher order processes.

2.2 Statistical Process Control

Statistical process control is a method for manufacturing a product with consistently uniform properties, using various statistical techniques to determine when process adjustments are required to set the process back on target. Examples of properties of interest include, for discrete item manufacturing: length, width and tensile strength; for chemical processes: denier, dye-depth and viscosity. SPC assumes that a process is in a state of control as long as the product quality variable deviates in a random fashion about a fixed mean, μ, with constant variance, σ^2. The use of a statistical test to determine whether control action is warranted stems from the economic argument that, in the discrete item manufacturing industry where SPC originated, there is often a significant cost associated with taking control action. A process shutdown is usually required to implement control action. This translates into lost product and hence, lost profit. Additionally, if a process were following the SPC model implementation of automatic control would result in increased process variance, which is undesirable.

In the discrete item manufacturing industry control charting techniques are the analytical tool of choice. There are, in general, three widely accepted procedures for charting process data: the Shewhart chart, the exponentially weighted moving average (EWMA) charts and the cumulative sum (CUSUM) charts. The basic theory underlying all three charting methods is similar. Each method can be represented as a procedure for testing a statistical hypothesis, the hypothesis being that the mean and variance of the PQV are maintaining their desired values. This results in testing whether an appropriate statistic falls within predetermined control limits. These limits are set at a level where there is only a small probability (i.e., 0.0027 for $\pm 3\sigma_x$ limits) that an in-control process will yield data that exceeds these limits on chance alone. As it is not the aim of this thesis to analyze the effectiveness of each charting technique or to compare each of the methods to the other, only a very brief summary of each technique will be presented. More detailed analyses of these charting techniques are available (Lucas and Saccucci, 1990; Roberts, 1959; Harris and Ross, 1991; Lucas and Crosier, 1982).

2.2.1 Shewhart Charts. The Shewhart chart, first introduced by W.A. Shewhart (1931), consists of sequentially plotting the mean and the range of the PQV (based on either individual observations or on a suitable subgroup) on a chart with upper and lower action (control) limits. These action limits are placed at plus or minus 3 times the standard deviation of the PQV being plotted where there is only a 0.27% chance that the limits would be exceeded on chance alone. We are interested in differentiating between the two hypotheses:

$$H_0: \ \mu_{PQV} = \mu_0 \tag{9}$$

versus

$$H_1: \ \mu_{PQV} \neq \mu_0 \tag{10}$$

Thus, if we reject the null hypothesis we have statistical evidence that a shift in the process mean has occurred and action should be taken to identify the cause and to remove it.

So-called "runs rules" are sometimes used in conjunction with the Shewhart chart in an effort to more quickly identify assignable cause. Runs rules use unusual sequences (runs) of data points as indicators of process upsets (eg., two out of three points on the same side of the mean falling between $2\sigma_a$ and $3\sigma_a$ is an indication of an out-of-control process). More such rules can be found in a paper by Nelson (1984) and a handbook by the Western Electric Company (1956). Caution must always be exercised when implementing runs rules because the more rules that are used the more likely you will make a type I error; type I errors occurring when you reject H_0 when H_0 is true.

Shewhart charts provide a rapid charting procedure for identifying large process disturbances ($\Delta \geq 3\sigma$). Additionally, they are easy to use, since process data can usually be charted directly and therefore plant personnel without extensive knowledge of SPC can use them. A prime disadvantage of using Shewhart charts is that they are very slow at identifying small process upsets, which are often the disturbances of greater interest.

2.2.2 Cumulative Sum Charts. The CUSUM charting technique consists of plotting the sum of the deviations of the PQV from target against time. This sum will remain close to zero as long as the process is only subject to random disturbances. If a shift does occur in the process mean then the cumulative sum will increase or decrease rapidly. Graphically a shift in mean is identified by overlaying a V-mask. Two parameters, d and θ, the lead time and half angle, respectively, determine the positioning and size of the V on the graph. If a point falls outside either of the arms of the V then this is taken as an indication of an assignable cause. A more extensive description of the graphical approach to CUSUM charting is given by Page (1954).

The algorithmic approach to CUSUM charting is a more reasonable means of identifying assignable cause in the CPI since data is usually collected, on-line, by computers. The test statistics used are:

$$S_{h,t} = \max[0\ ,\ y_t - k + S_{h,t-1}]$$
$$S_{l,t} = \max[0, -y_t - k + S_{l,t-1}] \tag{11}$$

where y_t is the PQV being charted, k is the slack or allowable variation in the process and max[a,b] is the maximum of a and b (Lucas and Crosier, 1982). If either of the test statistics exceeds a critical value, h, then a shift in the process mean has been indicated. The parameters h and k are related to d and θ and are chosen to minimize the number of false alarms for an in-control process (i.e., to minimize type I errors) while still being able to rapidly detect assignable cause (i.e., minimizing type II errors).

The advantage of CUSUM charts is that they are an effective method for identifying small process disturbances ($0.5\sigma \leq \Delta \leq 1.5\sigma$). The primary disadvantage of using CUSUM charts is that the test statistics and control limits are not as easy to understand as those for Shewhart charts.

2.2.3 Exponentially Weighted Moving Average. The exponentially weighted moving average (EWMA) charts were first introduced by Roberts (1959), but it was not until recently that they were used for quality control purposes (Hunter, 1986). This method is based on the test statistic

$$\bar{Z}_t = \lambda y_t + (1-\lambda)\bar{Z}_{t-1} \tag{12}$$

where $\bar{Z}_t$ is the EWMA statistic, y_t is the PQV and λ is the weighting constant ($0<\lambda<1$)

applied to past and present values of the PQV. When the control limits, $\pm L\sigma_{\hat{z}}$, are exceeded, an assignable cause is indicated, which may be indicative of a statistically significant shift in the process mean. Thus, the values of λ and the control limit parameter, L, must be chosen to minimize the occurrence of type I and type II errors. Tables of optimal values for λ and L, are available (Lucas and Saccucci, 1990), depending on the size of disturbance to be detected and the in-control run length desired.

The EWMA charts are also very effective at identifying small process disturbances ($0.5\sigma \leq \Delta \leq 1.5\sigma$). Like the CUSUM charts, the EWMA test statistic and control limits require a greater understanding of SPC to fully understand and use.

2.2.4 Choice of Charting Variable. When using a time series approach to process modelling and control one has essentially three choices for charting variables as suggested by MacGregor (1992): residuals, reconstructed outputs (equivalently, the disturbance) and the manipulated variable. Although one can think of many other possible charting variables, due to the nature of time series, these three variables are equivalent to all of the process variables not mentioned. For example, one might suggest that we chart the deviation from target of the controlled variable, but it can easily be shown that, when a minimum variance (MV) controller or a well tuned proportional plus integral plus derivative (PID) controller is used, the output deviation from target is equivalent to the residual.

Upon reviewing the literature, residuals appear to be the variable of choice for charting (Vander Wiel *et al.*, 1992; Harris and Ross, 1991 Box and Kramer, 1992). This choice of charting variable is probably due to the fact that, of the variables available for charting only the residuals yield data that are i.i.d. $N(0,\sigma_a^2)$. Thus, only the residuals satisfy the underlying assumptions of traditional charting procedures when we are dealing with correlated observations. However, as Harris and Ross (1991) indicated for highly positively correlated observations ($\phi > 0.7$), charts of residuals become ineffective at identifying assignable cause. Harris and Ross (1991) show that for the case when $\phi=0.5$ and $\Delta=1\sigma_z$ (ie., there is a 1σ step shift in the mean value of the disturbance) then the expected value of the residuals after the shift is 0.58 times the original shift, and 0.23 times for $\phi=0.9$. Shifts of this magnitude become increasingly more difficult to identify as ϕ increases.

The reconstructed output, which is equivalent to the disturbance, is also a popular choice for charting variable (Vander Wiel *et al.*, 1992; Harris and Ross, 1991). Unlike the residuals, this variable can only be used if the observations are generated by a stable common cause model. Thus, only ARMA (p,q) disturbances can be charted in this manner. As shown by Harris and Ross (1991), the presence of correlation greatly affects the in-control run length when using traditional control charts (CUSUM and EWMA), but does not affect the detection times when an assignable cause enters the process. The consequence of plotting correlated data on traditional charts is that the control limits have to be altered to allow longer, more reasonable, in-control run lengths. The result of this is slower detection times when assignable causes enter the process, slower in comparison to the detection times expected for the SPC model.

The only variable, of those suggested by MacGregor (1992), that has not been studied as a charting variable is the manipulated variable. None of the articles encountered by this author have employed the manipulated variable as a means for process monitoring. The charting properties of the manipulated variable are expected to be similar to those of the reconstructed output, since both sets of data are correlated. One of the strongest arguments that can be made for the use of the manipulated variable as a charting variable is that it can be employed with minimal knowledge of the process or the disturbances affecting it. A simple PID controller could be used to keep the process under continuous feedback control while the manipulated variable was being used to monitor the underlying process.

Finally, in dealing with nonstationary observations, various procedures have been suggested to transform the observations into stationary, chartable data. These include data differencing and residual calculations (Box and Jenkins, 1970; Box and Kramer, 1992). To date very little has been done, both theoretically and experimentally, in the area of SPC charting for nonstationary processes. The difficulty associated with identifying assignable cause in nonstationary processes is certainly one reason why very little has been done in this area. It also seems that nonstationary processes are indicative of a system that is not in a state of statistical control and thus should not be subject to SPC. However, until someone pursues this area of research a definitive answer cannot be obtained.

2.3 Automatic Process Control

APC is considered an active approach to process control, since it makes process adjustments after each new observation becomes available. Thus, unlike SPC, APC treats all deviations from target as being significant and implements control action based on the size and direction of the deviation. According to Stephanopoulos (1984) there are three classes of needs for such a control system which include: suppressing the influence of external disturbances, ensuring the stability of a chemical process and optimizing the performance of a chemical process. In the CPI the disturbances perturbing a process are often comprised of many smaller disturbances referred to as noise which, from an economic point of view, cannot feasibly be removed and therefore must be compensated for. The second need arises from the fact that some processes, when left to themselves, are unstable. Stability must be induced by actively controlling the process. Our last need is to be able to change the operation of the plant such that the economic objective function is maximized. Often, in batch processing, the optimal run condition is time dependent and thus requires a control algorithm to achieve optimal results.

2.3.1 Feedforward and Feedback Control. Two common types of automatic control configuration found in the chemical processing industry are feedback and feedforward. Figures 4 and 5 show the configurations of feedforward and feedback controllers, respectively. The main difference between these two types of controllers is that feedback controllers base control action on measurements of the process output variable, while feedforward controllers base control action on measurements of the input

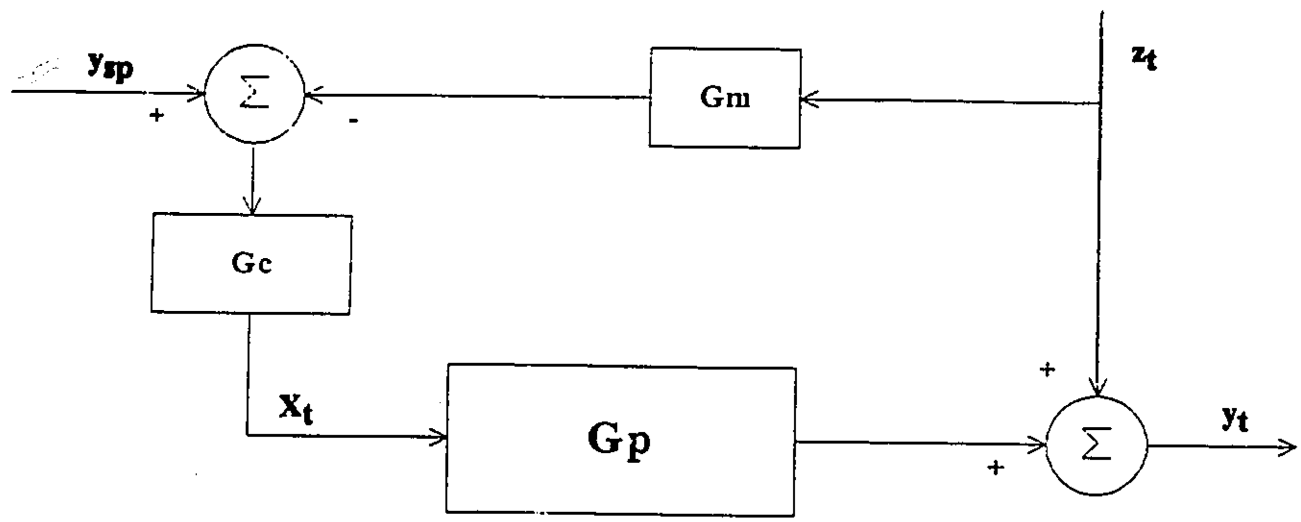


Figure 4: Block diagram of a feedforward control configuration.

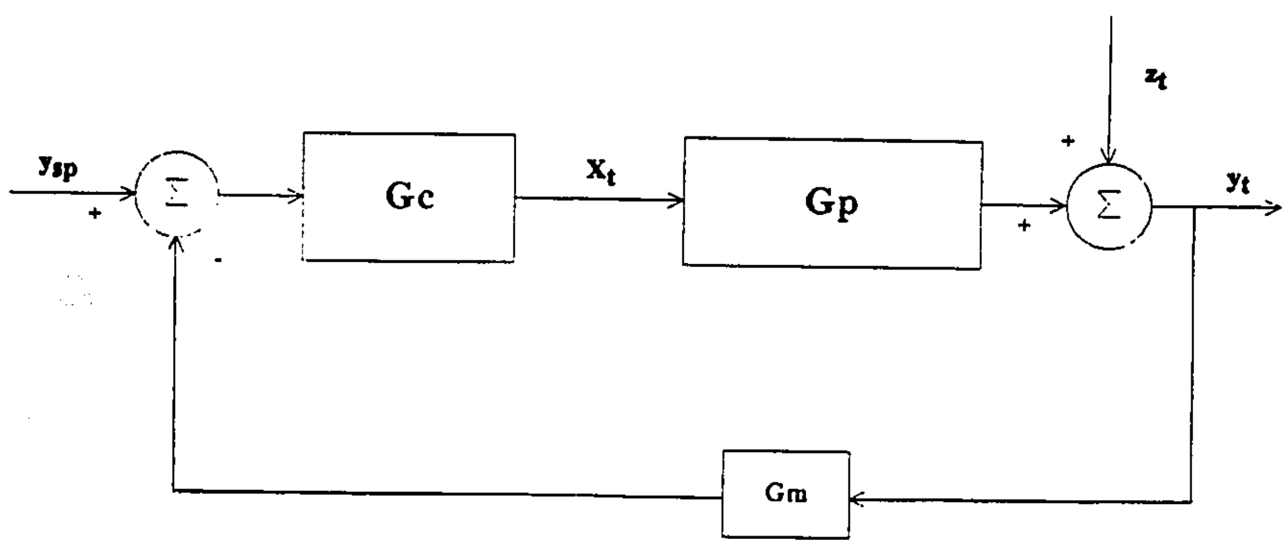


Figure 5: Block diagram of a feedback control configuration.

disturbances affecting the process. Thus, feedback control assumes that the disturbance cannot be measured directly and therefore must take control action after it has disturbed the system. On the other hand, feedforward control assumes that the input disturbances can be measured and that suitable compensatory action can be taken to nullify the effect of the disturbance. Theoretically, feedforward control can exactly eliminate the effect of a disturbance, given that the manipulated variable used to compensate for the disturbance affects the process at least as fast as the disturbance. However, perfect control is never achieved since it is impossible to measure all of the disturbances affecting the process and to acquire perfect knowledge of the process model(s). Therefore, a combination of feedforward and feedback control is often used to effectively regulate the process to target. The feedforward control compensates for the measurable disturbances while feedback control takes care of the unmeasurable or unexpected disturbances and model mismatch that are inevitably present in continuous processes.

2.3.2 PID Controllers. The most utilized controller in the chemical processing industry is the proportional plus integral plus derivative (PID) feedback controller. The form of this controller in the time domain is

$$X(t) = K_c y(t) + \frac{K_c}{\tau_I}\int_0^t y(t)dt + K_c \tau_D \frac{dy}{dt} \tag{13}$$

where K_c is the proportional gain constant, τ_I is the integral time constant, τ_D is the derivative time constant and y(t) is the output deviation from target of the controlled variable. For our purposes a more useful form of the PID controller equation is the discrete time equivalent, given by

$$X_t = K_c\{y_t + \frac{T}{\tau_I}\sum_{k=0}^{t} y_k + \frac{\tau_D}{T}(y_t - y_{t-1})\}. \tag{14}$$

By setting τ_D equal to zero we obtain a proportional plus integral controller, and by also setting τ_I equal to ∞ we obtain a proportional controller, two useful variations of the PID controller. PID controllers are the controllers of choice in industry because of their effectiveness in most applications and they can be applied to processes without prior knowledge of the types of disturbances affecting the process.

2.3.3 Minimum Variance Controllers. If we have gone to the trouble of modelling our process and the disturbances, we would normally like to make use of this information in setting up the controller(s). One appealing objective in designing the controller is minimization of the expected variance of the controlled variable (Box and Jenkins, 1970). Therefore, once the disturbance models and the process dynamics have been identified they may be used to derive minimum variance (MV) controllers. Minimum variance controllers have been suggested and derived in numerous articles related to quality improvement (MacGregor, 1988; Vander Wiel *et al.*, 1992; Harris, 1989). However, these controllers have typically been for very specific disturbance models and process dynamics. For example, MacGregor (1988) derived the MV controller for a FOPDT process subject to a first-order integrated moving average (IMA(1,1)) disturbance resulting in the control algorithm,

$$X_t = -\frac{(1-\theta)\delta}{\omega_0}[y_t - \frac{(1-\delta)}{\delta}\sum_{i=-\infty}^{t} y_i] \tag{15}$$

Interestingly, this turns out to be the discrete equivalent of the proportional plus integral controller.

2.4 SPC Versus APC

Many authors, in their discussions of the problem of integrating SPC with APC, have provided their own definitions of both SPC and APC. According to Vander Wiel *et al.* (1992), SPC is a collection of techniques especially useful in improving product quality by helping an analyst locate and remove root causes of quality variation. Box and Kramer (1992) view SPC as process monitoring that resembles a system of continuous statistical hypothesis testing. MacGregor (1988) gives us a more general definition, stating that SPC is the use of statistical methods to improve process productivity and product quality.

Although none of the above definitions is all encompassing, one gets a good idea of what SPC is by combining all three. In the most basic sense SPC involves the identification and subsequent removal of assignable cause. The techniques used to achieve this are based on statistical hypothesis testing. The final outcome is an improved process producing higher quality products.

On the other hand, APC has been defined as the application of appropriate compensatory adjustment to a process using statistical estimation of the current level of the process disturbance (Box and Kramer, 1992). APC can also be thought of as a collection of algorithms for manipulating the adjustable variables of a process to achieve the desired process behaviour (e.g., output close to a target value) (Vander Wiel *et al.*, 1992). MacGregor (1992) views APC as a short term solution that minimizes variability, not by removing its cause, but by transferring the variability into another variable - the manipulated variable.

One can see that there are some definite differences in the underlying philosophies of these process control techniques. SPC is thought of as a long term solution for process improvement whereas APC is considered a short term temporary solution to process upsets. However, one should bear in mind that SPC and APC techniques were developed in different industries, the discrete item manufacturing and continuous processing industries, respectively. In the discrete manufacturing industry, taking control action usually requires a shutdown of the process, which results in a loss of product and a cost to make the adjustments. The associated costs are often significant; thus, control action is only taken when deemed economically necessary. In the continuous processing industry, where control action usually takes the form of adjusting a valve, control action is essentially cost free. Thus, as long as the control action does not increase the variability in the product quality variable (PQV), control action can be implemented once each new observation becomes available. It can be shown, mathematically, that if the SPC model (equation 5) is representative of the disturbance affecting the process then the MV control algorithm is equivalent to a control chart, that is, do not take control action unless an assignable cause has been indicated (Box and Kramer 1992).

2.4.1 Criticisms of SPC and APC. Since the development of SPC and APC occurred in different industries, it is not surprising that advocates of these methods of process control have some criticisms of the other's method. Typically cited shortcomings of APC (Box and Kramer, 1992) include:

i) overcompensating for disturbances,

ii) compensating for disturbances rather than removing them,

iii) and concealing information that might be useful for quality improvement.

The first of these criticisms results if the controller is tuned too tightly or if the wrong controller is used. The solution to the first part of this problem is avoided if the controller tuning is relaxed. The second part can also be dealt with if accurate modelling of the process and disturbances is carried out. The second criticism, as indicated by Box and Kramer (1992), is not valid in the processing industry where elimination of all disturbances is not always economically feasible. Thus, compensation is required to adjust for the disturbances that cannot be removed. With regards to the last criticism, this author agrees fundamentally with Box and Kramer's (1992) notion that information should not be concealed, but disagrees with their implementation. The example used by Box and Kramer (1992) indicates that a plot of output deviations from target is sufficient to signal when an assignable cause has entered a process subject to an IMA (1,1) disturbance. However, it appears that such a plot only indicates assignable cause when the trend of the output deviation from target happens to be in the same direction as that of the shift, as seen in Figures 6a and 6b. Although Figure 6a indicates the presence of an assignable cause, at time $t=30$, for the same process Figure 6b does not identify the assignable

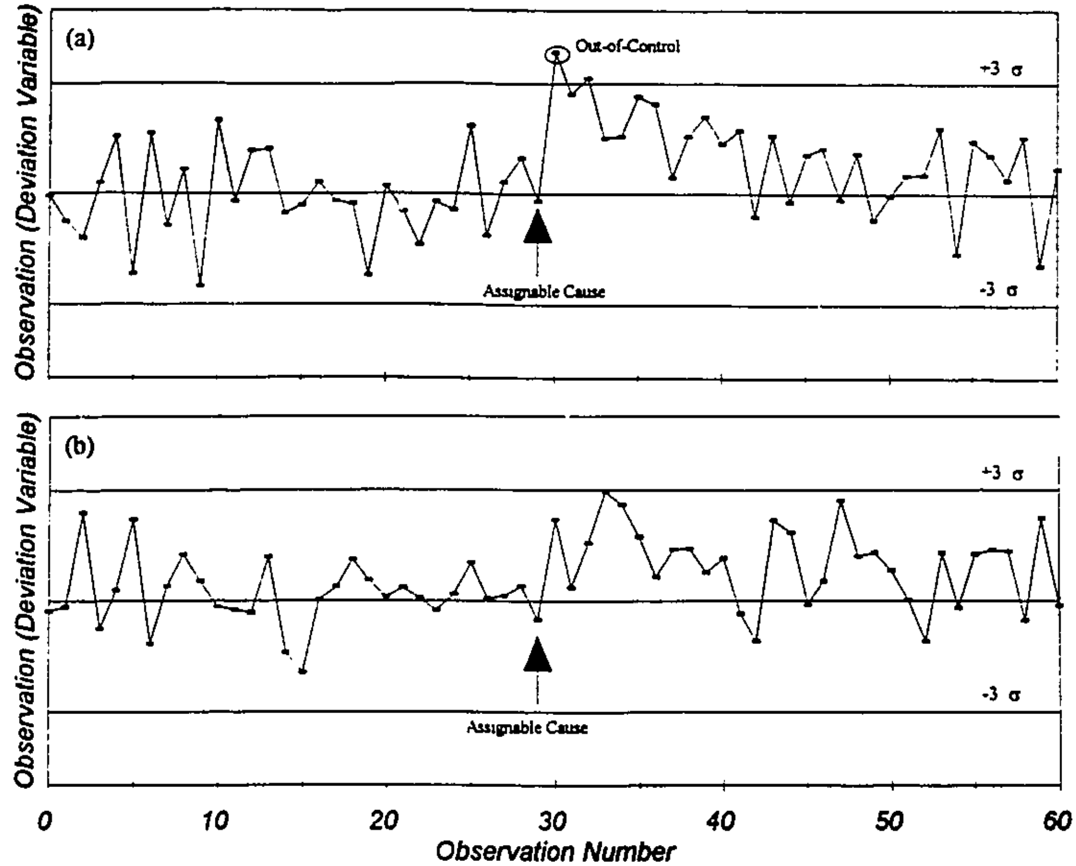


Figure 6: Plot of output deviations from target when a $3\sigma_a$ step disturbance is introduced in an IMA(1,1) when the disturbance trend is in (a) the same direction as the shift (Box and Kramer, 1992), (b) the opposite direction.

cause. The assignable cause being indicated by a point falling outside the $+3\sigma$ control limit (Figure 6a). The only difference between the two plots is the random number sets used to generate the IMA(1,1) disturbances. Therefore, figure 6b had its process upset enter when the observation was below the process mean while 6a had its introduced when the observation was above the mean. Supporting average run length data using a broader range of disturbances, would have provided more insight into potential limitations of such a charting procedure.

On the other hand, SPC has been accused of being inefficient at regulating a process (Box and Kramer, 1992). If, as Wardrop and Garcia (1992) point out, we accept SPC as a tool for process monitoring, then regulation using SPC should not be our goal. This simply means we should not ask SPC to perform a task it was not designed to do, and this is equally valid for APC. Thus, it is important to note that neither approach to process control is perfect. This provides the driving force behind the research into the integration of SPC with APC. As indicated by MacGregor (1992), it is important that one try to obtain the best of both worlds by actively controlling the process to target (APC) and then monitoring the resulting controlled process via SPC methods to identify and remove assignable cause.

2.5 Integration of SPC with APC

Although many authors have discussed the need for integration of SPC with APC (MacGregor, 1988; MacGregor, 1992; Palm, 1990), only a few (Vander Wiel et al., 1992; Box and Kramer, 1992) have actively pursued research in this area. However, much work (eg., Harris and Ross, 1991; English *et al.*, 1990) has been done in evaluating the effectiveness of traditional SPC methods when correlated measurements are encountered, which is quite often the case in the continuous processing industry. Palm (1990) provides a very good review of APC and SPC and the naive approaches that are sometimes taken in pursuit of both. He uses a fictitious example of the effect of oven temperature on the "golden-brownness" of cookies to outline how each method of process control might improve the process, APC for process regulation and SPC for process monitoring. In addition, Palm (1990) cites the work done by Vander Wiel *et al.*, which at the time was unpublished, on algorithmic statistical process control (ASPC) as a means of achieving process improvement. The important conclusion that Palm reached was that neither approach alone would have done as well without the help of the other.

The way in which MacGregor (1992) envisions obtaining the best of both worlds, SPC and APC, is by applying control charts to the manipulated variables, the reconstructed outputs, and the residuals (prediction errors). In addition to these methods he also suggests using the autocorrelation function to examine the time dependent behaviour of the process. The use of the autocorrelation function is an effective indicator of whether one's controller has been correctly tuned or if there have been any changes in the process or disturbances. The example cited by MacGregor (1992) is that of basis-weight control on a paper machine. This example shows how statistical process monitoring schemes compliment automatic process control schemes. The automatic control is effective in keeping the process output close to the target value, while the autocorrelation function and power spectrum are used to identify assignable causes, such as an alignment problem with the scanning basis weight gauge on the industrial paper machine. This example indicates the usefulness of using statistical techniques to monitor both the process and the control systems.

The paper by English and Case (1990) is a good example of a misguided attempt at the integration of SPC with APC. The authors used SPC as a feedback filter, taking control action only when an out-of-control signal was given. As stated by MacGregor (1991) control should be based on efficient control algorithms rather than simply applying a feedback compensation whenever an alarm is given by the SPC chart. If there is no cost associated with taking control action and the process is not already in a state of statistical control, then information is wasted when control action is not taken after each new observation becomes available. In addition, when an out-of-control signal was given in the examples of English and Case (1990), compensatory action was taken, but no attempt was made to identify and remove the cause of the process upset. If no attempt is made to find the cause of the process upset and subsequently remove it then process improvement is not realized and SPC does not serve its purpose.

In the continuous processing industry observations are taken over very short sampling intervals which yields observations that are usually highly autocorrelated, thus making research in the area of correlated data and SPC very relevant. Harris and Ross (1991) provided insight into the effect of serially correlated data on the performance of cumulative sum and exponentially weighted moving average charting methods. This work differs from others in the form of the model used to describe the stochastic disturbances. Harris and Ross (1991) interpreted the disturbance as a sequence of load changes on top of which is superimposed inherent variability,

$$\begin{aligned} y_t &= \eta_t + \alpha_t \\ \eta_t - \tau &= \phi(\eta_{t-1} - \tau) + a_t + \delta_{t_0}[\Delta]; \qquad -1 \le \phi \le 1 \end{aligned} \tag{16}$$

where $\{\alpha_t, a_t\}$ are each randomly and identically distributed random variables. ϕ is the autoregressive parameter, η_t is the process mean at time t, τ is the nominal value for the mean and $\delta_{t0}[\Delta]$ is a sporadically non-zero process upset. In contrast, Goldsmith and Whitfield (1971) considered a model which can be interpreted as abrupt shifts in the mean level, on top of which is superimposed a correlated inherent variability,

$$
\begin{aligned}
y_t &= \eta_t + \zeta_t \\
\zeta_t &= \phi\zeta_{t-1} + a_t
\end{aligned}
\tag{17}
$$

where a_t is a randomly and identically distributed random variable. Given observations of only y_t it is not possible to discriminate between these two models, the difference lies in the significance of the in-control average run length. For the Harris and Ross (1991) model the in-control run length, ARL(0), cannot be interpreted as the frequency of false alarms, but rather as the number of observations that pass before the stochastic process crosses the critical boundary. For the Goldsmith and Whitfield model the ARL(0) does represent the frequency of false alarms. Harris and Ross (1991) showed that, although the abilities of the EWMA and CUSUM to detect step changes in the disturbance mean are not significantly affected by the presence of correlation, the ARL(0) is very sensitive to the presence of even mild correlation.

Harris and Ross (1991) also showed that the detection of step changes using residual analysis becomes increasingly difficult as the positive correlation between observations becomes larger. Residuals are the difference between the actual value of the process variable and the predicted value, $y_t - y_{t/t-1}$. The difficulty in detecting assignable cause arises from the fact that, for a first-order autoregressive (AR(1)) process given by

$$
y_t = \phi y_{t-1} + a_t \tag{18}
$$

The size of the intervention required to produce an ultimate shift of $\Delta\sigma_y$ in the y's is $\Delta\sigma_y(1-\phi)$ (Harris and Ross, 1991). Thus, the size of the shift appearing on the chart of the residuals is significantly reduced as the magnitude of ϕ increases.

English *et al.* (1990) looked at the effect of correlated data on Shewhart charts with "corrected" limits. These "corrected" limits were calculated using the standard deviation of the observations, σ_y, such that the control limits were placed at $\pm 3\ \sigma_y$. This gave larger ARL(0)'s, but it also yielded longer detection times for real shifts. The main findings in this paper were that significantly fewer false alarms are given when the "corrected" control limits are used instead of the uncorrected limits. The uncorrected limits were based on the variance of the white noise sequence generating the AR(p) disturbance. However, in order to effectively compare the impact of correlation on SPC charts one must use a common starting point. Thus, a more effective method would be to establish control limits such that the ARL(0) is the same for all values of ϕ.

The claim made by English *et al.* (1990) that the use of residuals will allow the application of practically all of the existing SPC techniques with results equivalent to those given by the SPC model, is misleading. Although the residuals are Guassian white noise, Harris and Ross (1991) showed that the magnitude of the step disturbance in the residuals decreases as the data becomes more highly positively correlated. Thus, application of all existing SPC techniques will not yield results equivalent to those given by the SPC model.

Montgomery and Mastrangelo (1991) proposed the use of the exponentially weighted moving average test statistic, in certain situations, as a means for estimating the one-step-ahead forecast for autocorrelated processes. This is based on the fact that the EWMA is the exact one-step-ahead predictor for an IMA(1,1) model, with the optimal weighting function being $\lambda = 1\text{-}\theta$. Thus, for other members of the ARIMA family selecting values of λ which minimize the sum of the squares of the errors yields appropriate one-step-ahead model predictions. The resulting one-step-ahead prediction errors are plotted on control charts. Two problems with this approach should be immediately evident. The first is that these plots are equivalent to residual plots, which have been shown by Harris and Ross (1990) to be ineffective for large amounts of autocorrelation at identifying step shifts in the mean of the process. The second problem is due to model mismatch. If one is trying to model an AR(1) process, with say $\phi=0.5$, using the EWMA test statistic for forecasting there will be a certain amount of model mismatch. Such a mismatch will yield correlated data and therefore the calculated control limits will not be accurate. Moreover, Montgomery and Mastrangelo (1991) do not present any supporting ARL data for their conclusions, nor do they indicate the relative magnitudes of the so-called disturbances that they identify in their three examples.

Deshpande (1993) and Deshpande *et al.* (1993) have indicated three approaches to SPC monitoring of continuous processes with autocorrelated data. The first is to plot an autocorrelogram to see how the correlation reduces as sampling interval increases. From this plot a sampling interval is selected with an autocorrelation coefficient, ϕ, sufficiently small. Traditional SPC charts can then be used with this data. A potential drawback, identified by Deshpande (1993), is that the sampling interval could be too large, meaning the process could go out of control before the next sampling interval. The second approach is to model the observations with time series and apply control charts to the resulting residuals. The final approach is to utilize the EWMA test statistic as a one-step-ahead predictor, as suggested by Montgomery and Mastrangelo (1991). These last two approaches have essentially the same problem, plots of the residuals are not efficient at identifying step shifts in the mean value of the ARMA model when large positive autocorrelation exists.

Most of the work done by Box and Kramer (1992) dealt with economics and optimal sampling periods when the cost of adjustment and measurement are not negligible. This type of work is very important for the discrete item manufacturing industry, where such costs are commonly encountered. However, in the continuous processing industry where adjustments are essentially cost free, the optimal control scheme is to make adjustments as each new observation becomes available. Nevertheless, Box and Kramer (1992) did discuss the integration of SPC with APC in their discussion of the criticisms of SPC and APC. This reference to integration only employed a single example, and no ARL data were presented in support of the findings for this one example.

Vander Wiel *et al.* (1992) are probably the only group to have published research on a real process describing an attempt to integrate feedforward/feedback control while monitoring the complete system to identify and remove special causes. The terminology Vander Wiel *et al.* (1992) chose for this integration was algorithmic statistical process control (ASPC). The process used in this work was that of a batch polymerization, in which the intrinsic viscosity of the polymer was the quality variable of interest. The disturbance model was found to be an ARMA(1,1) model

$$z_t = \frac{(1-\theta B)}{(1-\phi B)} a_t \tag{19}$$

where $a_t \sim N(0,\sigma_a^2)$. The process was modelled as pure-gain with zero or one unit of dead-time

$$y_t = g(B^b X_{t-1}) \tag{20}$$

where y_t is the output viscosity deviation from target, g is the process gain constant, b is the process dead-time and X_{t-1} is the change in the manipulated variable.

The model parameters were verified by fitting a second set of test data and comparing both sets of parameters. In reviewing the model parameter estimates and the standard errors associated with each, one might question the validity of including θ, since zero was a plausible value (Table 1). The unnecessary inclusion of an extra parameter

Table 1: Table of Parameter Estimates and Standard Errors for ARMA(1,1) Model Used by Vander Wiel *et al.* (1992)

Parameters	g	ϕ	θ	σ_a
Estimates	1.087	0.859	0.164	2.798
Std. error	0.223	0.071	0.122	0.192

will result in an inflated variance for the predicted value of the disturbance, z_t. Once the model parameters were obtained, a minimum variance feedback control scheme was derived for the case with zero units of dead-time

In terms of process monitoring, Vander Wiel *et al.* (1992) chose the cumulative sum charting procedure, monitoring both the output deviation from target and the

$$X_{t-1} = \phi X_{t-2} - [\frac{(\phi-\theta)}{g}]y_{t-1} \tag{21}$$

reconstructed output as charting variables; reconstructed outputs being the value the output variable would have if no control action were taken. Since the process was modeled with an ARMA disturbance model, advantage could be taken of the offset that occurs in the output deviations from target when a step change enters the process. The offset occurs because a minimum variance controller was used, which will effectively compensate for the ARMA disturbance, but, will not correct for sporadic shifts in the level of the mean. The size of this offset is proportional to $[(1-\phi)/(1-\theta)]$, which in this case is not very large. Therefore, the disadvantage of using a minimum variance controller, when occasional shifts in mean are expected, is that from the time the step change enters until the time it is located and removed product is being made at a level other than the target (or set point). This can result in lower quality material being made, thus rendering the compensatory abilities of APC ineffective when assignable causes are present. CUSUM charts were chosen because plant personnel were already familiar with them. However, if they had not been familiar with any charting procedure, then Shewhart charts would be the charts of choice since they are easy to implement, effective and can expose types of non-randomness of a totally unexpected kind (Box and Kramer, 1992). Vander Wiel *et al.* reported that ASPC resulted in a 35% reduction in viscosity variation and virtual elimination of off-spec material. However, a breakdown of how much of the improvement was due to the introduction of SPC and how much was due to the APC was not available as both methods were introduced at the same time.

In a more recent publication Vander Wiel *et al.* (1993) use their polymerization process as a basis for a four step approach to integration of SPC with APC. The four steps presented are:

1) modelling,
2) model identification and estimation,
3) control rule design, and
4) process monitoring.

They provide a thorough evaluation of the steps required for setting up ASPC on a polymerization process. However, the schèma is not as general as might be required for achieving an integrated APC/SPC system on a process significantly different from Vander Wiel's. Although there is mention of ARIMA disturbance models, ARMA models are used throughout. The problems associated with having nonstationary disturbances present in a process are of far greater interest, since very little work (if any) has been done on process monitoring in this area. Additionally, no explanation behind the choice of monitoring variable(s) was given. The selection of an appropriate variable for process monitoring may appear trivial (i.e., choose the PQV) but, when feedback control is continually being applied to the PQV, it no longer becomes the obvious "best" choice.

One should bear in mind that the algorithmic portion of ASPC in the processing industries is well established and that the bulk of the research remains in the area of SPC. In terms of process monitoring Vander Wiel *et al.* (1993) suggested that, at the very least, one would be interested in detecting a change in the mean squared error (MSE) of the controlled variable. Such a change in the MSE would indeed be of interest.

However, as Vander Wiel *et al.* (1993) point out, how exactly to best conduct process monitoring remains largely an open question. Many suggestions have been made as to what should be monitored in a process, but very little has been done to identify the feasibility of these approaches.

2.6 Summary

One can see that many authors have talked about what should be done to integrate SPC with APC, however, very little has been done experimentally or through simulations, to verify the benefits of integration. It is clear from the work done by Vander Wiel *et al.* (1992 and 1993)), MacGregor (1988) and others that integration of SPC with APC is a highly desirable goal. Nevertheless, there are still many questions that have been left unanswered. Which process variable should be used to monitor the process? Can nonstationary processes be monitored effectively? Do minimum variance controllers have to be used?

Thus, in terms of the layout of this project, it will begin with an investigation into which of the process variables can effectively be monitored, for both stationary and nonstationary process data, on traditional SPC charts. This will provide a better understanding of which variables are the best to monitor, under which circumstances and why. Next the unique problems encountered when dealing with nonstationary data are investigated. Finally, everything is tied together through the use of an industrial example. In this example a six-step procedure is established to set up an integrated system of SPC and APC on a new or existing process. This example provides a feel for the magnitude of such an undertaking, the difficulties that are inevitably encountered and the amount of improvement that is possible once such a scheme has been implemented.

Chapter 3

THEORY AND METHODOLOGY

In this chapter, the methodology involved in the selection of charting variables for first-order processes with minimum variance controllers, subject to ARIMA(1,1,1) or ARMA(1,1) disturbances is presented. The theory and methodology underlying the n^{th}-difference charts is also presented. Then two generalized minimum variance controllers are derived in section 3.3. The first controller is for the case of an ARMA(1,1) disturbance perturbing either a pure-gain or first-order plus dead-time process. The second case involves a situation were either a PG or first-order process is subject to an ARIMA(1,1,1) disturbance. Finally, in section 3.4 the simulation software is discussed.

3.1 Selection of Charting Variables

One of the greatest problems encountered in trying to decide which of the process variables is the most efficient at detecting assignable cause is that measurement noise does not allow one to see how well the disturbance propagates to the process monitoring variables. However, one can observe how a shift propagates using simulations. The time series models used to describe process disturbances in the CPI industry are comprised of a deterministic (predictable) component and a stochastic (random) component. An example is the first-order autoregressive moving average or ARMA (1,1) model,

$$z_t = \phi z_{t-1} + a_t - \theta a_{t-1} \tag{22}$$

where the term $a_t - \theta a_{t-1}$ comprises the stochastic component and ϕz_{t-1} is the deterministic component. If we remove the stochastic component and focus on the deterministic component of the disturbance we will be able to see what effect a step change in the mean value of the disturbance has on the process variables that have been suggested for charting. Simultaneously, we can investigate the effect of the random component, or noise, on each of the process variables, since this will also affect our choice of charting variable. The more noise associated with a process variable, due to the random component, the less attractive it becomes for charting. The perfect charting variable would be stationary, have very little noise, while at the same time be able to show the full magnitude of a shift in the mean of the process disturbance. Figure 7 shows how a $1\sigma_a$ step shift in the mean value of an ARMA(1,1) disturbance propagates to the manipulated variable of a first-order process subject to MV feedback control, with and without the random component of the disturbance. Clearly, for this example, the manipulated variable would be an appropriate charting variable since the data is stationary, does not have a significant amount of noise and the size of the shift is about 60% of that occurring in the disturbance. Control limits are not indicated on the plot shown in Figure 7 because the purpose of this section of work is to indicate the relative size of the disturbance noise to the shift size.

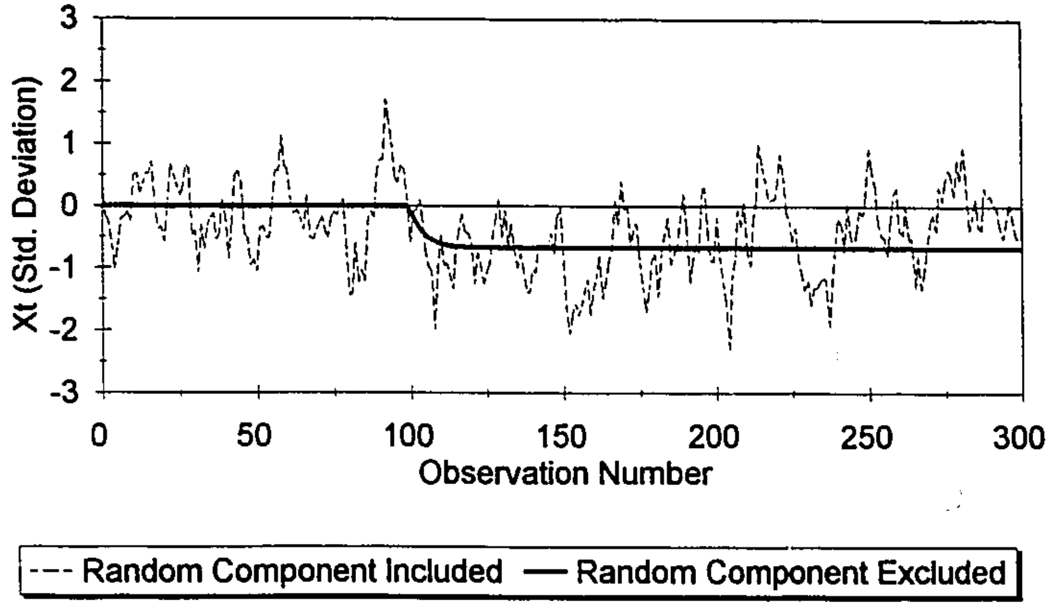


Figure 7: Plots of the manipulated variable of a first-order process subject to minimum variance feedback control and perturbed by an ARMA(1,1) disturbance with a $1\sigma_a$ step shift introduced at observation 100, with and without the random component.

The method described above for the selection of charting variables is important since it allows us to determine why certain types of disturbances, when charted in the traditional fashion, do not permit the identification of assignable cause. This is a critical step because it enables one to identify the limitations of a particular process so that changes can be implemented to yield a more capable process or compensation, such as appropriately scaling the control limits to allow for faster identification of assignable cause, can be made. Obviously, if no suitable charting variables are available then fundamental changes must be made to the process before successful integration can be achieved.

3.2 N^{th}-Difference Charts

For nonstationary disturbances, the greatest weakness in trying to identify assignable cause is the transformation needed to yield stationary, chartable data. These transformations only allow the process shifts to be observable on control charts over one or two time periods. This is usually not long enough for identification and raises the question whether there is an alternative method to transform nonstationary data into stationary data while at the same time improving the probability of identifying an assignable cause. N^{th}-difference charts were proposed and developed in this work in an attempt to integrate SPC with APC when nonstationary disturbances are present. The n^{th}-difference charts are very similar to the differencing method referred to in Chapter 2 as a means of transforming nonstationary data. The chances of identifying assignable cause in nonstationary processes would be greatly improved if the transformation method allowed the assignable cause to appear on the charts for a longer period of time. One way to do this is to difference the data over a longer time period. Rather than differencing successive observations, data is differenced over 5, 10 or more time intervals. Using the observations of the manipulated variable for a first-order process subject to an IMA(1,1) disturbance model, shown in Figure 8a, one can see how taking the 10^{th}-difference results in stationary, chartable data (Figure 8b) as does the first-difference (Figure 8c). However, the shift (magnitude $1\sigma_a$) introduced at observation 100 (Figures 8a, b and c) shows that 10^{th}-differencing allows the assignable cause to appear on the chart for a longer period of time than the first-difference. Additionally one can note that, although the control limits for the 10^{th}-difference chart are wider than those

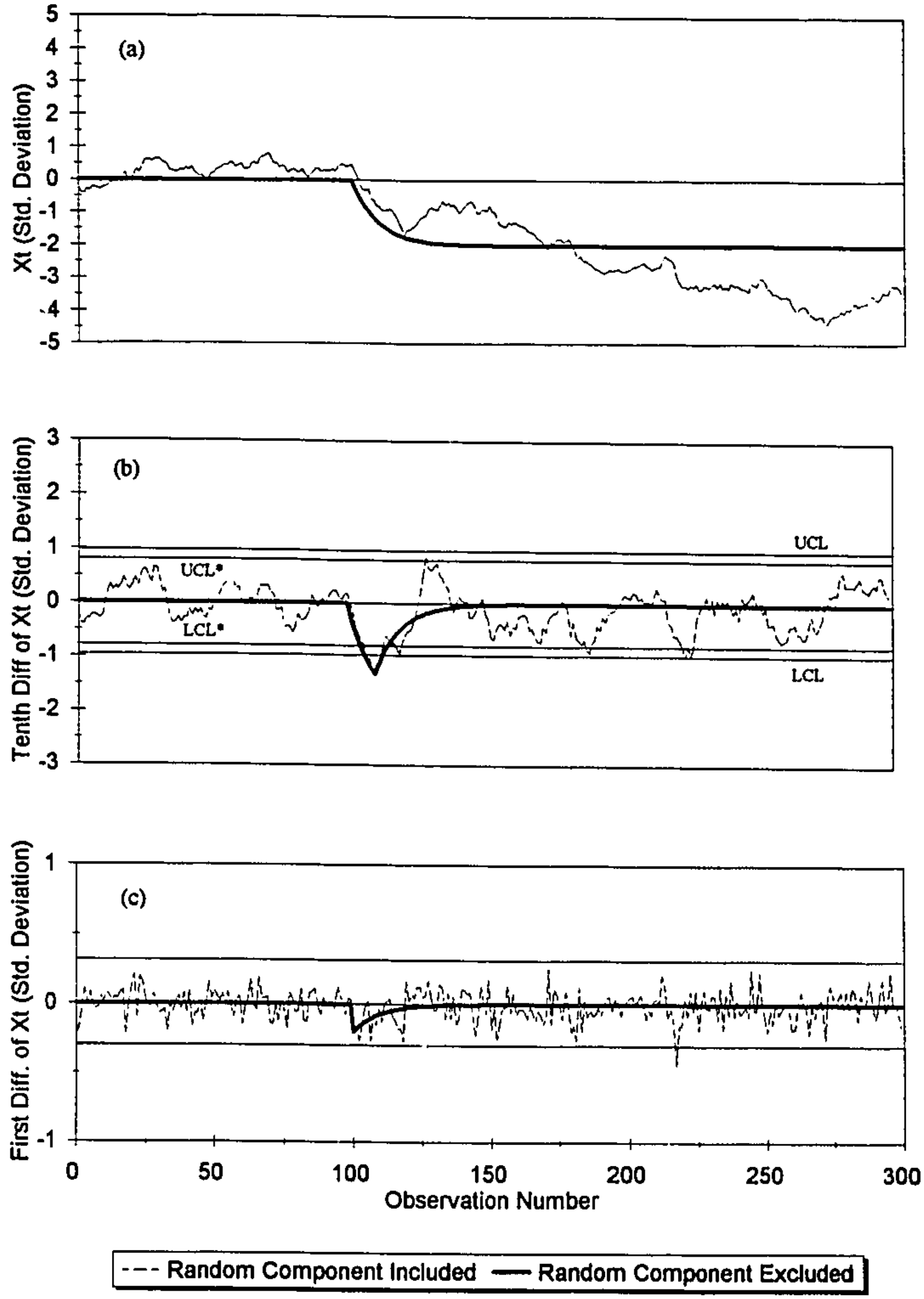


Figure 8: (a) The manipulated variable for a simulated process, subject to an IMA(1,1) disturbance, θ=0.9 and δ=0.0 (b) the 10^{th}-difference of the manipulated variable (c) the first difference of the manipulated variable, each with their corresponding underlying shifts when a $2\sigma_a$ shift in the mean value of the disturbance occurs.

for the first-difference chart, the ratio of the underlying shift to the control limit width is significantly greater for the 10^{th}-difference chart. Both of these properties in the 10^{th}-difference chart allows for shorter detection times when an assignable cause enters the process.

The control limits (CL) for n^{th}-difference charts can be established analytically, using the variance of the charting variable (Appendix A), or through the use of simulations. Simulations allow CL to be adjusted to yield predetermined in-control run lengths. An ARL(0)=370.4 is commonly used as it corresponds to the in-control run length of a process following the SPC model with $\pm 3\sigma_a$ control limits. Control limits arrived at through simulations are done by trial and error. The CL are estimated and then the simulation is run, a good initial estimate is the analytically determined limits. Depending on whether the ARL(0) is higher or lower than desired, the next set of CL are chosen to compensate. This procedure is repeated until an appropriate ARL(0) is obtained. Analytically determined control limits, although simpler to obtain, allow for less flexibility.

Appendix A shows the derivation of the 5^{th}-difference variance of the manipulated variable for the above mentioned process. The upper and lower control limits (UCL and LCL) determined analytically and through simulations (UCL^* and LCL^*) are both displayed on Figure 8b. The analytically determined CL would yield ARL(0)s longer than 370.4 and thus would also give longer detection times when an assignable cause is present. This point is supported by the work done by English and Case (1990) on charting correlated data. Even though the paper by English and Case (1990) did not deal with differenced data, the similarity of the correlation structure between data generated by an AR(1) model and n^{th}-differenced data allows similar conclusions to be drawn.

3.3 Generalized Derivation of Minimum Variance Controllers

A general evaluation of MV controllers in quality improvement applications was not found in the literature. In order to implement such a controller in a simulation program it would be much more useful if general MV controllers could be derived and used for a wider range of process dynamics and disturbances. Thus, two controllers will be explicitly derived, the first will be for the case of an ARMA(1,1) disturbance perturbing either a PG or FOPDT process. The second will be able to control either a PG or first-order process subject to an ARIMA (1,1,1) disturbance.

Comparing equations 7 and 8 one can see that a PG process is obtained by setting b=0 and δ=0 in equation 8. Thus, we use equation 8 to describe the process dynamics in our general derivation. For the FOPDT process

$$y_{t+b+1} = \frac{\omega_0}{(1-\delta B)} X_t + z_{t+b+1}. \tag{23}$$

We can see that the effect of the disturbance, z_{t+b+1}, will be exactly eliminated if we set y_{t+b+1} to zero. The necessary control action to achieve this would be

$$X_t = -\frac{(1-\delta B)}{\omega_0} z_{t+b+1}. \tag{24}$$

However, this control action is not realizable since it would require knowledge of a future value of the disturbance. Box and Jenkins (1970) showed that by substituting the b+1 step ahead forecast of the disturbance for z_{t+b+1}, the minimum variance of output deviations from set point is obtained. Thus, the appropriate control action becomes,

$$X_t = -\frac{(1-\delta B)}{\omega_0}\hat{z}_{t+b+1/t} \tag{25}$$

where $z_{t+b+1/t}$ is the b+1 step ahead forecast of the disturbance and is determined by taking the conditional expectation given the information up to time,t, given by

$$\hat{z}_{t+b+1/t} = E[z_{t+b+1}|z_t,\ z_{t-1}, \ldots, a_t,\ a_{t-1}, \ldots]\,. \tag{26}$$

Expanding equation 6, with d=0, at time, t+b+1, we have

$$z_{t+b+1} = \phi z_{t+b} + a_{t+b+1} - \theta a_{t+b}. \tag{27}$$

Taking the conditional expectation of both sides of equation 27 gives

$$\begin{aligned}\hat{z}_{t+b+1/t} &= \phi E[z_{t+b}] + E[a_{t+b+1}] - \theta E[a_{t+b}] \\ &= \phi \hat{z}_{t+b/t}\end{aligned} \tag{28}$$

since the expected values of future a_t's are equal to the mean, $\mu = 0$. Again, taking the conditional expectation of both sides of the previous equation gives

$$\begin{aligned}\hat{z}_{t+b+1/t} &= \phi\{\phi E[z_{t+b-1}] + E[a_{t+b}] - \theta E[a_{t+b-1}]\} \\ &= \phi^2 \hat{z}_{t+b-1/t}.\end{aligned} \tag{29}$$

We continue in this way until we no longer have forecasted values on the right hand side of equation 29, which yields

$$\hat{z}_{t+b+1/t} = \phi^b[\phi z_t - \theta a_t]\,. \tag{30}$$

Substituting equation 30 into equation 25 yields the minimum variance control action

$$X_t = -\frac{(1-\delta B)\phi^b}{\omega_0}[\phi z_t - \theta a_t]\,. \tag{31}$$

Substituting equation 6, b=0, into equation 31 for z_t yields

$$X_t = -\frac{(1-\delta B)\phi^b}{\omega_0}[\ \phi\frac{(1-\theta B)}{(1-\phi B)}a_t - \theta a_t\ ]\,. \tag{32}$$

Multiplying both sides of equation 32 by (1- ϕB) and expanding gives

$$X_t-\phi X_{t-1} = -\frac{\phi^b}{\omega_0}\{\phi[a_t-(\delta+\theta)a_{t-1}+\delta\theta a_{t-2}]-\theta[a_t-(\phi+\delta)a_{t-1}+\phi\delta a_{t-2}]\}\,. \tag{33}$$

Rearranging and simplifying gives

$$X_t - \phi X_{t-1} = -\frac{\phi^b(\phi-\theta)}{\omega_0}[1 - \delta B]\,a_t. \tag{34}$$

Equation 34 is the MV controller, in terms of a_t 's, for a PG or FOPDT process subject to an ARMA(1,1) disturbance. However, one cannot measure the values of the random noise, a_t, generating the ARMA disturbance. Thus, another variable is required, one that is readily measurable, to substitute for a_t. Many authors (e.g., MacGregor, 1988; Harris, 1987) have shown for the case when there is no dead time that, by substituting equations 31 and 27 into equation 23, $y_t = a_t$. However, the more general case for any dead time is of greater interest. Thus, substituting equation 31 into equation 23, gives

$$y_{t+b+1} = -\phi^b(\phi z_t - \theta a_t) + z_{t+b+1}. \tag{35}$$

Substituting the expanded form of equation 27 for z_{t+b+1} ,

$$z_{t+b+1} = \phi^{b+1} z_t - \theta\phi^b a_t + \{1 + (\phi-\theta)\,[B+\phi B^2+\phi^2 B^3+ \ldots +\phi^{b-1} B^b]\}\, a_{t+b+1} \tag{36}$$

into equation 35 gives

$$y_{t+b+1} = \{1 + (\phi-\theta)\,[B+\phi B^2+\phi^2 B^3+ \ldots +\phi^{b-1} B^b]\}\, a_{t+b+1}. \tag{37}$$

Thus using equation 37 to substitute for a_t in equation 34 yields

$$X_t - \phi X_{t-1} = \frac{\phi^b(\phi - \theta)(1 - \delta B) y_t}{\omega_0\{1 + (\phi-\theta)\,[B+\phi B^2+\phi^2 B^3+ \ldots +\phi^{b-1} B^b]\}}. \tag{38}$$

Multiplying both sides by $\{1+(\phi-\theta)[B+\phi B^2+\phi^2 B^3+ \ldots +\phi^{b-1} B^b]\}$and simplifying yields the general form of the MV controller in terms of output deviations from target and previous control actions,

$$X_t = \theta X_{t-1} + (\phi-\theta)\phi^b X_{t-b-1} - \frac{\phi^b(\phi-\theta)}{\omega_0}[y_t - \delta y_{t-1}]. \tag{39}$$

One can see that, if b=0, the control action shown in equation 34 with y_t substituted for a_t is obtained.

In a similar manner a MV controller for a process being perturbed by an ARIMA(1,1,1) disturbance can be derived. Since the case with dead time is not of interest, the process dynamics are now represented as

$$y_{t+1} = \frac{\omega_0}{(1-\delta B)} X_t + z_{t+1}. \tag{40}$$

One can minimize the variance of the controlled variable deviations from set point by setting y_{t+1} to zero, yielding the following control action

$$X_t = -\frac{(1-\delta B)}{\omega_0} z_{t+1}. \tag{41}$$

Again, this control action is not realizable, because it requires a future value of the disturbance. Therefore, z_{t+1} must be replaced by the one step ahead prediction of the disturbance yielding

$$X_t = -\frac{(1-\delta B)}{\omega_0} \hat{z}_{t+1/t}. \tag{42}$$

Using equation 6 and expanding we obtain

$$z_{t+1} = (1+\phi) z_t - \phi z_{t-1} + a_{t+1} - \theta a_t. \tag{43}$$

Taking the conditional expectation of both sides of equation 43 gives

$$\begin{aligned} \hat{z}_{t+1/t} &= (1+\phi) E[z_t] - \phi E[z_{t-1}] + 0 - \theta a_t \\ &= (1+\phi) z_t - \phi z_{t-1} - \theta a_t. \end{aligned} \tag{44}$$

Substituting equation 44 into equation 42 yields

$$X_t = -\frac{(1-\delta B)}{\omega_0} \{ (1+\phi) z_t - \phi z_{t-1} - \theta a_t \}. \tag{45}$$

Using equation 6 to substitute for z_t and z_{t-1} in equation 45 gives

$$X_t = -\frac{(1-\delta B)}{\omega_0} \{ (1+\phi) \frac{(1-\theta B)}{\nabla(1-\phi B)} a_t - \phi \frac{(1-\theta B)}{\nabla(1-\phi B)} a_{t-1} - \theta a_t \}. \tag{46}$$

Multiplying both sides by $\nabla(1-\phi B)$ and expanding yields

$$\nabla(1-\phi B)X_t = -\frac{1}{\omega_0}\{(1+\phi)[1-(\delta+\theta)B+\delta\theta B^2]\ a_t - \phi[1-(\delta+\theta)B \quad \textbf{(47)}$$
$$+\delta\theta B^2]\ a_{t-1} - \theta[1-(1+\delta+\phi)B+(\delta+\delta\phi+\phi)B^2-\delta\phi B^3]\ a_t\}.$$

Grouping similar terms and simplifying gives

$$X_t = (1+\phi)X_{t-1}-\phi X_{t-2}-\frac{1}{\omega_0}\{(1+\phi-\theta)a_t+(\delta\theta-\phi-\delta-\phi\delta)a_{t-1}+\phi\delta a_{t-2}\}. \quad \textbf{(48)}$$

By substituting equations 45 and 43 into equation 40 it can be shown that $y_t = a_t$, which when substituted into equation 48 finally gives the MV controller

$$X_t = (1+\phi)X_{t-1}-\phi X_{t-2}-\frac{1}{\omega_0}\{(1+\phi-\theta)y_t+(\delta\theta-\phi-\delta-\phi\delta)y_{t-1}+\phi\delta y_{t-2}\}. \quad \textbf{(49)}$$

When one looks at the complexity of this problem, one is surprised to see that the MV control action is simply a function of two previous control actions and three values of the output deviations.

Equations 39 and 49 will be used throughout the study of the integration of SPC and APC.

3.4 Simulations

All of the simulations were carried out using SPCSIM software developed by the author. The software was written in FORTRAN and is able to simulate FOPDT processes subject to ARMA(1,1) disturbances or first-order processes subject to ARIMA(1,1,1) disturbances. Pseudo-random numbers, from a Normal distribution, were generated using the IMSL subroutine RNNOA and were passed through suitable filters (ie., equation 6) to yield the stochastic disturbance models. Both cases implement minimum variance feedback control; PID control is also available, however, tuning is required. All three traditional methods of statistical process control charting (Shewhart, EWMA and CUSUM) are available for process monitoring, in addition to the n^{th}-difference charting procedure. A listing of the software code along with a typical input file are found in Appendix B.

The simulation software was utilized to obtain average run length (ARL) data for the processes investigated. Average run lengths are the number of observations of the monitored variable that pass, on average, before an out-of-control signal is given. The average run lengths were calculated based on 4000 simulated experiments. This number of simulations was sufficient to provide an accurate and precise value for the ARL (Slocomb, 1991). Assignable causes introduced into the simulated processes consisted of step shifts in the mean value of the disturbance. The sizes of these step shifts, expressed in terms of the standard deviation of the white noise generating the disturbance, were $1\sigma_a$, $2\sigma_a$ and $3\sigma_a$ which in traditional SPC environments are the magnitudes generally of interest.

The software was developed initially to determine the effectiveness of the n^{th}-difference charting procedure for identifying assignable cause in nonstationary disturbances. The disturbance model chosen for the initial tests was an IMA(1,1), since it was suggested by MacGregor (1988) that this type of disturbance is prevalent in SPC environments. The two process variables in an integrated system available for differencing are the manipulated variable and disturbance. Thus, the first task was to determine which of the two variables, if any, was better for process monitoring. Once this was accomplished, an evaluation of the effectiveness of this charting procedure at varying levels of differencing was carried out. Upon completion of these simulations other nonstationary disturbances, such as ARIMA(1,1,0) and ARIMA(1,1,1), were investigated.

A Quattro spreadsheet was utilized to demonstrate graphically how assignable causes propagated to the potential charting variables (see Appendix C). The required random numbers were generated using the SPCSIM software. The spreadsheet allowed the use of a first-order dynamic model and a choice between ARMA(1,1) and ARIMA(1,1,1) disturbance models. Minimum variance controllers were utilized. The available charting variables were the manipulated variable, the deviation from target of the controlled variable and the reconstructed output.

Chapter 4

RESULTS AND DISCUSSION

Chapter 4 consists of the presentation and discussion of the results obtained for this work. The first results are those obtained from the study on selection of charting variables. This discussion is broken down further based on the type of disturbance model affecting the process, ARMA(1,1) or ARIMA(1,1,1). In the following section the results for the n^{th}-difference charting procedure are presented, first for processes subject to IMA(1,1) disturbances and then for ARIMA(1,1,1) disturbances. In the last section, results from the study of the effect of sampling interval on disturbance detection in ARMA(1,1) models are presented and evaluated.

4.1 Disturbance Propagation

The purpose of this section is to outline qualitatively how one chooses a process monitoring variable for an integrated system of control. When minimum variance control is employed, only three variables are available for process monitoring: the reconstructed output (i.e., the value the output variable would take if no automatic control was taken), the manipulated variable and the deviation of the controlled variable from target (i.e., the residual). Therefore, these three variables are plotted against time along with the underlying deterministic shift that results when a shift in the mean value of the disturbance of size $\Delta = 1\sigma_a$ occurs (Figures 9-22). Many different combinations of parameter values (ϕ, θ and δ) were used to determine the effect of the disturbance model on the potential charting variables. The results for the stationary, ARMA(1,1) disturbance are presented and discussed first, then the nonstationary, ARIMA(1,1,1) disturbance is addressed. For both cases a first-order model was used for the process dynamics and the required MV controllers were those derived in Section 3.3.

4.1.1 First Order ARMA Disturbance Models The reconstructed outputs are shown in Figures 9 and 10 for $\theta = 0.6$, $\phi = 0.3$ and $\theta = 0.3$, $\phi = 0.6$, respectively. One can see that the larger the value of the autoregressive parameter, ϕ, the further the data drifts temporarily from the mean (i.e., the more positively correlated the data becomes). This results in either wider control limits or shorter in-control run lengths, ARL(0)s, as compared to those obtained for the SPC model. Thus, it would be expected that the effectiveness of this variable for process monitoring decreases as ϕ increases and θ decreases (ie., as positive correlation increases) due to the widening of the control limits required to accommodate the drift in the data. It is also quite apparent that the full effect of the deterministic disturbance is felt in the reconstructed output. Additionally, the reconstructed output is not affected by process inertia, δ. This is as expected since the reconstructed output is equivalent to the disturbance, whose equation (equation 6) does not contain the term for process inertia.

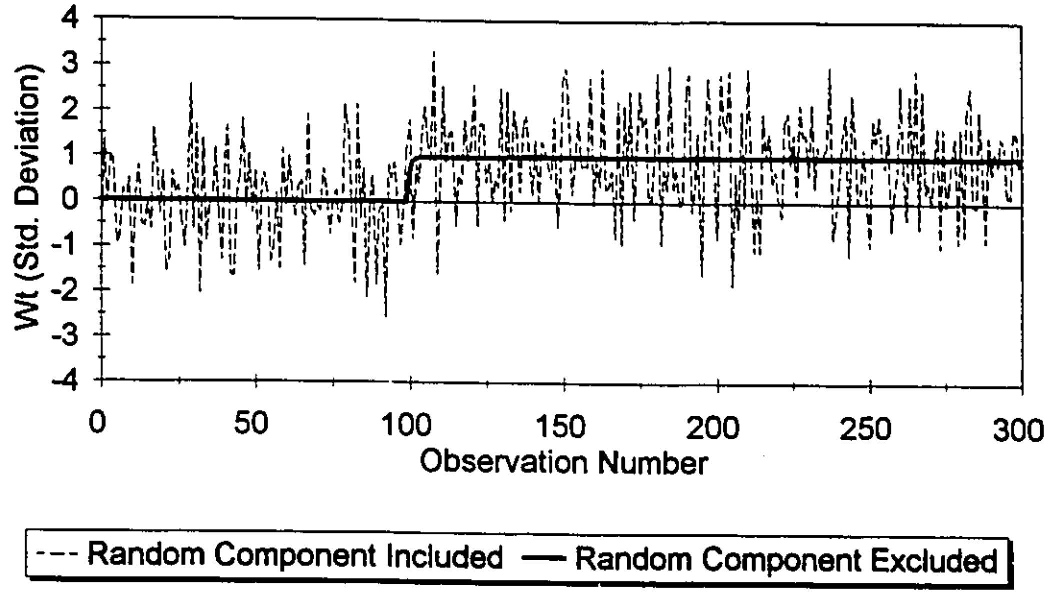


Figure 9: Reconstructed output and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARMA(1,1) disturbance, $\theta=0.6$ and $\phi=0.3$.

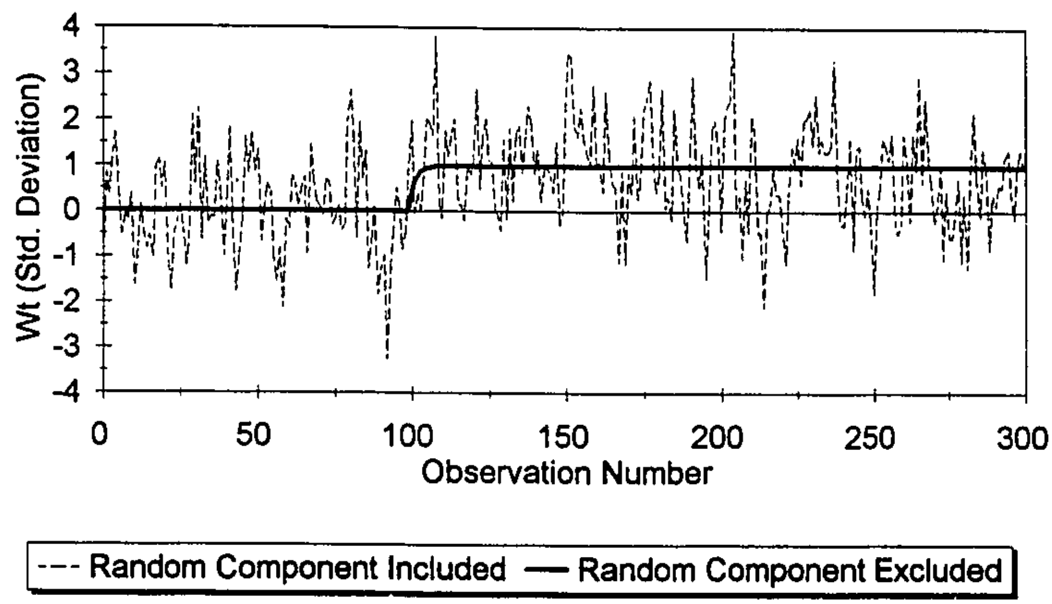


Figure 10: Reconstructed output and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARMA(1,1) disturbance, $\theta=0.3$ and $\phi=0.6$.

The effectiveness of the manipulated variable as a charting variable depends not only on the values of the moving average and autoregressive parameters but also on the process inertia, δ. Figures 11 and 12 show that as δ is increased from 0.3 to 0.8 the variability of the manipulated variable almost doubles. Therefore, although the $1\sigma_a$ shift in the disturbance mean propagates identically in both cases, the size of the disturbance no longer appears significant when $\delta = 0.8$. Thus, for processes with large amounts of process inertia (i.e., large time constants) the manipulated variable is not an effective charting variable. It is also interesting to note that the manipulated variable performs better than the reconstructed output when δ is small. Table 2 shows the ARL results for a process subject to an ARMA(1,1) disturbance (ϕ=0.3 and θ=0.6) with δ=0.3 and 0.8.

Table 2: Comparison of ARL($3\sigma_a$), using Shewhart charts, for the reconstructed output and manipulated variable for two different values of process inertia, δ.

δ	**Reconstructed Output, W_t**	**Manipulated Variable, x_t**
0.3	2.27	1.34
0.8	2.27	14.34

With regards to the deviation from target of the controlled variable (CV) or equivalently the residuals, none of the parameters have an affect as long as the process is following its stable common cause model. However, once an assignable cause enters, the response of the controlled variable differs markedly depending on the values of θ and

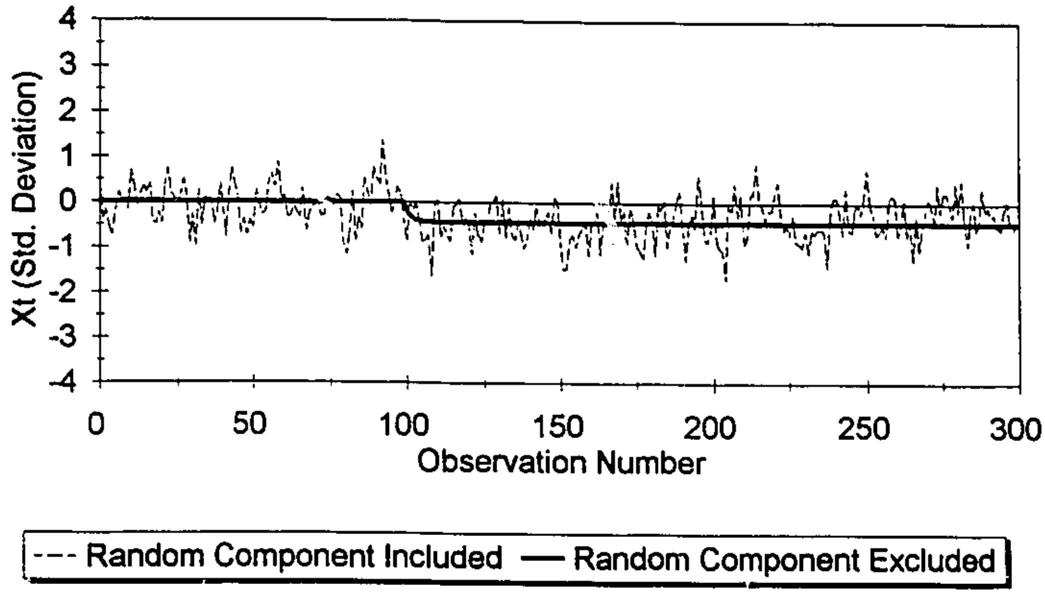


Figure 11: Manipulated variable and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARMA(1,1) disturbance, $\theta=0.3$, $\phi=0.6$ and $\delta=0.3$.

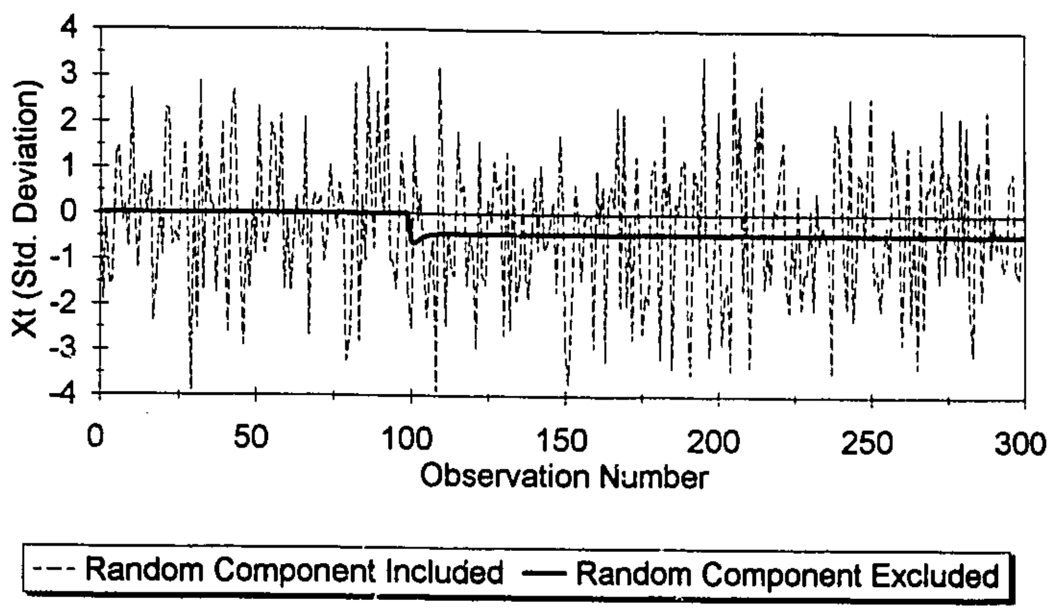


Figure 12: Manipulated variable and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARMA(1,1) disturbance, $\theta=0.3$, $\phi=0.6$ and $\delta=0.8$.

ϕ. Figure 13 shows that, when θ is larger than ϕ, the shift in the CV becomes larger than the original shift in the disturbance, that is the shift is magnified. However, when ϕ is greater than θ the shift in the CV becomes smaller than the original shift in the mean value of the disturbance (Figure 14). This shift, or offset, in the controlled variable, resulting from step shifts in the mean of the disturbance, may appear as a good indicator of when an assignable cause has entered the process. However, since this is the controlled variable one should be concerned with an offset. An offset in the controlled variable indicates that the automatic control algorithm is not performing as it should. If such deterministic shifts in the mean of the disturbance are expected on a regular basis, then the control algorithm should be designed to compensate for them. Once a control algorithm has been designed to compensate for the periodic shifts in the mean of the disturbance then the residuals can be used to show the offset (i.e., indicate assignable cause).

In terms of choosing a charting variable(s) for processes subject to ARMA(1,1) disturbances, the choice is highly dependant on the parameter values. When the moving average parameter, θ, exceeds the autoregressive parameter, ϕ, residuals should be utilized for process monitoring. When the AR parameter is greater than the MA parameter and there is a large process inertia then the reconstructed outputs should be utilized. Otherwise the manipulated variable should be used.

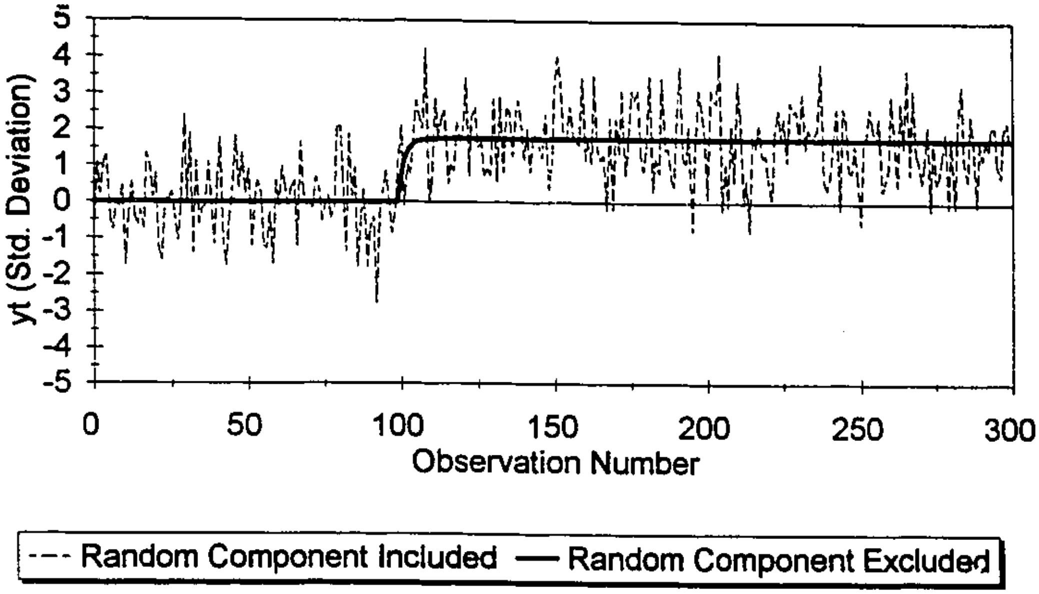


Figure 13: Residuals and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARMA(1,1) disturbance, $\theta=0.6$ and $\phi=0.3$.

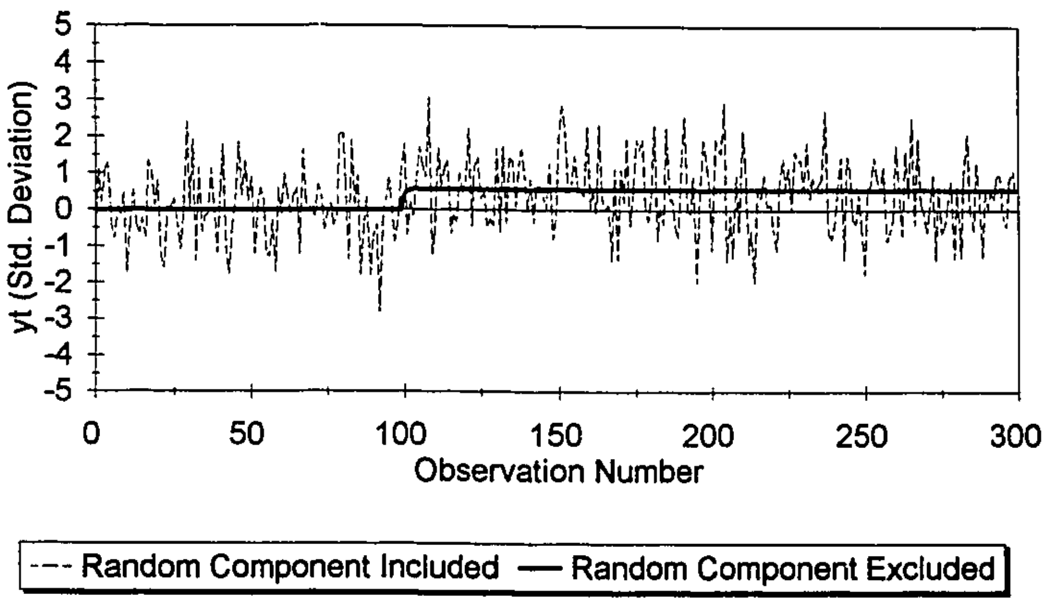


Figure 14: Residuals and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARMA(1,1) disturbance, $\theta=0.3$ and $\phi=0.6$.

4.1.2 First Order ARIMA Disturbance Models As mentioned previously, nonstationary data cannot be plotted on traditional SPC charts without first being transformed into stationary data. However, it is worth plotting the nonstationary data along with the underlying shift resulting from a step change in the mean value of the disturbance to determine the relative magnitude of the process variable drift to the underlying shift. In doing this one is able to identify whether data transformations will yield effective charting variables or whether the nonstationarity should be investigated for the purpose of removing its cause. Nonstationary data, generated using ARIMA(1,1,1) disturbance models, for several different combinations of parameter values were plotted (Figures 15-22) to acquire a good sense of the "extent of nonstationarity" in the data.

The reconstructed outputs for several combinations of parameter values are shown in Figures 15, 16 and 17. These Figures are displayed in order of increasing nonstationarity. Figure 15, $\theta=0.8$ and $\phi=0.3$, shows that the size of the underlying shift is about 20% of the process drift. For Figure 16, $\theta=0.5$ and $\phi=0.8$, and Figure 17, $\theta=0.0$ and $\phi=0.8$, the shifts are about 4% and 2% of the process drift, respectively. One can see that as ϕ increases and θ decreases the data drifts further from its nominal value; hence, the smaller the relative magnitude of the underlying shift. This is exemplified in Figure 17 as one can see that the process drifts more than 50 units between time 270 and 300. In comparison, over the same time period, a $3\sigma_a$ step shift in the mean value of the disturbance will only shift this process by 3 units. In practice, if such a nonstationary disturbance is encountered, the integrity of the process should be questioned. Such a disturbance is indicative of a process that is already under the influence of one or several assignable causes and an effort should be made to remove these causes before evaluating the process further. If, on the other hand, a disturbance with a large value of θ and a small ϕ is representative of the process and one is willing to accept a nonstationary disturbance then it will be shown in Section 4.2 that the n^{th}-difference charts could be implemented for charting purposes.

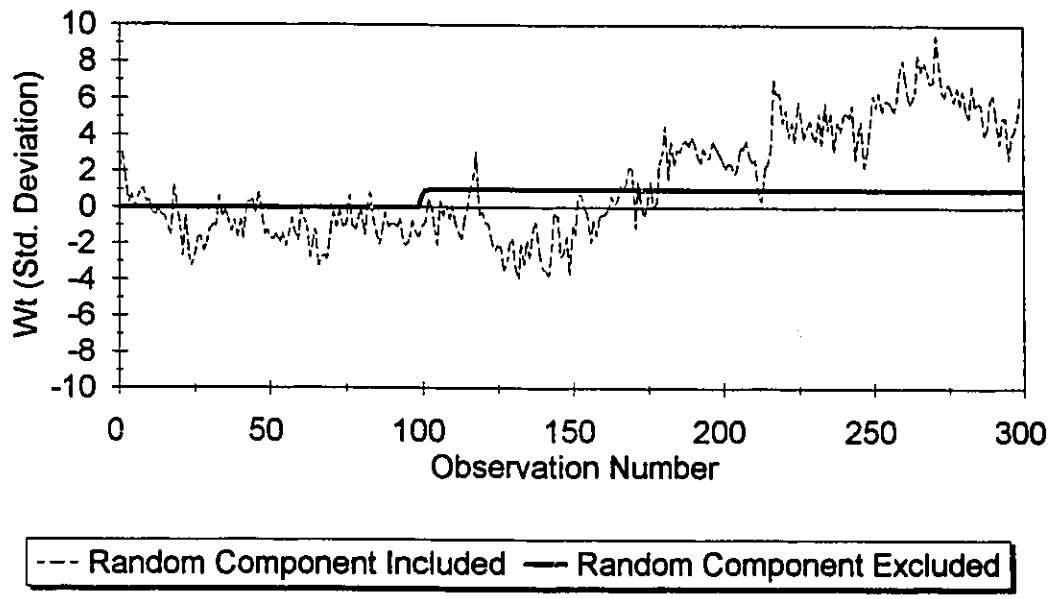


Figure 15: Reconstructed output and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARIMA(1,1,1) disturbance, θ=0.8 and ϕ=0.3.

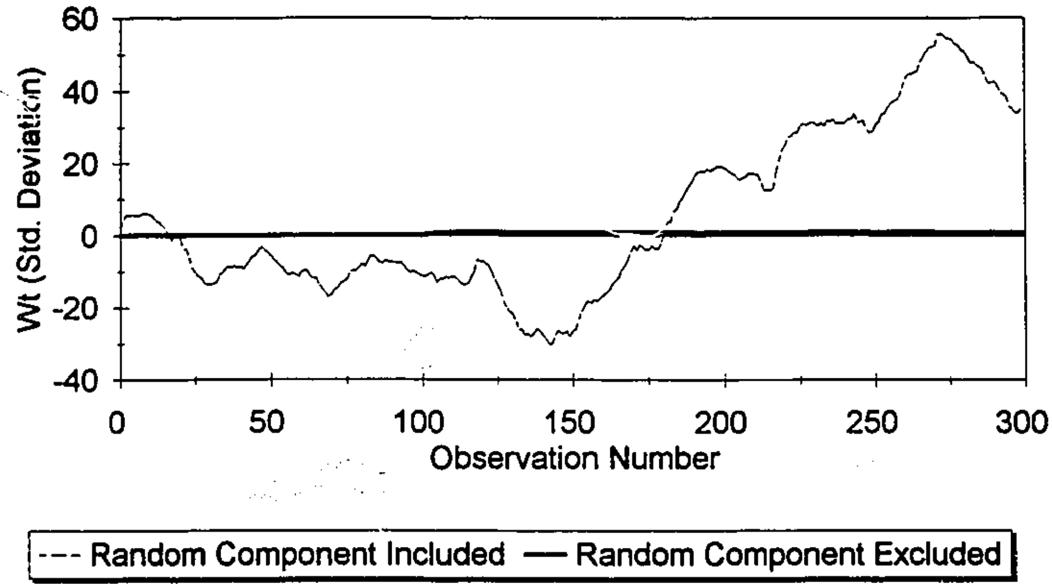


Figure 16: Reconstructed output and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARIMA(1,1,1) disturbance, $\theta=0.5$ and $\phi=0.8$.

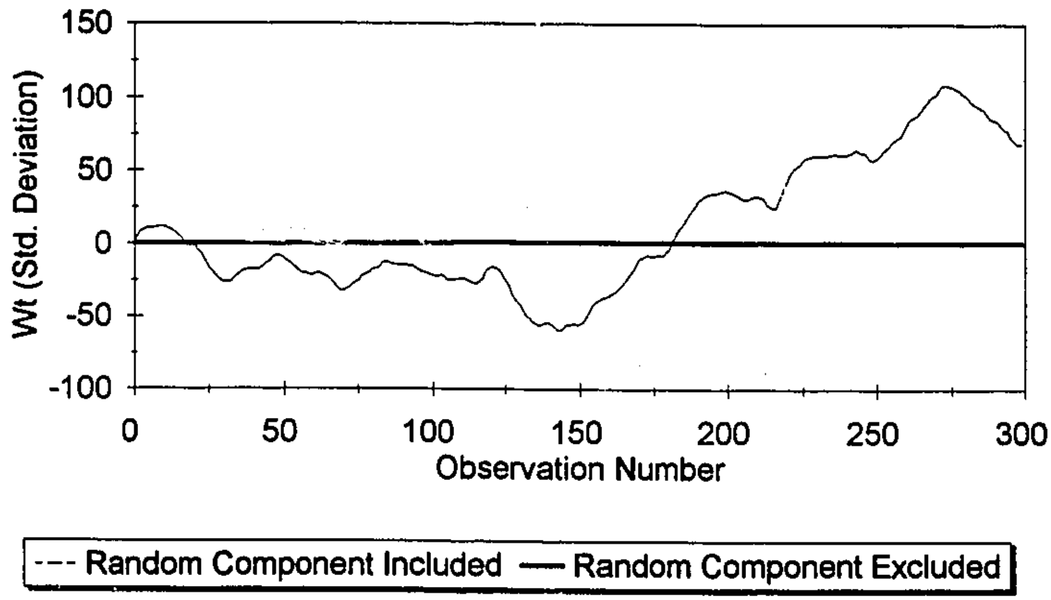


Figure 17: Reconstructed output and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARIMA(1,1,0) disturbance, $\theta=0.0$ and $\phi=0.8$.

Similar comments to those made for the reconstructed outputs can be made for the manipulated variable (Figures 18, 19 and 20). Comparing Figures 18 and 19 one can see that as ϕ increases and θ decreases the degree of nonstationarity increases. A comparison between Figures 18 and 20 shows that as the process inertia, δ, increases so does the amount of manipulation required to control the process output. Although the trend in the process data is the same in both cases, the variability from point to point is greater when δ is large. Thus, an additional point, concerning the manipulated variable, is that it can drift further from its nominal value than the reconstructed output when δ is sufficiently large. An obvious drawback to having the manipulated variable drift considerably from its nominal value is that the physical limitations of the final control element may be exceeded, that is, the manipulated variable will be regularly saturated. If this occurs, effective automatic process control is sacrificed.

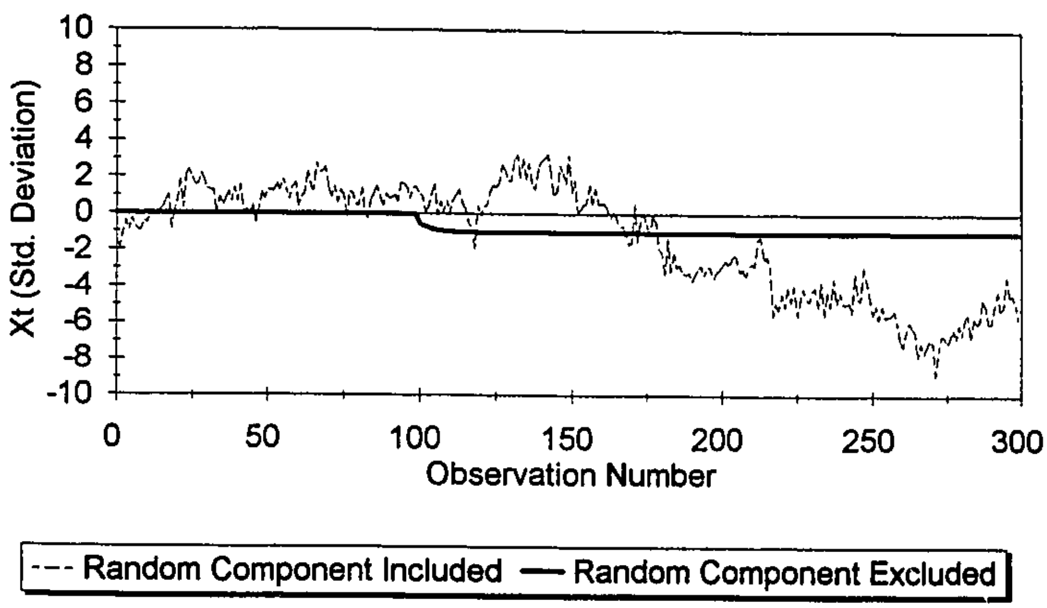


Figure 18: Manipulated variable and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARIMA(1,1,1) disturbance, θ=0.8, ϕ=0.3 and δ=0.3.

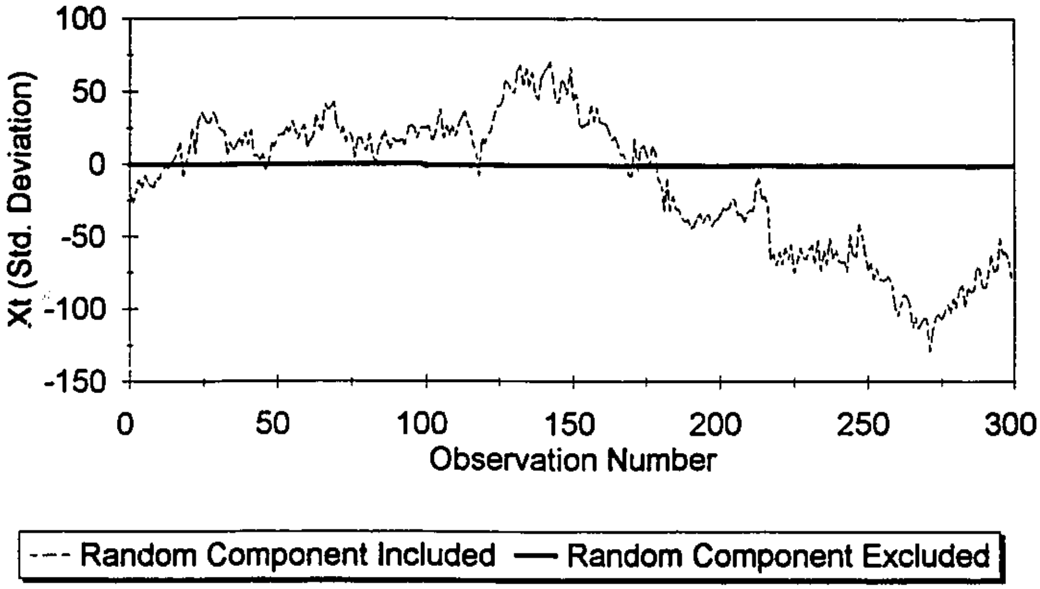


Figure 19: Manipulated variable and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARIMA(1,1,1) disturbance, θ=0.0, ϕ=0.8 and δ=0.8.

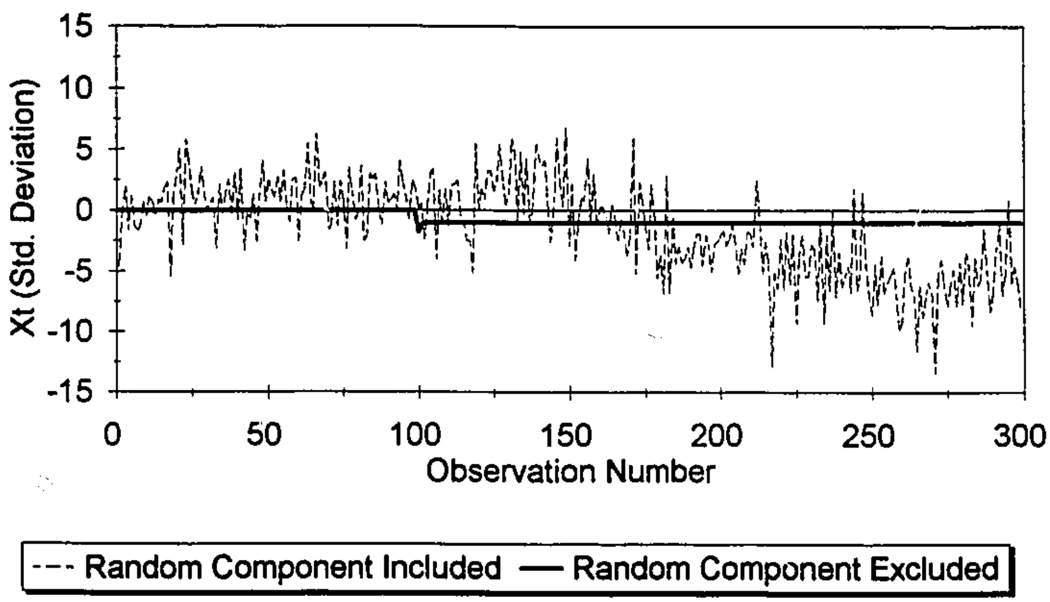


Figure 20: Manipulated variable and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARIMA(1,1,1) disturbance, θ=0.8, ϕ=0.3 and δ=0.8.

The only stationary data available for charting, when a nonstationary disturbance is affecting the process, are the deviations from target of the controlled variable (Figures 21 and 22). However, the underlying shift is only present for a few sampling intervals. The shift is present for such a short time because the APC algorithm is performing as it should, compensating for the process upsets. Additionally, the size of the underlying shift, for the first sampling interval after the shift in the mean of the disturbance occurs, is given by $(1-\phi)\Delta\sigma_a$ and subsequently decays exponentially by $(1-\phi)^n\sigma_a$. Therefore it is very difficult to identify assignable cause using the deviation from target of the controlled variable.

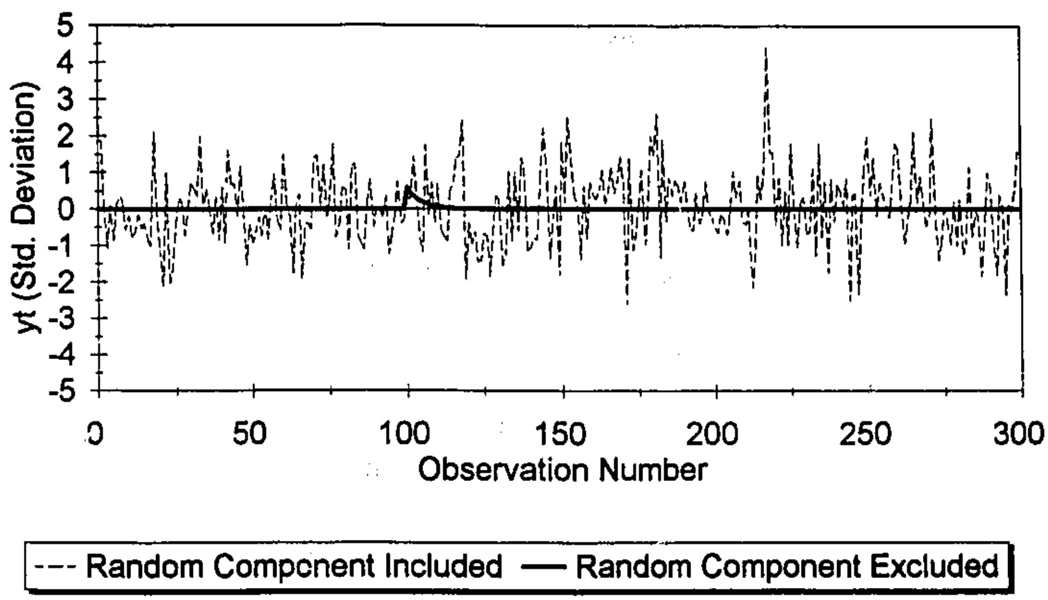


Figure 21: Residuals and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARIMA(1,1,1) disturbance, $\theta=0.8$, $\phi=0.4$.

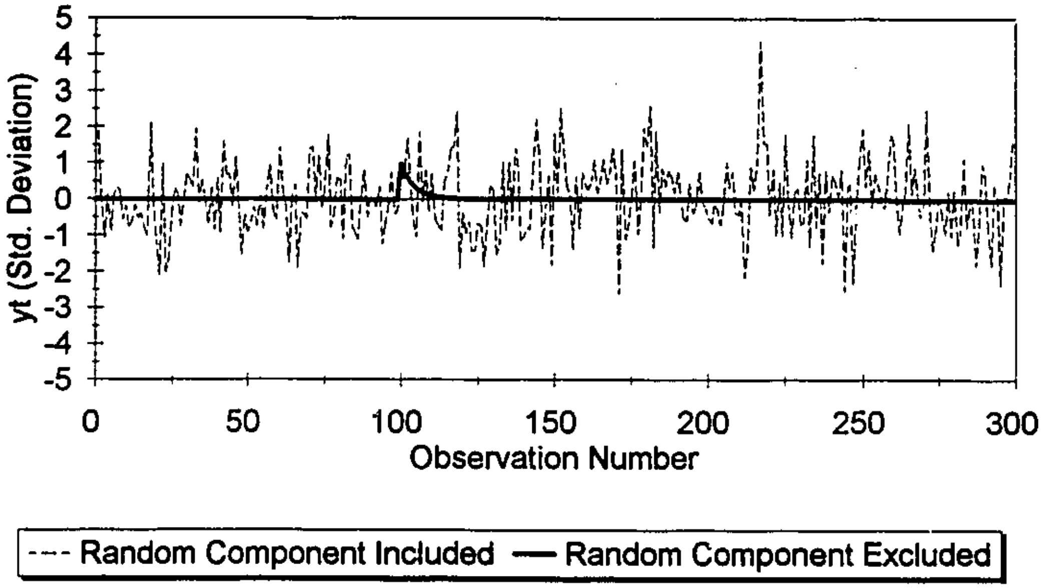
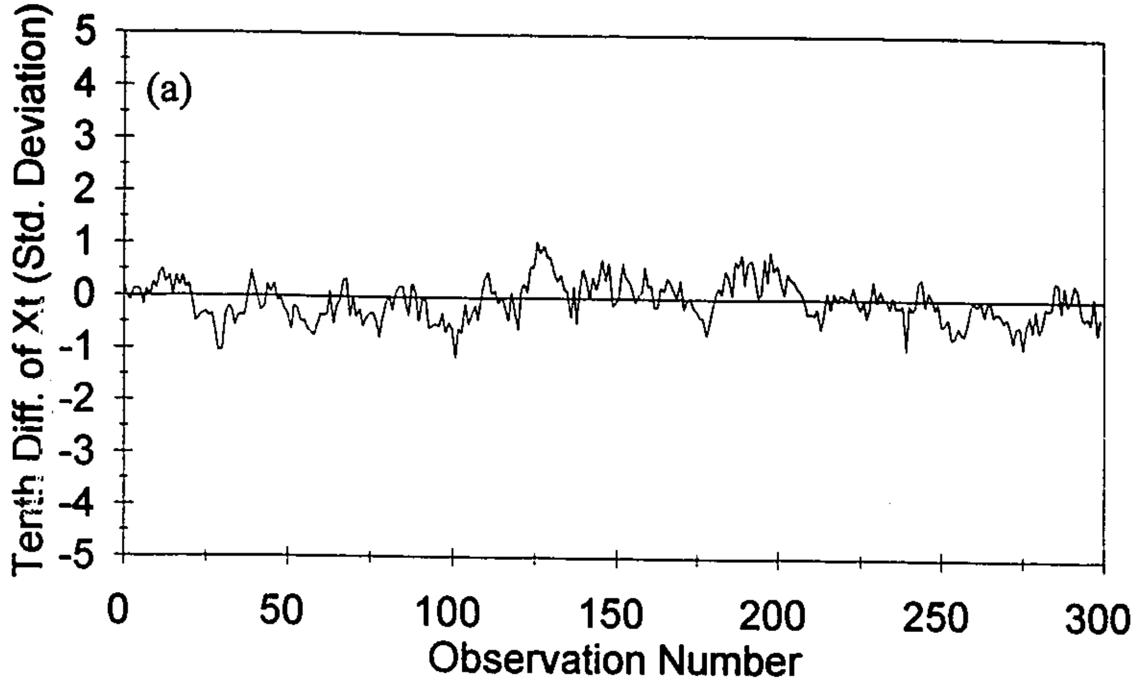


Figure 22: Residuals and the corresponding underlying shift resulting from a $1\sigma_a$ step shift in the mean value of the ARIMA(1,1,1) disturbance, $\theta=0.8$, $\phi=0.0$.

4.2 Nth-Difference Charts

Residuals are not a candidate for differencing since they are already stationary. Since there are two remaining variables available for nth-differencing, the manipulated variable and the reconstructed output, the first goal is to determine which variable is the most effective for identifying assignable cause. Figures 23a and 24a show the results of taking the 10th-difference of the manipulated variable and reconstructed output, respectively, for a first-order process employing MV feedback control and subject to an IMA(1,1) disturbance. The original undifferenced data is displayed in Figures 23b and 24b. The manipulated variable shows significantly less variability than the reconstructed output, which is indicative of a good charting variable. Subsequent process simulations



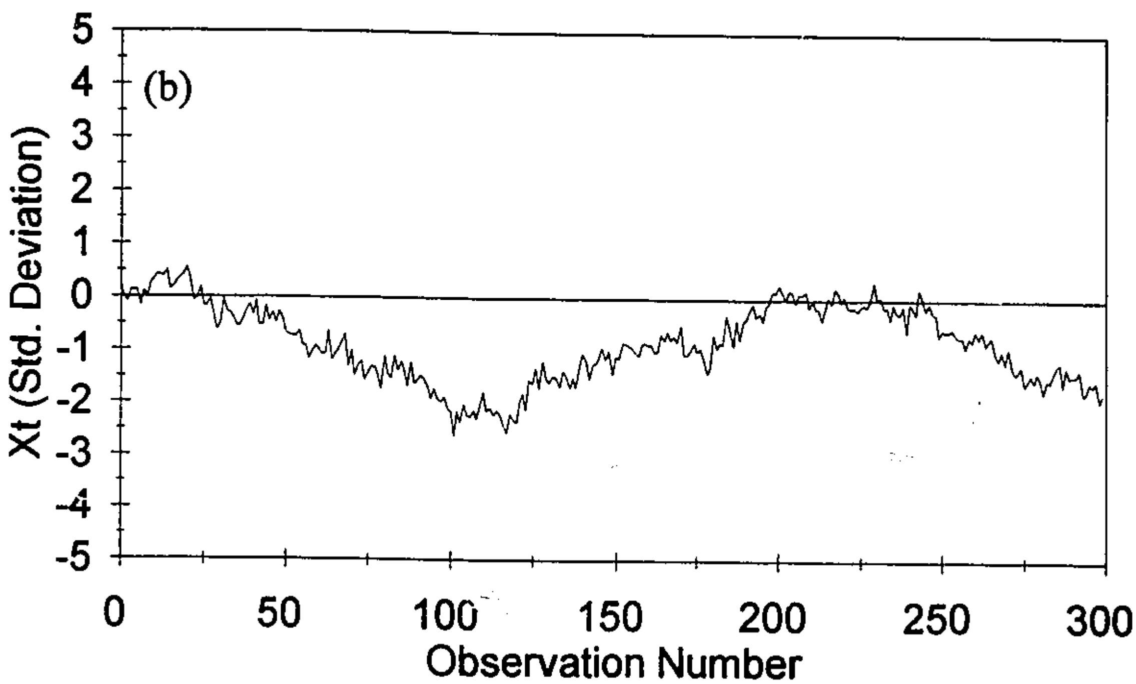


Figure 23: (a) The 10^{th}-difference of the manipulated variable and (b) the manipulated variable for a first-order process employing MV feedback control and subject to an IMA(1,1) disturbance, $\theta=0.9$ and $\delta=0.5$.

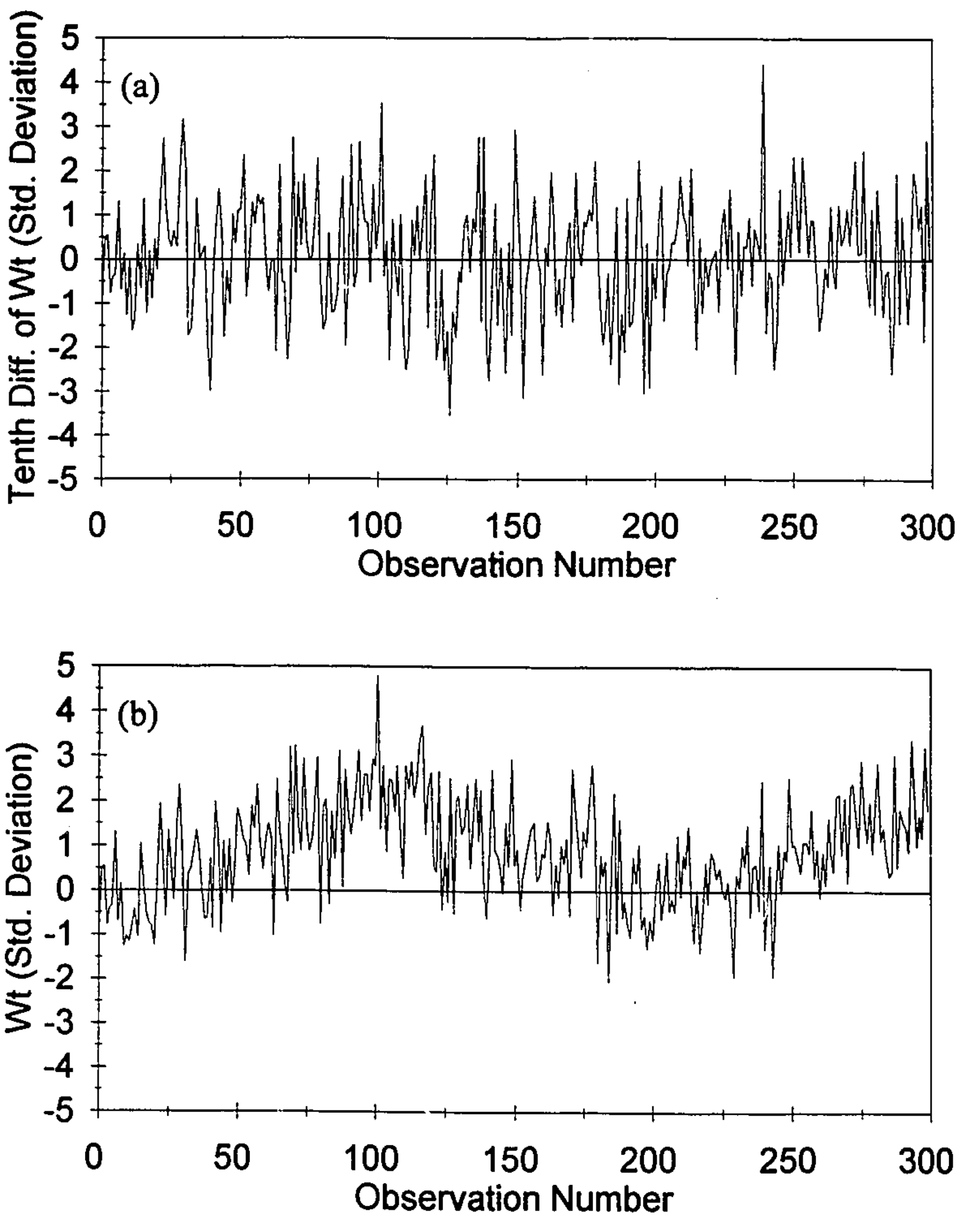


Figure 24: (a) The 10^{th}-difference of the reconstructed output and (b) the reconstructed output for a first-order process employing MV feedback control and subject to an IMA(1,1) disturbance, $\theta=0.9$ and $\delta=0.5$.

(Table 3) verified that indeed the manipulated variable was the most effective at identifying assignable cause, even when the process inertia is large. The control limits for these simulations were determined through trial and error so that an ARL(0) = 371.4 was obtained. All of the results that follow will be for the n^{th}-difference of the manipulated variable.

Table 3: Comparison of the effectiveness of the n^{th}-difference of the reconstructed output and the manipulated variable at identifying assignable cause, for a first-order process subject to an IMA(1,1) disturbance, θ=0.9 and δ=0.7.

Shift Size	Reconstructed Output	Manipulated Variable
0	371.6	371.1
$1\sigma_a$	359.9	356.6
$2\sigma_a$	291.2	267.7
$3\sigma_a$	146.2	104.9

Tables 4-7 show the average run length (ARL) and median run length (MRL) results for the n^{th}-difference charting procedure for a first-order process subject to an IMA(1,1) disturbance under MV feedback control. The MRL is the value for which 50 % of the simulated run lengths are smaller. The ARL coupled with the MRL gives one a good idea of the skewedness of the run length distribution. Thus, looking at the first two values in Table 4 for n=20, θ=0.5 and Δ = 0.0, one can see that on average 373.2 observations are required before an out of control signal is given, however, 50 % of the time fewer than 275 observations are required. Therefore the run length distribution is

Table 4: Average run length results for the n^{th}-difference of the manipulated variable for a first-order process subject to an IMA(1,1) disturbance, $\delta=0.0$.

θ	n	Δ			
		0.0 ARL / MRL	1.0σ ARL / MRL	2.0σ ARL / MRL	3.0σ ARL / MRL
0.5	20	373.2 / 275.0	361.6 / 260.5	325.1 / 216.0	267.4 / 134.0
	10	372.3 / 268.5	360.0 / 257.0	316.8 / 202.5	229.3 / 75.0
	6	371.8 / 265.0	358.0 / 251.0	301.0 / 183.0	187.5 / 11.0
	5	372.7 / 270.0	358.5 / 252.0	297.1 / 178.0	177.5 / 5.0
	4	373.0 / 273.0	359.1 / 254.0	291.7 / 174.0	165.5 / 4.0
	1	371.9 / 268.0	362.7 / 258.0	303.8 / 192.0	169.3 / 1.0
0.7	20	373.2 / 275.0	342.9 / 240.0	259.4 / 119.0	136.4 / 12.0
	10	372.3 / 268.5	343.3 / 235.0	226.1 / 66.0	86.4 / 6.0
	6	371.8 / 265.0	344.1 / 234.0	210.2 / 45.0	57.3 / 4.0
	5	372.7 / 270.0	343.9 / 234.0	212.0 / 46.0	50.6 / 3.0
	4	373.0 / 273.0	343.3 / 235.0	213.5 / 48.0	51.3 / 3.0
	1	371.9 / 268.0	359.2 / 255.0	283.1 / 166.0	137.7 / 1.0
0.75	20	373.2 / 275.0	331.4 / 223.0	217.8 / 59.0	86.7 / 9.0
	10	372.3 / 268.5	334.0 / 222.5	182.2 / 10.0	46.6 / 5.0
	6	371.8 / 265.0	335.9 / 225.0	172.1 / 6.0	27.2 / 3.0
	5	372.7 / 270.0	335.8 / 225.0	176.4 / 5.0	31.1 / 3.0
	4	373.0 / 273.0	337.2 / 228.0	182.9 / 5.0	31.6 / 3.0
	1	371.9 / 268.0	257.3 / 254.0	273.5 / 152.0	118.2 / 1.0
0.8	20	373.2 / 275.0	312.7 / 194.0	158.7 / 15.0	35.1 / 7.0
	10	372.3 / 268.5	315.6 / 199.0	127.3 / 8.0	14.1 / 4.0
	6	371.8 / 265.0	320.3 / 208.0	128.2 / 5.0	9.8 / 3.0
	5	372.7 / 270.0	322.2 / 208.0	132.1 / 5.0	11.2 / 3.0
	4	373.0 / 273.0	325.7 / 218.0	145.4 / 4.0	12.8 / 3.0
	1	371.9 / 268.0	354.6 / 251.0	262.6 / 133.0	97.0 / 1.0

Table 4 (Continued):

θ	n	Δ			
		0.0 ARL / MRL	1.0σ ARL /MRL	2.0σ ARL / MRL	3.0σ ARL /MRL
0.9	20	373.2 / 275.0	218.5 / 56.0	21.5 / 8.0	4.4 / 5.0
	10	372.3 / 268.5	227.9 / 70.0	22.0 / 6.0	2.9 / 4.0
	6	371.8 / 265.0	255.2 / 115.0	28.4 / 5.0	2.1 / 3.0
	5	372.7 / 270.0	268.1 / 136.0	36.7 / 4.0	2.1 / 3.0
	4	373.0 / 273.0	283.2 / 158.0	42.6 / 4.0	2.2 / 3.0
	1	371.9 / 268.0	340.2 / 235.0	198.7 / 31.0	35.6 / 1.0
0.95	20	373.2 / 275.0	96.0 / 15.0	6.4 / 7.0	3.8 / 5.0
	10	372.3 / 268.5	124.6 / 10.5	4.4 / 5.0	2.6 / 4.0
	6	371.8 / 265.0	169.5 / 14.0	4.1 / 4.0	1.9 / 3.0
	5	372.7 / 270.0	186.3 / 20.0	4.6 / 4.0	1.7 / 3.0
	4	373.0 / 273.0	205.6 / 33.0	7.8 / 4.0	1.5 / 3.0
	3	371.9	230.1	13.0	1.35
	2	373.0	272.2	36.4	1.27
	1	371.9 / 268.0	311.4 / 201.0	114.7 / 7.0	6.4 / 1.0

Table 5: Average run length results for the n^{th}-difference of the manipulated variable for a first-order process subject to an IMA(1,1) disturbance, $\delta=0.25$.

θ	n	Δ 0.0 ARL / MRL	1.0σ ARL / MRL	2.0σ ARL / MRL	3.0σ ARL / MRL
0.8	20	371.0 / 269.0	311.3 / 192.0	159.0 / 15.0	33.9 / 7.0
	10	370.5 / 267.5	315.7 / 199.0	131.9 / 8.0	16.8 / 4.0
	6	367.7 / 262.0	317.9 / 209.0	131.6 / 6.0	12.5 / 3.0
	5	372.8 / 268.0	324.8 / 212.0	139.4 / 5.0	13.5 / 3.0
	4	370.5 / 269.0	327.6 / 220.0	156.4 / 4.0	18.0 / 3.0
	1	370.7 / 264.0	360.2 / 254.0	299.1 / 180.0	165.3 / 2.0
0.85	20	371.0 / 269.0	282.8 / 156.0	86.0 / 11.0	9.9 / 6.0
	10	370.5 / 267.5	286.0 / 157.0	71.8 / 7.0	5.1 / 4.0
	6	367.7 / 262.0	293.8 / 175.0	78.4 / 5.0	4.3 / 3.0
	5	372.8 / 268.0	307.3 / 193.0	92.2 / 4.0	5.9 / 3.0
	4	370.5 / 269.0	312.7 / 202.0	113.8 / 4.0	7.3 / 3.0
	1	370.7 / 264.0	357.5 / 251.0	291.8 / 169.0	145.5 / 2.0
0.9	20	371.0 / 269.0	220.5 / 57.0	21.6 / 8.0	4.3 / 5.0
	10	370.5 / 267.5	230.6 / 74.0	22.7 / 6.0	2.7 / 4.0
	6	367.7 / 262.0	260.4 / 122.0	32.3 / 4.0	2.3 / 3.0
	5	372.8 / 268.0	274.7 / 148.0	39.7 / 4.0	1.8 / 3.0
	4	370.5 / 269.0	287.0 / 169.0	59.6 / 4.0	2.8 / 2.0
	1	370.7 / 264.0	354.0 / 246.0	271.1 / 139.0	109.8 / 2.0
0.95	20	371.0 / 269.0	94.5 / 15.0	6.3 / 7.0	3.6 / 5.0
	10	370.5 / 267.5	122.8 / 11.0	4.4 / 5.0	2.5 / 3.0
	6	367.7 / 262.0	182.4 / 17.0	4.3 / 4.0	1.8 / 3.0
	5	372.8 / 268.0	195.1 / 26.0	6.1 / 4.0	1.6 / 3.0
	4	370.5 / 269.0	221.9 / 61.0	11.4 / 4.0	1.4 / 2.0
	3	371.9	252.6	22.6	1.37
	2	373.0	297.8	78.9	2.56
	1	370.7 / 264.0	341.5 / 231.0	212.7 / 56.0	55.0 / 2.0

Table 6: Average run length results for the n^{th}-difference of the manipulated variable for a first-order process subject to an IMA(1,1) disturbance, δ=0.50.

θ	n	Δ 0.0 ARL / MRL	1.0σ ARL / MRL	2.0σ ARL / MRL	3.0σ ARL / MRL
0.8	20	376.9 / 275.0	317.8 / 200.0	171.1 / 16.0	38.8 / 7.0
	10	371.5 / 268.0	319.7 / 211.0	143.6 / 8.0	20.8 / 4.0
	6	371.4 / 270.0	329.3 / 222.0	158.3 / 6.0	22.5 / 3.0
	5	371.7 / 262.0	334.6 / 224.0	168.1 / 5.0	24.1 / 3.0
	4	371.4 / 263.0	340.3 / 228.0	193.6 / 12.0	32.3 / 3.0
	1	371.0 / 270.0	366.1 / 265.0	325.7 / 218.0	220.6 / 64.0
0.85	20	376.9 / 275.0	291.3 / 166.5	92.3 / 11.0	10.6 / 6.0
	10	371.5 / 268.0	292.9 / 171.0	85.2 / 7.0	5.8 / 4.0
	6	371.4 / 270.0	314.6 / 201.0	105.9 / 5.0	6.1 / 3.0
	5	371.7 / 262.0	315.8 / 204.0	120.6 / 5.0	10.5 / 3.0
	4	371.4 / 263.0	330.7 / 219.0	150.7 / 4.0	15.3 / 2.0
	1	371.0 / 270.0	364.1 / 264.0	321.5 / 200.0	215.9 / 57.0
0.9	20	376.9 / 275.0	228.1 / 70.0	25.2 / 8.0	4.4 / 5.0
	10	371.5 / 268.0	242.6 / 100.0	26.4 / 6.0	2.6 / 3.0
	6	371.4 / 270.0	287.0 / 160.0	54.5 / 5.0	2.6 / 3.0
	5	371.7 / 262.0	294.3 / 176.0	65.5 / 4.0	3.0 / 3.0
	4	371.4 / 263.0	310.6 / 199.0	97.5 / 4.0	4.3 / 2.0
	1	371.0 / 270.0	362.4 / 260.0	315.2 / 205.0	203.1 / 36.0
0.95	20	376.9 / 275.0	98.7 / 16.0	6.4 / 7.0	2.5 / 4.0
	10	371.5 / 268.0	146.4 / 12.0	5.0 / 5.0	2.3 / 3.0
	8	372.5	163.2	5.4	2.1
	6	371.4 / 270.0	210.4 / 38.0	7.4 / 4.0	1.7 / 3.0
	5	371.7 / 262.0	229.5 / 75.0	15.2 / 4.0	1.5 / 2.0
	4	371.4 / 263.0	261.0 / 121.0	29.6 / 4.0	1.5 / 2.0
	1	371.0 / 270.0	358.0 / 254.0	297.2 / 183.0	173.0 / 10.0

Table 7: Average run length results for the n^{th}-difference of the manipulated variable for a first-order process subject to an IMA(1,1) disturbance, $\delta=0.75$.

θ	n	Δ			
		0.0 ARL / MRL	1.0σ ARL / MRL	2.0σ ARL / MRL	3.0σ ARL / MRL
0.8	20	371.0 / 265.0	328.3 / 215.0	200.2 / 20.0	60.9 / 6.0
	10	370.8 / 266.0	336.7 / 231.5	206.6 / 39.0	54.4 / 4.0
	6	370.0 / 267.0	348.5 / 240.0	237.8 / 92.0	72.0 / 3.0
	5	372.0 / 269.0	350.9 / 244.0	255.4 / 112.0	83.2 / 3.0
	4	371.9 / 270.0	353.0 / 249.0	270.8 / 147.0	110.7 / 3.0
	1	371.2 / 265.0	364.7 / 259.0	337.5 / 227.0	267.3 / 136.0
0.85	20	371.0 / 265.0	302.7 / 182.5	122.0 / 13.0	16.1 / 5.0
	10	370.8 / 266.0	321.5 / 212.0	152.0/ 9.0	20.3 / 4.0
	6	370.0 / 267.0	340.3 / 232.0	199.2 / 25.0	37.6 / 3.0
	5	372.0 / 269.0	343.0 / 237.0	221.2 / 59.0	49.6 / 3.0
	4	371.9 / 270.0	350.0 / 245.0	246.6 / 108.0	78.0 / 3.0
	1	371.2 / 265.0	364.1 / 259.0	336.2 / 226.0	265.8 / 134.0
0.9	20	371.0 / 265.0	252.8 / 109.0	40.3 / 9.0	4.4 / 4.0
	10	370.8 / 266.0	292.2 / 175.0	72.5 / 7.0	3.4 / 3.0
	6	370.0 / 267.0	326.1 / 218.0	141.5 / 6.0	12.9 / 3.0
	5	372.0 / 269.0	334.6 / 227.0	169.1 / 5.0	19.9 / 3.0
	4	371.9 / 270.0	343.0 / 238.0	211.6 / 53.0	42.2 / 3.0
	1	371.2 / 265.0	364.4 / 259.0	335.7 / 224.0	264.0 / 132.0
0.95	20	371.0 / 265.0	131.7 / 18.0	6.7 / 7.0	3.0 / 4.0
	15	371.6	165.8	6.2	2.9
	10	370.8 / 266.0	218.6 / 60.0	14.0 / 6.0	2.1 / 3.0
	8	372.5	249.1	24.7	2.25
	6	370.0 / 267.0	293.0 / 175.0	63.6 / 5.0	2.3 / 3.0
	5	372.0 / 269.0	304.7 / 186.0	97.7 / 5.0	4.1 / 2.0
	4	371.9 / 270.0	328.1 / 223.0	149.8 / 5.0	14.2 / 2.0
	1	371.2 / 265.0	363.4 / 258.0	333.1 / 222.0	234.4 / 118.0

negatively skewed as was also demonstrated by Harris and Ross (1991) and Slocomb (1991). Selected results are shown graphically in Figures 25-28. Figure 25 indicates that the ARLs are highly dependant on the degree of differencing used as well as the size of the step shift to be detected. As the size of the step shift in the mean value of the disturbance increases, the optimal degree of differencing decreases. This result is expected since the smaller the disturbance affecting the process the longer the time interval needed for identification.

Comparing Figures 25 and 26 one notices that the amount of process inertia, δ, has a significant effect on the amount of differencing needed as well as the speed at which the assignable cause is identified. The larger the process inertia (process time constant) the slower the step disturbance propagates to the charted variable, and hence the more time required for identification.

A comparison between Figures 25, 27 and 28 shows that as the amount of nonstationarity increases, that is as θ decreases, the less effective the n^{th}-difference charts become. One can see that at $\theta=0.95$, a $3\sigma_a$ step shift is identified in just over 1 time interval whereas for $\theta=0.5$ the same shift requires, on average, almost 200 time units. Therefore, the n^{th}-difference charts, although useful, should not be used on processes displaying more than moderate nonstationarity. For this reason only a limited number of ARIMA(1,1,1) models were studied, since they display significantly more nonstationarity than the IMA(1,1) disturbance.

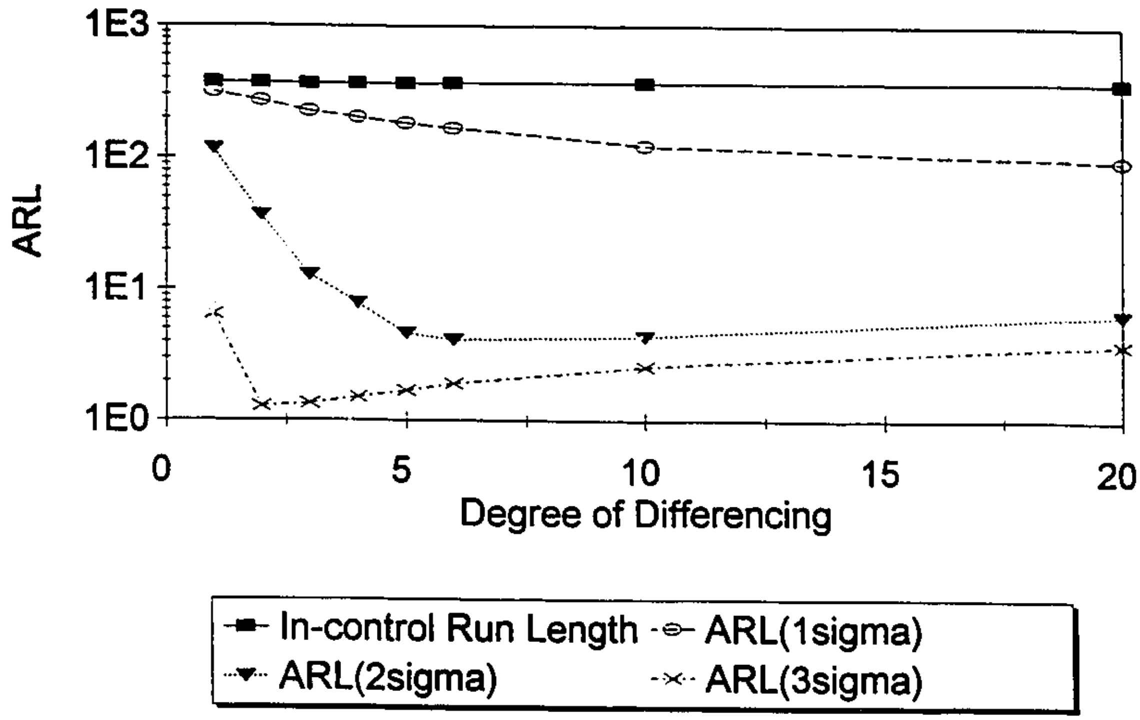


Figure 25: ARL results versus degree of differencing for a first-order process subject to an IMA(1,1) disturbance, $\theta=0.95$ and $\delta=0.0$.

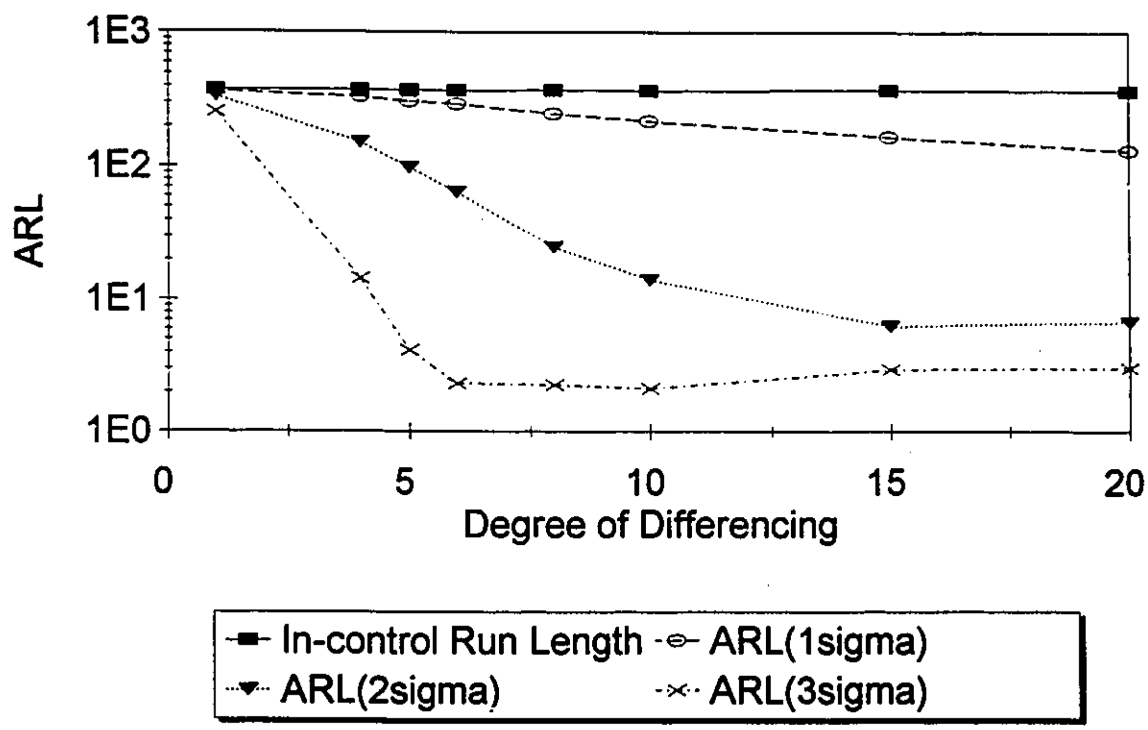


Figure 26: ARL results versus degree of differencing for a first-order process subject to an IMA(1,1) disturbance, $\theta=0.95$ and $\delta=0.75$.

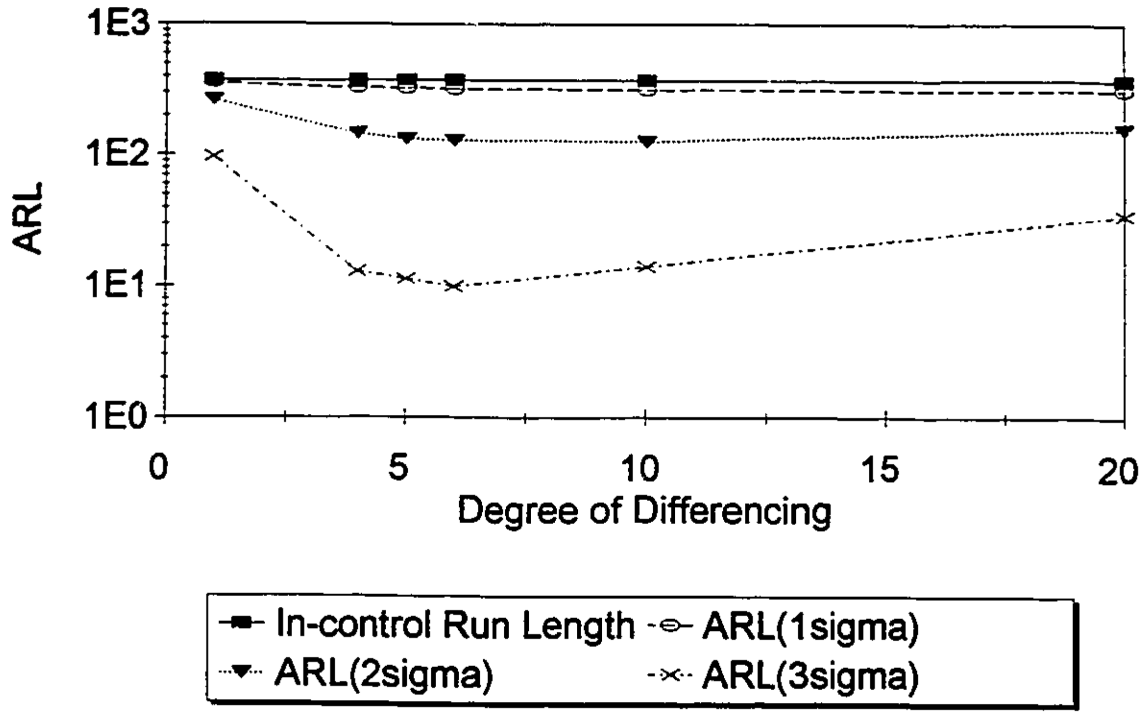


Figure 27: ARL results versus degree of differencing for a first-order process subject to an IMA(1,1) disturbance, $\theta=0.80$ and $\delta=0.0$.

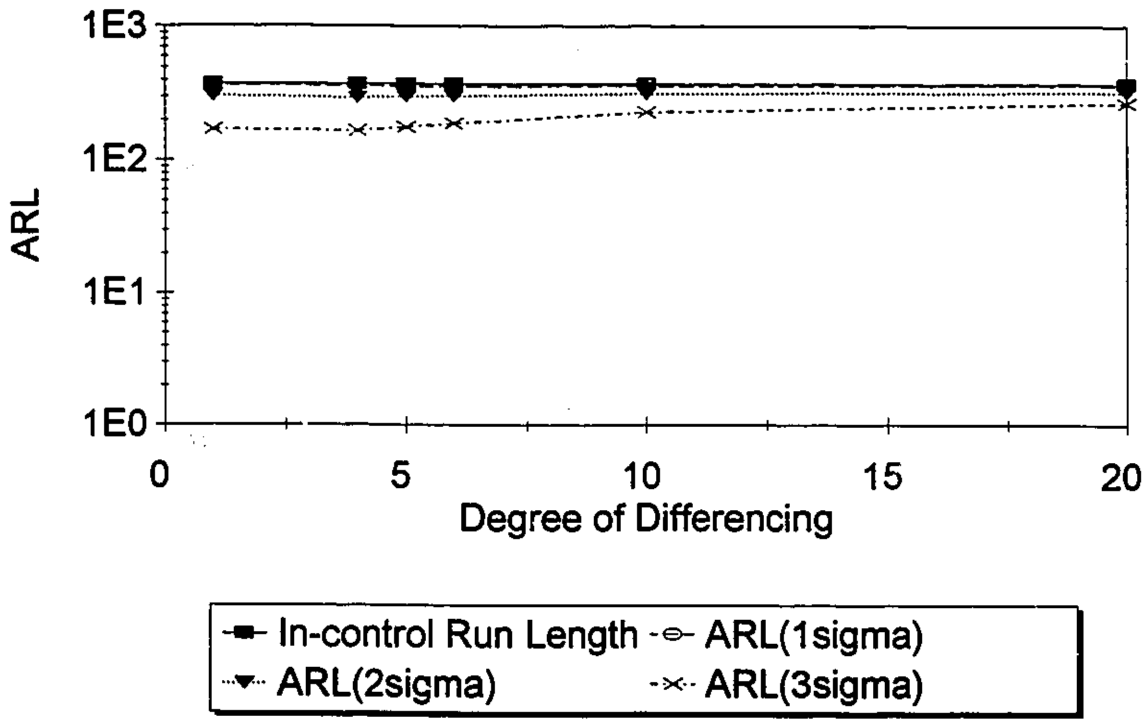


Figure 28: ARL results versus degree of differencing for a first-order process subject to an IMA(1,1) disturbance, $\theta=0.50$ and $\delta=0.0$.

Table 8 shows the ARL results of the 5th-difference of the manipulated variable for a pure gain process ($\delta=0$) subject to an ARIMA(1,1,1) disturbance. In comparing these results to those obtained for IMA(1,1) disturbances, one can see that even very small values of the autoregressive term, ϕ, yield a significant decrease in the ability of the nth-difference chart to detect assignable cause. This is expected since the degree of nonstationarity of a process increases as ϕ increases and θ decreases.

Table 8: Average run length results of the 5th-difference of the manipulated variable of a pure gain process ($\delta=0$) subject to an ARIMA(1,1,1) disturbance, based on ARL(0) $\approx$ 371.

θ / ϕ	ARL($1\sigma_a$)	ARL($2\sigma_a$)	ARL($3\sigma_a$)
0.9 / 0.1	309.6	92.3	3.95
0.9 / 0.2	333.0	181.6	31.9
0.9 / 0.4	354.2	293.9	163.4
0.8 / 0.1	331.4	177.0	32.7
0.8 / 0.2	345.1	235.9	78.9

4.3 Effect of Sampling Interval on Disturbance Detection in ARMA(1,1) Models

Deshpande (1993) suggested two ways to overcome problems arising due to autocorrelation. The first is to fit an appropriate time series model to the observations and then apply the control charts to the residuals. The second method is to select a sampling interval, based on the sample autocorrelogram, such that the autocorrelation coefficient is sufficiently small to warrant use of traditional SPC techniques. Although, such a method does produce data that follow the basic assumptions underlying traditional SPC charting techniques, Deshpande (1993) does not provide any further support for this technique. Thus, simulations were carried out in order to determine whether there does exist an optimal sampling interval when there are no costs associated with sampling.

Table 9 shows the ARL results for three sampling schemes, the first sampling all of the data, the second using every fifth data point and the last using every tenth data point. These results are also shown graphically in Figure 29. The AR parameter, ϕ, for the full data set is 0.9, which is a very large degree of autocorrelation. In sampling every fifth data point the AR parameter is reduced to ~ 0.6 and for every tenth point to ~ 0.35. Deshpande (1993) hypothesized that increasing the sampling time and hence reducing the autocorrelation allows for more efficient detection of process upsets. However, the results of this work show that appropriately adjusted control limits, using the full data set, yield identical detection times for assignable cause as the reduced correlation data sets. One should note that if it has been determined that the in-control run length, ARL(0), for the full data set is say 370.4, then the ARL(0) for the data sets sampled every fifth and tenth interval will be 74.08 and 37.04, respectively. Reducing the ARL(0) by increasing the sampling interval results in real time ARL(0)s of 370.4 for all cases, and thus gives a common starting point for comparison.

Table 9: Effect of sampling interval on disturbance detection in ARMA(1,1) models.

Size of Shift	Sampling Interval		
	1 time unit (ARL)	5 time units (ARL / Real time)	10 time units (ARL / Real time)
$0\ \sigma_a$	371.8	74.43 / 372.15	37.22 / 372.2
$1\sigma_a$	253.35	51.2 / 256.0	25.51 / 255.1
$2\sigma_a$	121.4	24.9 / 124.5	12.89 / 128.9
$3\sigma_a$	64.4	13.6 / 68.0	7.07 / 70.7

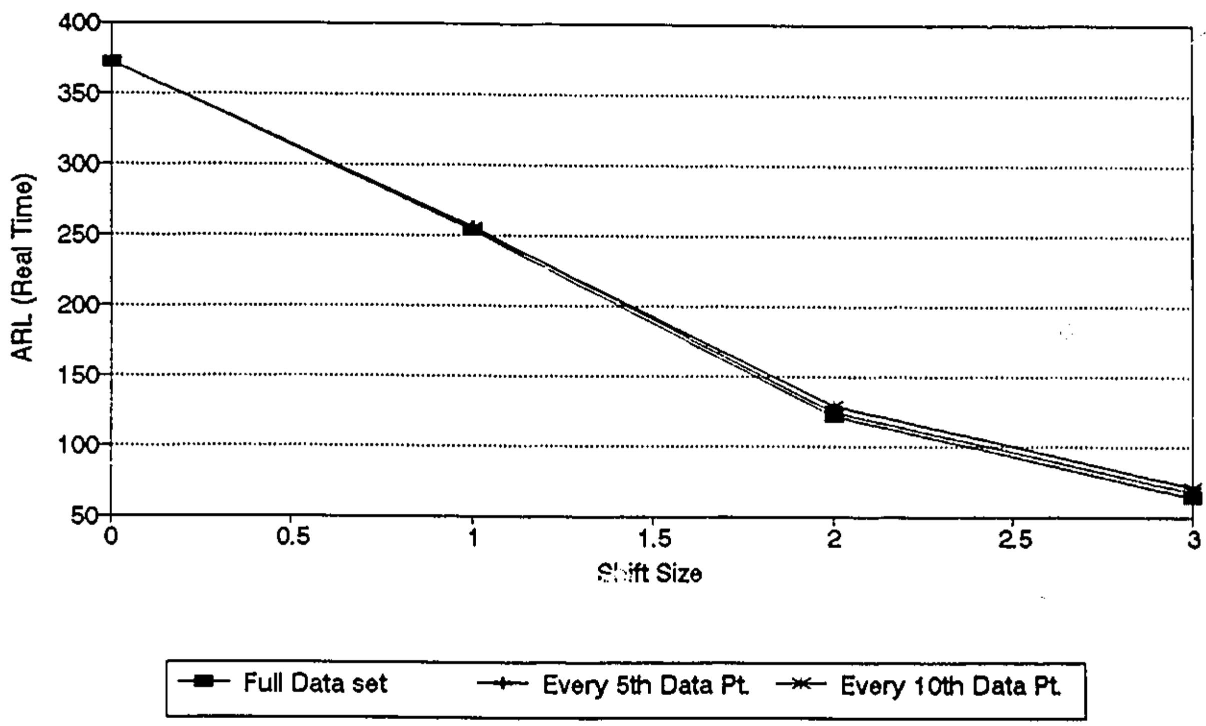


Figure 29: Effect of sampling interval on disturbance detection in ARMA(1,1) models.

4.4 Summary

Three important findings can be identified from the results and discussion presented in the preceding sections. First, with regards to selection of charting variable, it was shown that the choice is dictated by the model parameters (ϕ, θ and δ) when the disturbance is characterized by an ARMA(1,1) model. The choice of charting variable should be; the residuals when θ is greater than ϕ, the reconstructed output when ϕ is greater than θ and δ is large and the manipulated variable when δ is small.

Secondly, n^{th}-difference charts may be utilized for identification of assignable cause when the disturbance is an IMA(1,1) and $\theta < 0.7$. Although it is preferable to remove the cause of any nonstationary disturbances, the nth-difference chart allows another alternative. In terms of achieving an integrated system of process control the nth-difference charts should be chosen only if the cause of the nonstationarity cannot be identified (or removed) or if process improvements cannot be implemented immediately.

And lastly, there does not exist an optimal sampling scheme for identification of assignable cause when there is a high degree of positive correlation between observations. Therefore, if there is minimal cost associated with sampling, all of the observations should be utilized for process monitoring. Although the data may not satisfy the independence requirement for traditional SPC charts, appropriately scaled control limits will yield identical results to those obtained when the same observations are sampled less often, to induce independence.

Chapter 5

APC/SPC INTEGRATION CASE STUDY:

Shell Canada C_3 Splitter

To develop a strategy for implementing an integrated SPC/APC system a simulator for a C_3 splitter at the Shell Canada operations in Corunna, Ontario was used. The simulation software, provided by Cott (1992), formed the basis for the model identification workshop given at the 1992 Canadian Chemical Engineering Conference in Toronto was chosen. The main reasons for choosing this process were that it was relatively simple, enabled the demonstration of the necessary points concerning the integration of SPC with APC and because it was available.

Although a few authors (e.g.,Vander Wiel *et al.*, 1992) have developed integrated SPC/APC systems for their specific processes, only Vander Wiel and his associates (1993) have explicitly identified a strategy for developing an integrated system on a new, or existing process. It should be noted that processes are different and there is no unique recipe for integrating SPC with APC. Nevertheless, a basic framework for integration is desirable. A systematic approach to all processes for integrating SPC and APC is developed and presented in this section.

Six-steps are proposed:

1) disturbance identification and modelling,

2) process evaluation (Is the process in a state of statistical control?),

3) identification and modelling of process dynamics,

4) choice of automatic process control,

5) choice of charting variable(s) and charting procedures,

6) continuous process improvement.

Each of these steps will be addressed by setting up an integrated SPC/APC system for the C_3 splitter.

5.1 Process Description

The purpose of the distillation column is to remove a light key impurity from the column's feed stream so that is does not reach a reaction system downstream. Figure 30 shows a simplified piping and instrumentation diagram as provided by Cott(1992). The column has 35 trays with the feed entering at tray 5. Since the current feedrate is running well above design specifications, the condenser cooling rate is kept at its maximum. For this process the feed flowrate is assumed constant and the two available manipulated variables are the reboiler duty, Q, and the overhead vapour flowrate, D. The control objectives for this column are:

1) to control column pressure, P,

2) to control impurity level in the bottoms, x,

3) to minimize overhead vapour flowrate, D.

Typical operating ranges and steady-state values are listed in Table 10.

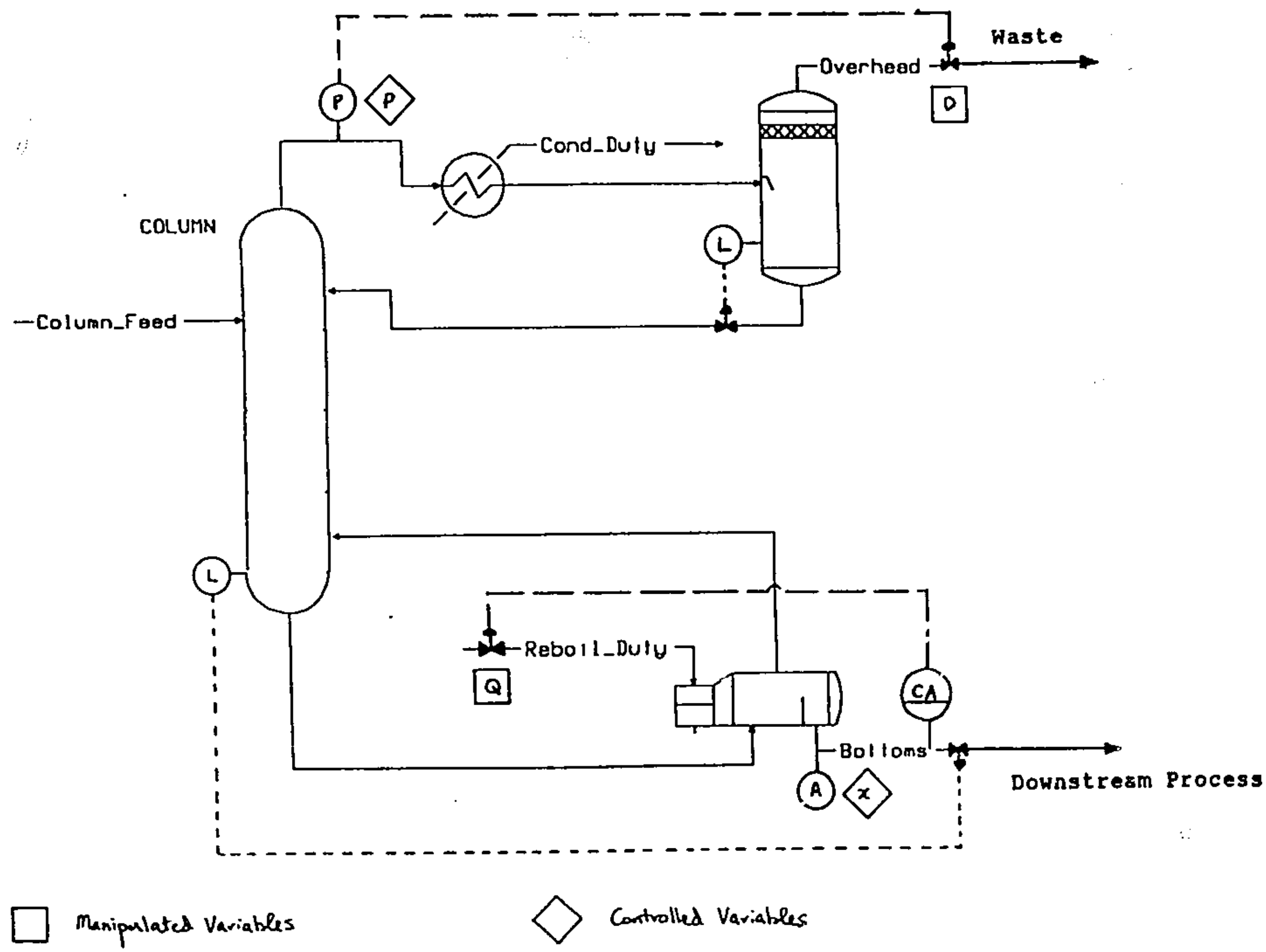


Figure 30: Piping and Instrumentation Diagram for Shell C_3 Splitter.

Table 10: Operating ranges and steady-state values for Shell Canada simulation software.

Variable Name	Operating Range	Design Steady State
Reboiler Duty, Q (kW-hr/tonne/day)	2000-3000	2500
Overhead vapour flow, D (tonnes/day)	10-30	20
Impurity composition, x (ppm)	250-1000	500
Column pressure, P (kPa)	2700-2900*	2800

*Pressure relief at 3200 kPa, dumps to flare.

The software contains three programs, the first operating at the full noise level (100%), the second operating at half of the full noise level (50%) and the third operating at 20%. Process sampling occurs every 5 minutes and is determined by the speed at which the analyzer is able to measure the impurity level. The simulations always start with the variables at their steady-state values, given in Table 10. The INPUT.DAT file included in the simulation package allows step changes to be made in both D and Q, enabling initial estimates of process dynamics.

5.2 Six-Step Strategy for Integration

Although all three noise levels in the simulation software were representative of typical operating conditions, depending upon seasonal changes in the cooling water temperature, the 50% noise level was chosen for modelling. Nevertheless, the control algorithms derived at the 50% noise level would be effective for controlling all three situations. This is because the model forms for the disturbances at all three noise levels were the same, the only difference being the magnitude of the white noise, a_t, generating the disturbances. This will become more evident once the models have been identified.

STEP 1: Disturbance Identification and Modelling

The first step was to collect open-loop data at steady state. Steady state implies that all of the input variables are at their nominal operating values and no changes are made to them over the duration of the experiment, however, disturbances are still allowed to enter the process. Although this is not a strict definition of steady state it is the definition used for this work. These experiments allow the identification of the disturbance models affecting the column pressure, P, and the bottoms impurity composition, x. The statistical analysis software StatGraphics® was employed to obtain parameter estimates for the stochastic disturbance models.

In developing the disturbance models one can start with the most complex model form and work back towards a simpler more parsimonious model, however, this can be very tedious. An easier method is to first analyze the autocorrelation functions (ACF) and partial autocorrelation functions (PACF) of the process outputs for trends suggesting a suitable starting model form. Appendix D contains definitions and estimation techniques for both the PACF and ACF. Characteristic trends for various model forms have been given by Ledolter and Abraham (1984). Table 11 shows trends to look for when evaluating ACFs and PACFs for model identification. For this problem, sample ACF and PACF plots of the column pressure and bottoms composition are shown in Figures 31-34, respectively. The failure of the ACFs for both P and x to die out quickly are indicative of nonstationary disturbances. Additional support for this conclusion is provided by the large single spike at lag one, in both PACFs. Thus, the data must first

Table 11: Summary of ACF and PACF patterns of various ARMA models (Ledolter and Abraham, 1984).

Process	ACF	PACF
AR(1)	Exponential decay	Cut off at lag 1
AR(2)	Expo. decay/ damped sin wave	Cut off at lag 2
.	.	.
.	.	.
AR(p)	Expo. decay/ damped sin wave	Cut off at lag q
MA(1)	Cut off at lag 1	Exponential decay
MA(2)	Cut off at lag 2	Expo. decay/ damped sin wave
.	.	.
.	.	.
MA(q)	Cut off at lag q	Expo. decay/ damped sin wave
ARMA(1,1)	Expo. decay after lag 0	Expo. decay after lag 0
.	.	.
.	.	.
ARMA(p,q)	Expo decay/ damped sin wave after lag q-p	Expo decay/ damped sin wave after lag p-q

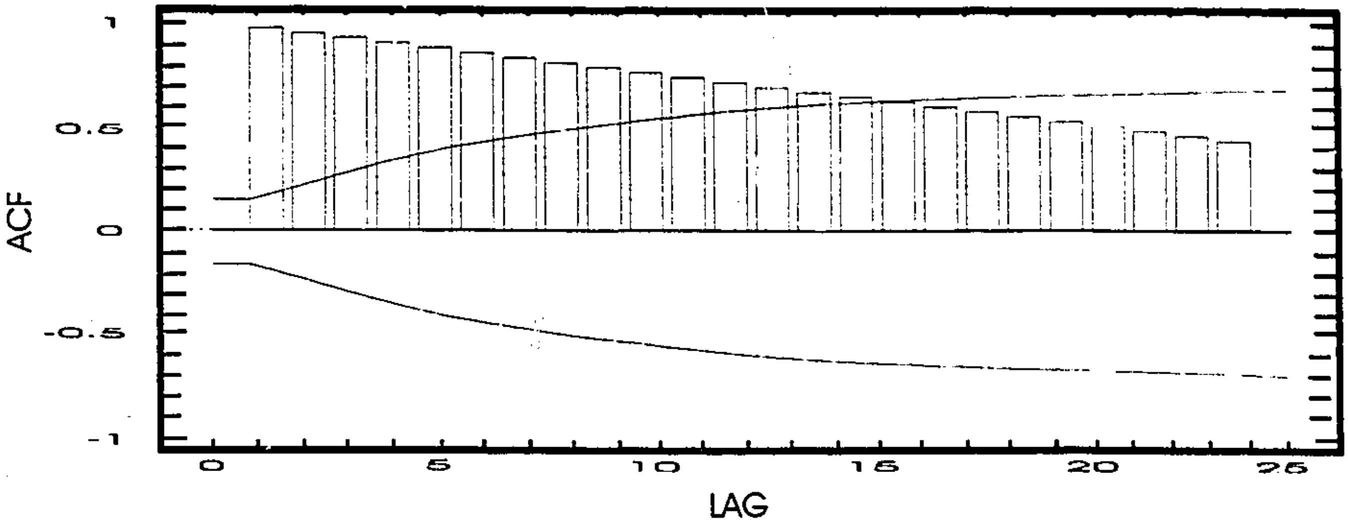


Figure 31: Sample Autocorrelation Function for Column Pressure at Steady State.

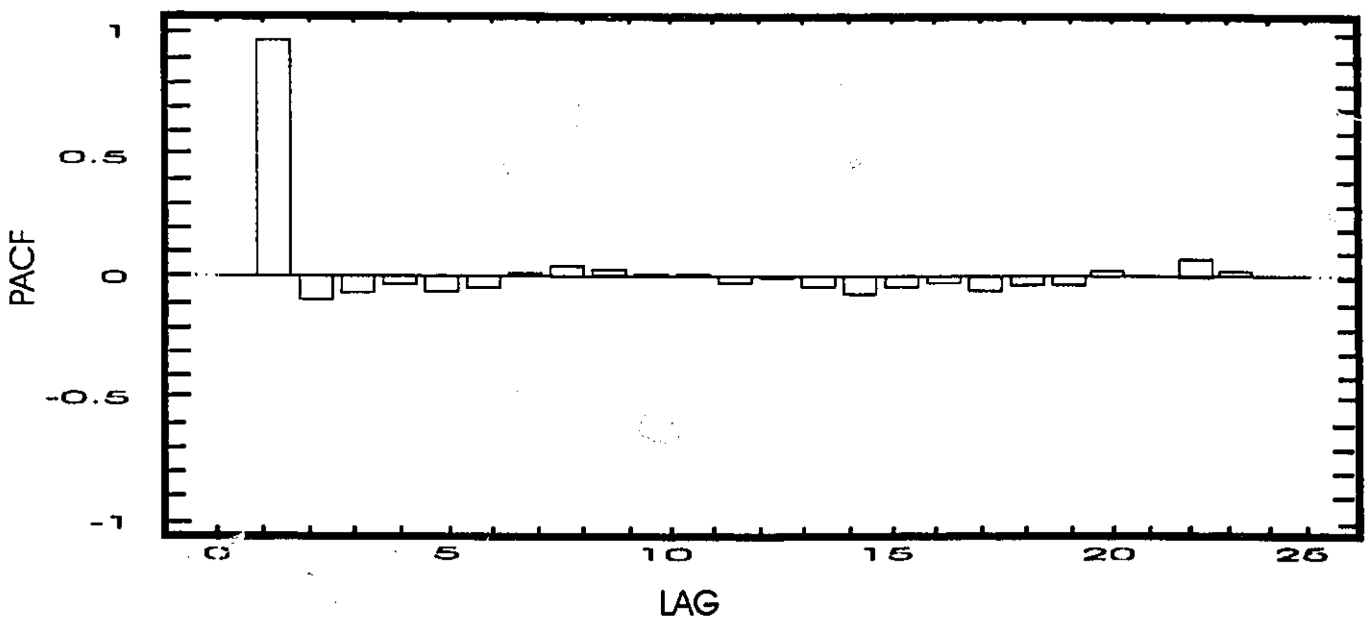


Figure 32: Sample Partial Autocorrelation Function for Column Pressure at Steady State.

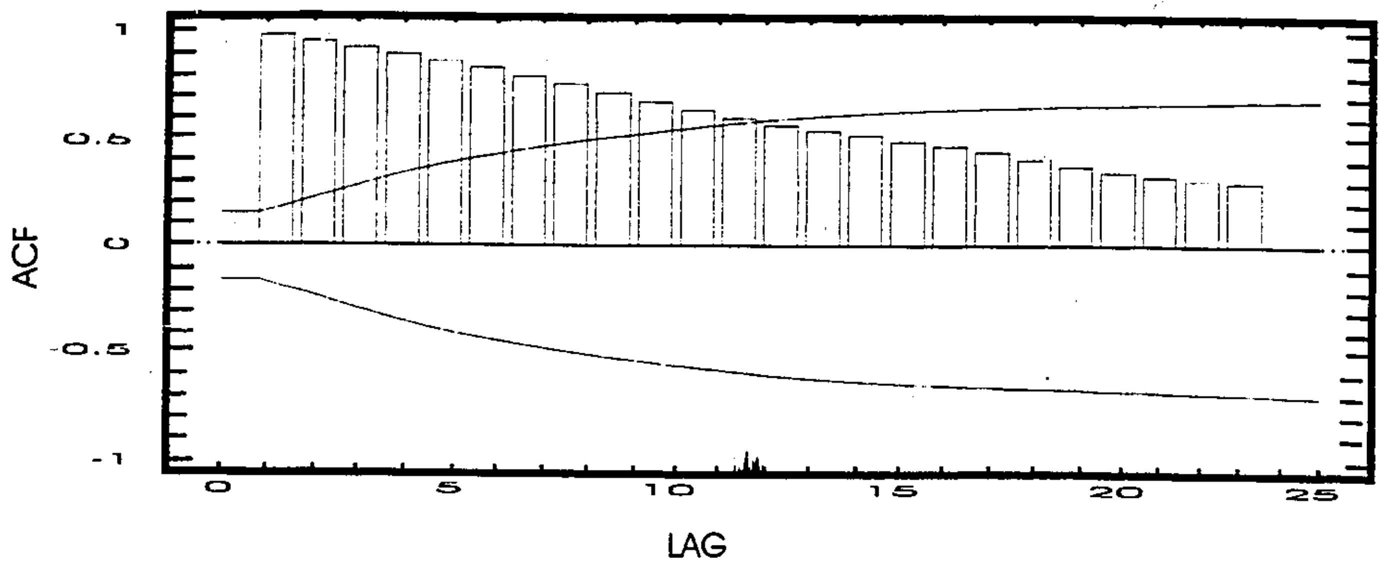


Figure 33: Sample ACF for Bottoms Composition at Steady State.

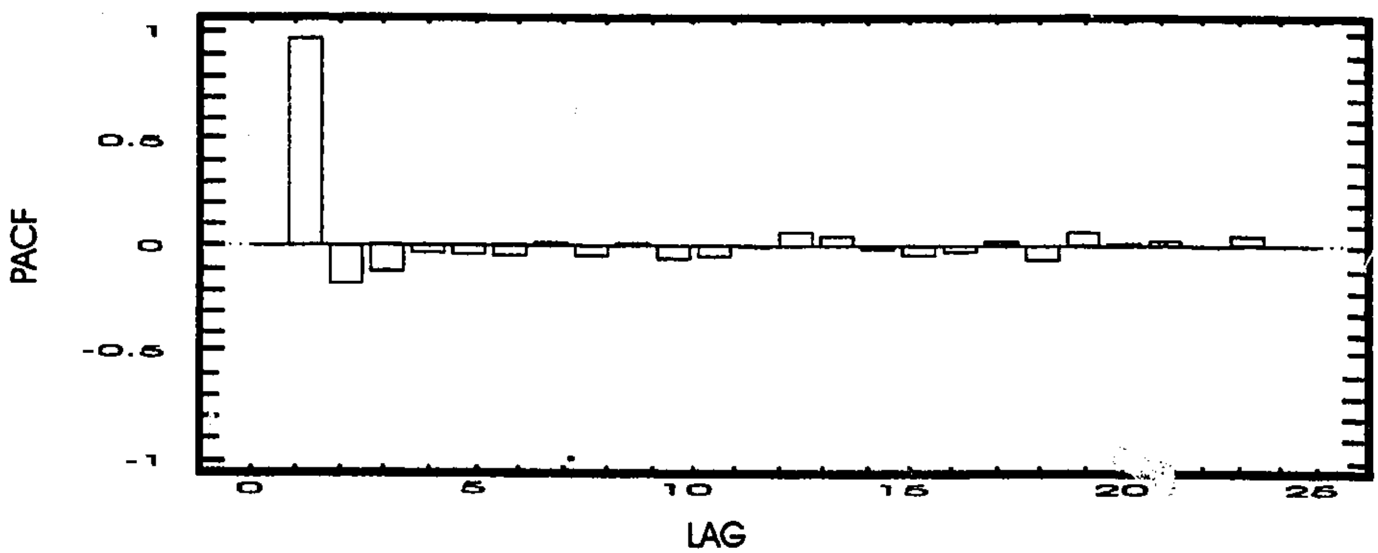


Figure 34: Sample PACF for Bottoms Composition at Steady State.

be differenced and then the ACFs and PACFs, for the differenced data, should be evaluated. The exponential trend in the ACF, for the differenced P and x data (Figures 35 and 37), is representative of the presence of autoregressive terms, and the single spike at lag one in the PACF (Figures 36 and 38) indicates that there is only one such term. Therefore, the initial disturbance model form suggested by the data is ARIMA(1,1,0),

$$(1-\phi_1)\nabla z_t = a_t \tag{50}$$

for both P and x. Upon analysis of several, simulated experiments it was determined that the ϕ_1 values for the two disturbances were $\phi_{1x} = 0.66$ and $\phi_{1p} = 0.60$ with both parameter estimates having a standard error of 0.02. The standard deviations of the white noise generating the disturbance for the column pressure and the bottoms composition were 3.05 and 1.73, respectively.

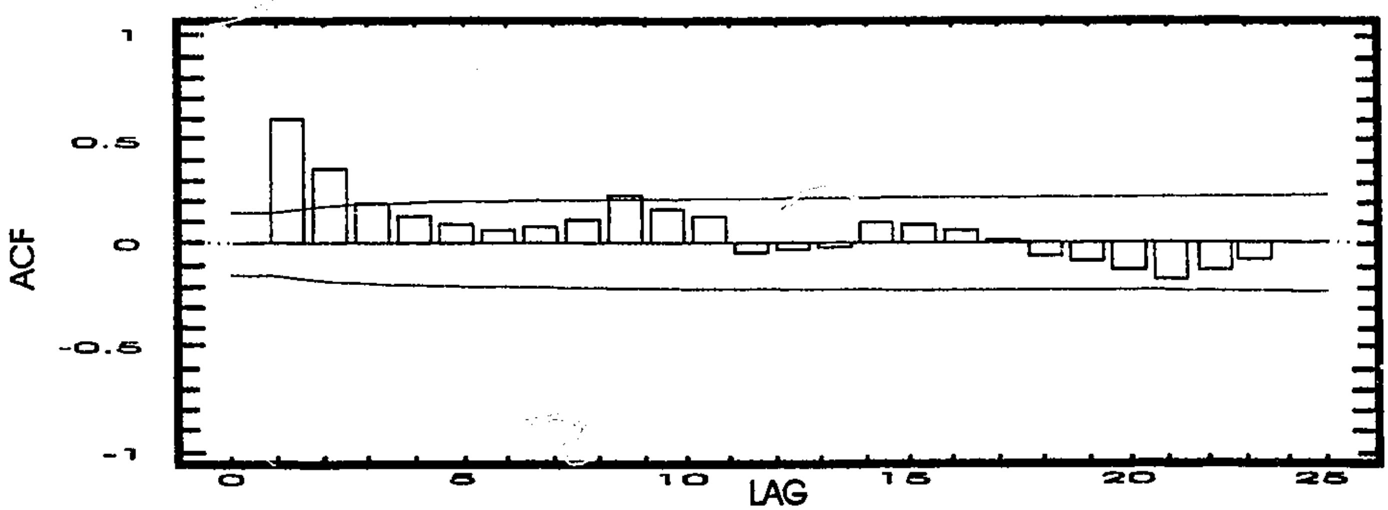


Figure 35: ACF for the First-Difference of the Steady-State Column Pressure Data.

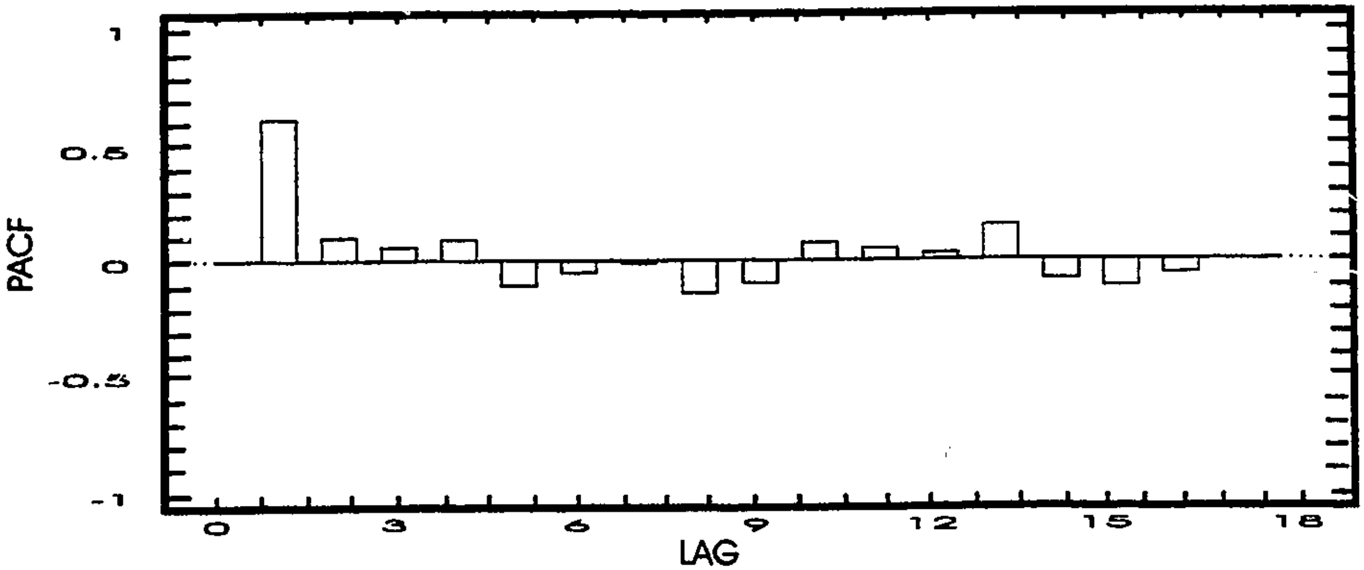


Figure 36: PACF for the First-Difference of the Steady-State Column Pressure Data.

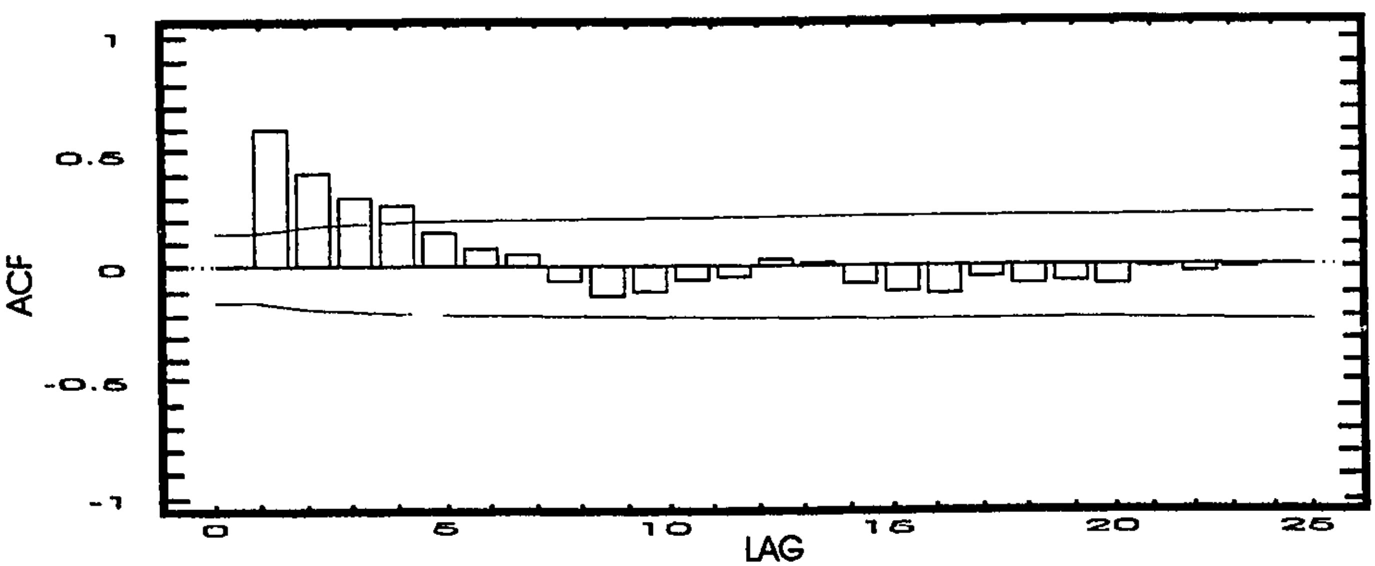


Figure 37: ACF for the First-Difference of the Steady-State Bottoms Composition Data.

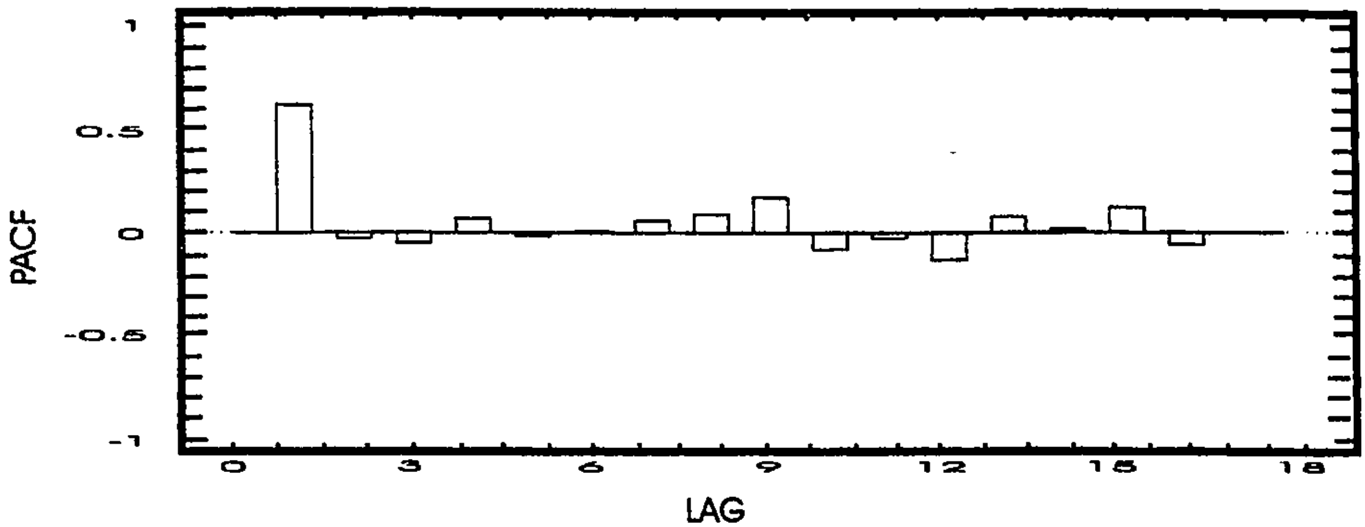


Figure 38: PACF for the First-Difference of the Steady-State Bottoms Composition Data.

One should bear in mind that this is a simulated problem and we are sure that the process is operating at steady state. However, when dealing with real process data, one must ensure that the process is indeed running at steady state. If an assignable cause enters the process during the collection of the steady-state data, incorrect disturbance models may be obtained, depending on the severity of the process upset. One way to verify the steady-state assumption would be to collect two or more sets of data and check the similarity of the models obtained from each.

STEP 2: Process Evaluation

To this point, the disturbances affecting both controlled variables have been determined to be nonstationary. Based on the results presented in Chapter 4 these disturbances are not of the form that can be monitored on n^{th}-difference charts, since θ ($= 0$) is less than 0.7. Therefore one must decide whether it is worthwhile continuing integration of SPC with APC or whether the origin of the nonstationarity should be investigated. If it is possible to remove the cause of the nonstationarity, one would greatly improve the control of the process and chance of achieving an integrated SPC/APC system. For the C_3 splitter, the source of the nonstationarity is quite obvious; the cooling capacity of the overhead condenser is much less than required for the amount of material being processed. Thus, it would be beneficial for one to first increase the cooling capacity of the overhead condenser and then repeat step 1. However, since this is an existing process, one may not be able to implement changes to the process immediately. Therefore, it may be appropriate to continue through steps 3 and 4, such that an APC scheme can be introduced to stabilize the process until appropriate changes can be made to the system. Thus, it may preferable to have the process evaluation as Step 4 rather than as Step 2.

STEP 3: Identification and Modelling of Process Dynamics

A very popular method of identifying dynamic models is the reaction curve method. This method consists of introducing a step change into the process input and fitting the resulting change in the output to a FOPDT model. This method was used for our example since it is very easy to employ, and appeared suitable for this work. Caution must be exercised in using this method since serious error in parameter estimates may result if significant noise exists. A pseudo-random binary sequence (PRBS) can also be used as an input forcing function for the purpose of identifying process dynamics. This type of experimentation usually takes place in plant situations, where a limited amount of disruption to normal operation is required. An additional method of identifying process dynamic models when dealing with time series data involves using ordinary processing data and the method of prewhitening the input(s). Box and Jenkins (1970) provide an extensive outline of this method. This method was not used in this work because the input data for the simulated process was deterministic, not stochastic.

Once the disturbance models have been identified and verified, experiments were carried out in order to determine the effect of existing or potential manipulated variables on the output variables, P and x. In this case, the distillate flow and reboiler duty had been identified as potential manipulated variables. Initial analysis of the time plots of the outputs, P and x, when subject to step disturbances indicated that the column pressure is affected by both distillate flow and reboiler duty while the bottoms composition is only affected by reboiler duty (see Figures 39-44). Additionally, it is noted that negative shifts in the reboiler duty have a greater effect on bottoms composition than positive shifts, which indicates a nonlinear relationship between x and Q. All three of the input/output relationships appear to obey a first-order plus dead time relationship. Recalling equation 8, it is noted that this model is nonlinear in the parameters, δ and g. Thus, the Levenberg-Marquardt nonlinear regression technique in StatGraphics® was

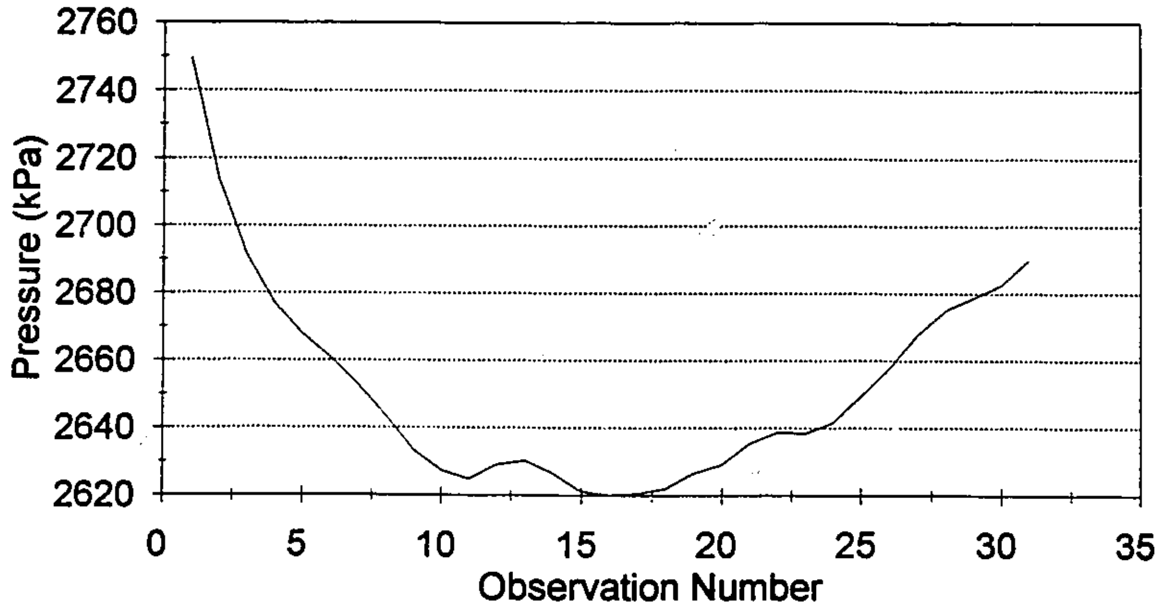


Figure 39: Dynamic response of column pressure to a 500 unit step decrease in reboiler duty.

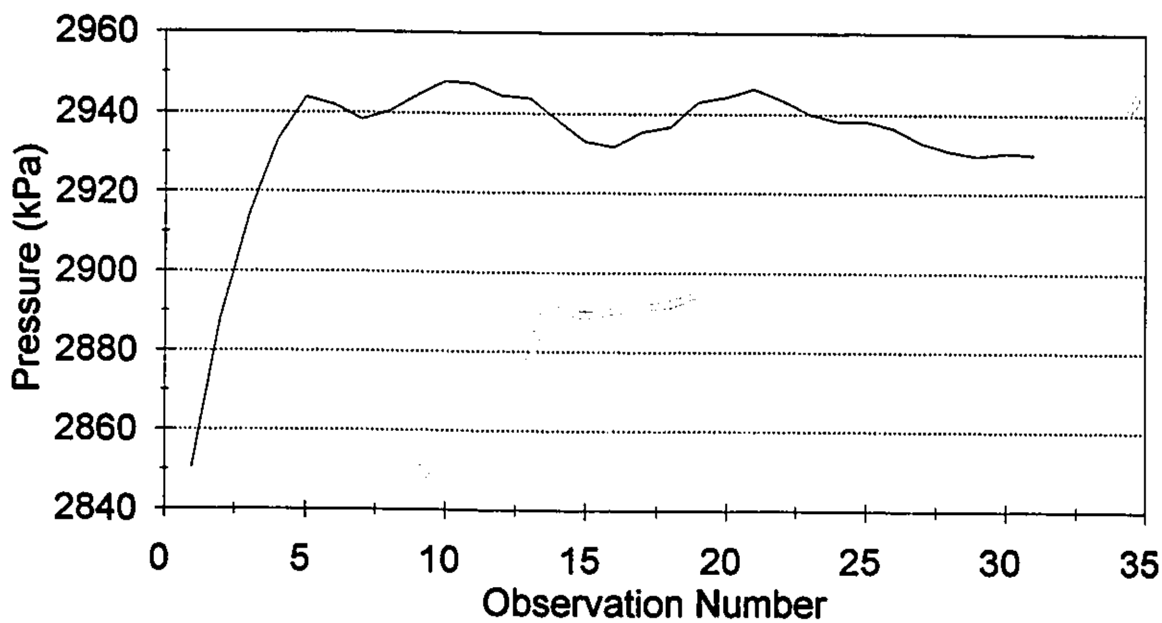


Figure 40: Dynamic response of column pressure to a 500 unit step increase in reboiler duty.

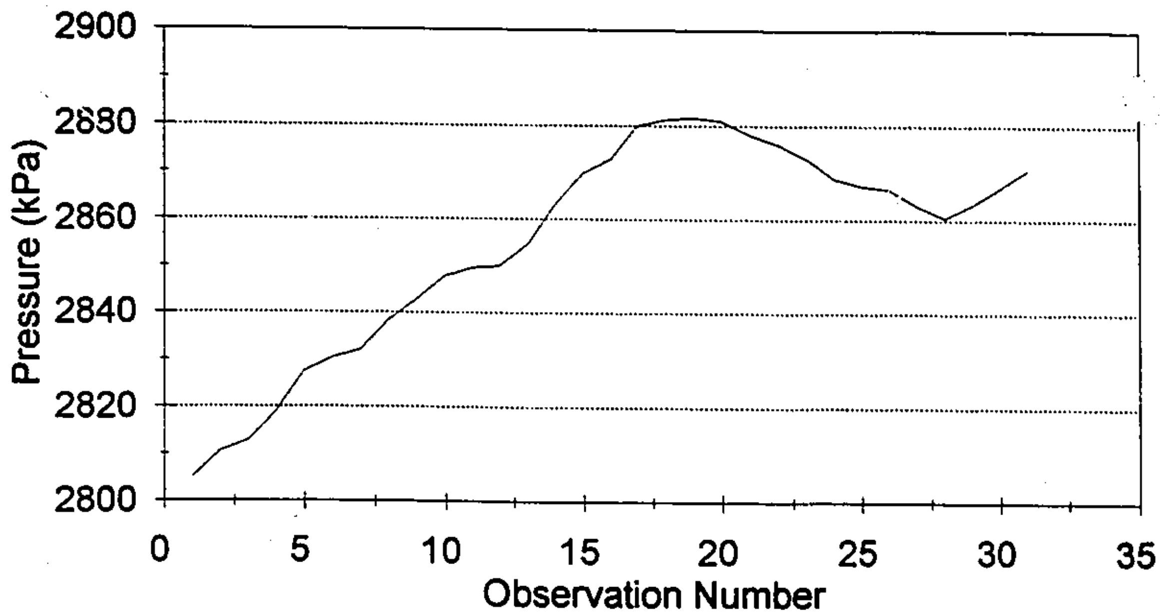


Figure 41: Dynamic response of column pressure to a 10 unit step decrease in the distillate flow.

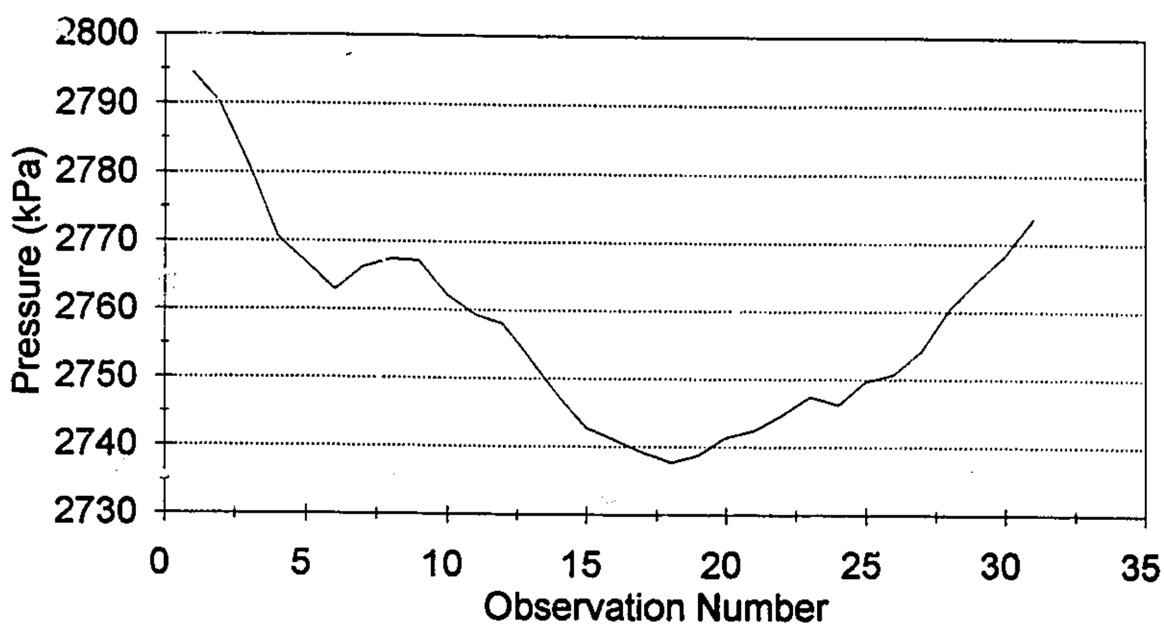


Figure 42: Dynamic response of column pressure to a 10 unit step increase in the distillate flow.

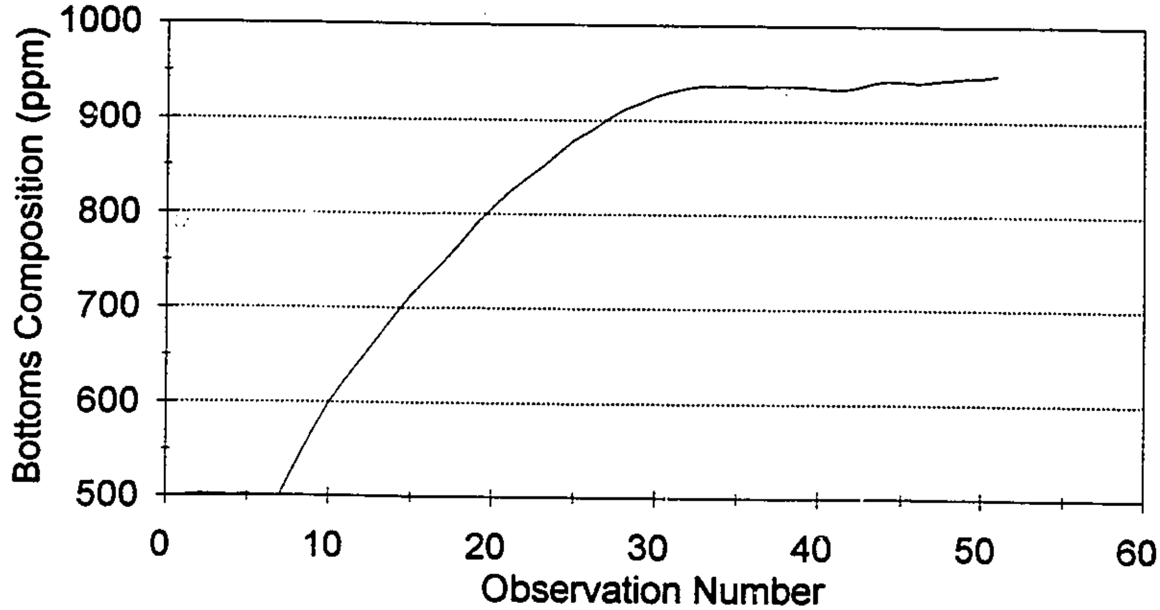


Figure 43: Dynamic response of the bottoms composition to a 500 unit step decrease in reboiler duty.

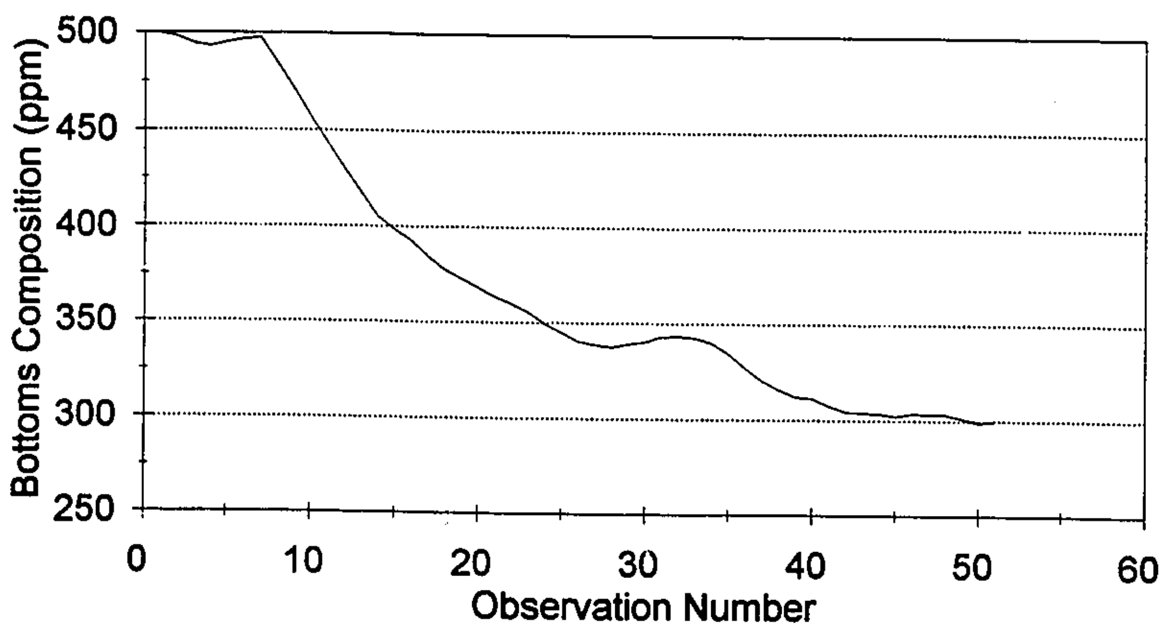


Figure 44: Dynamic response of the bottoms composition to a 500 unit step increase in reboiler duty.

used. The resulting transfer functions were

$$P_t = 2800 - \frac{0.67}{(1-0.85B)}(D_{t-1}-D^{ss}) \tag{51a}$$

$$P_t = 2800 + \frac{0.1}{(1-0.76B)}(Q_{t-1}-Q^{ss}) \tag{51b}$$

$$x_t = 500 - \frac{0.05}{(1-0.945B)}(Q_{t-8}-Q^{ss}) \tag{51c}$$

where Q^{ss} and D^{ss} are the steady-state values of the reboiler duty and distillate flow, respectively. Perhaps a more useful representation of equation 51b would be obtained by equating equation 51b to 51a to determine the relationship between reboiler duty and distillate flow, giving

$$D_t^* = -0.15\,\frac{(1-0.85B)}{(1-0.76B)}\,Q_t^* \tag{52}$$

where variables with stars are deviation variables (e.g., $D_t^* = D_t - D^{ss}$). Equation 52 will later be used to decouple the effects of the reboiler duty on the column pressure. The nonlinearity between the bottoms composition and reboiler duty, mentioned earlier, was handled by taking an average of the two parameters, δ and g, for the step increase and step decrease experiments.

STEP 4: Choosing an APC Algorithm

The next step was to identify a suitable automatic control scheme to regulate the process outputs, P and x. As was mentioned previously, if one possesses information about the disturbances and process dynamics then some form of MV controller should be used. This does not mean traditional PID controllers could not be used, but information about the process disturbances would be wasted. In a similar manner to that shown in Section 3.3, we derive MV feedback controllers for the distillation column. Since there is no dead time associated with the column pressure transfer functions we can simply use the controller shown in equation 49,

$$(1.0-(1+\phi_{1P})B+\phi_{1P}B^2)D_t^* = -\frac{1}{\omega_{PD}}\{(1+\phi_{1P})P_t^* - (\phi_{1P}+\delta_{PD}+\phi_{1P}\delta_{PD})P_{t-1}^* + \phi_{1P}\delta_{PD}P_{t-2}^*\} \tag{53}$$

However, this is the non-decoupled form of the controller, that is, this controller does not account for the interaction between reboiler duty, Q, and column pressure, P. Thus, utilizing equation 52, and noting that D^*_t must be premultiplied by $(1.0-(1+\phi)B+\phi B^2)$, to be consistent with equation 52, we obtain the decoupled form of the controller,

$$D_t^* = (1.0+\phi_{1P}B)D_{t-1}^* - \phi_{1P}D_{t-2}^* - \frac{1}{\omega_{PD}}\{(1.0+\phi_{1P})P_t^* - (\phi_{1P}+\delta_{PD}+\phi_{1P}\delta_{PD})P_{t-1}^* + \phi_{1P}\delta_{PD}P_{t-2}^*\} + \frac{\omega_{PQ}(1.0-\delta_{PD}B)\ (1.0-(1.0+\phi_{1P})B+\phi_{1P}B^2)}{\omega_{PD}(1.0-\delta_{PQ})}Q_t^* . \tag{54}$$

Substituting the parameter values obtained through modelling

$$D_t^* = 1.6D_{t-1}^* - 1.96D_{t-2}^* + 0.51D_{t-3}^* + 1.5(1.6P_t^* - 3.176P_{t-1}^* + 1.9996P_{t-2}^* - 0.3876P_{t-3}^*) + 0.15(Q_t^* - 2.45Q_{t-1}^* + 1.96Q_{t-2}^* - 0.51Q_{t-3}^*) . \tag{55}$$

Similarly, the controller for bottoms composition is

$$Q_t^* = 2.8713Q_{t-8}^* - 1.8713Q_{t-9}^* + 20.0\{2.8713x_t^* - 4.5847x_{t-1}^* + 1.7684x_{t-2}^*\} . \tag{56}$$

Due to the complexity of the derivation of equation 56 it has been presented in Appendix E.

A simulation program was developed once the disturbance models, process models and automatic process control schemes were identified. Thus, all of the data presented henceforth will be generated using the simulation software COLMSIM (see Appendix F).

The dashed line in Figure 45 shows the fluctuations in column pressure, in the absence of control, and the solid line indicates the effect of minimum variance control. Likewise, Figure 46 indicates graphically how well the MV controller does in keeping the bottoms composition close to target One can see that both of these controllers perform very well in keeping the controlled variable on target. However, a significant amount of autocorrelation still exists in the controlled bottoms composition, x_t. This autocorrelation is due to the process dead time. Since one must forecast the disturbance 8 units into the future, the controlled variable, x_t, becomes correlated with the previous 8 a_ts.

Figures 47 and 48 indicate the manipulations of the reboiler duty and distillate flow, respectively, required to maintain MV control. One can see that the amount of manipulation is quite excessive, for both manipulated variables. As one might expect there are stringent constraints placed on each of the manipulated variables. These constraints are $|Q_t| \leq 500$ and $|D_t| \leq 10$. Such constraints usually arise due to physical limitations of the final control elements (e.g., a valve can only open so far). Re-evaluation of Figures 47 and 48 indicates that the reboiler duty is operating within its designed limits, whereas the distillate flow does not perform within its specified limits. The dotted line in Figure 45 illustrates that control of the column pressure is greatly affected by the introduction of these constraints, while control of the bottoms composition is unaffected. Figure 49 shows the resulting distillate flow for the constrained situation.

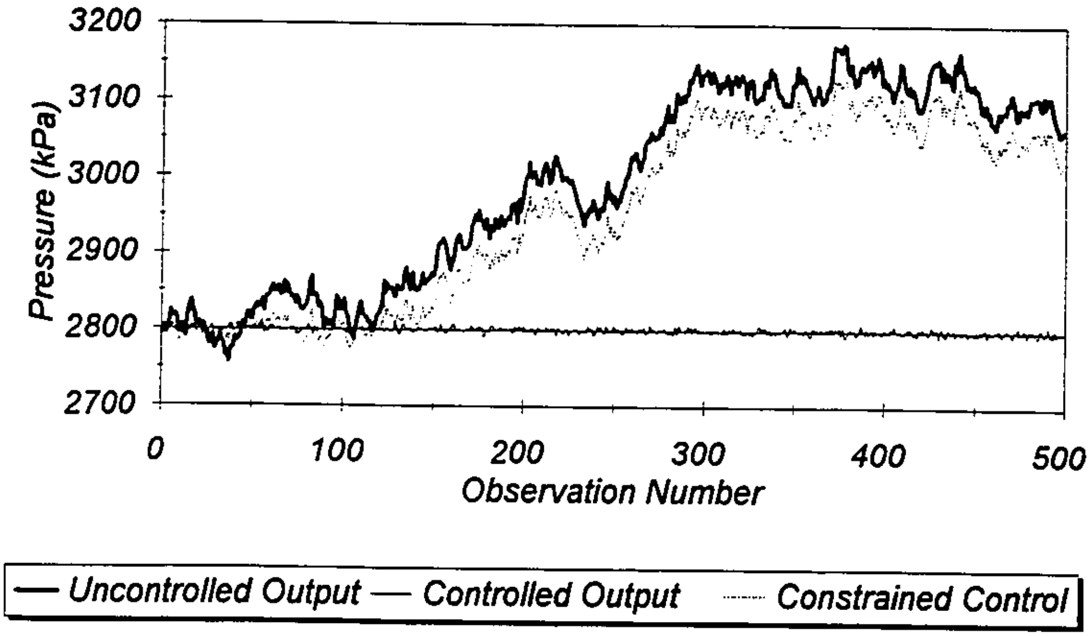


Figure 45: Column pressure; without automatic control, with MV control and with constrained control.

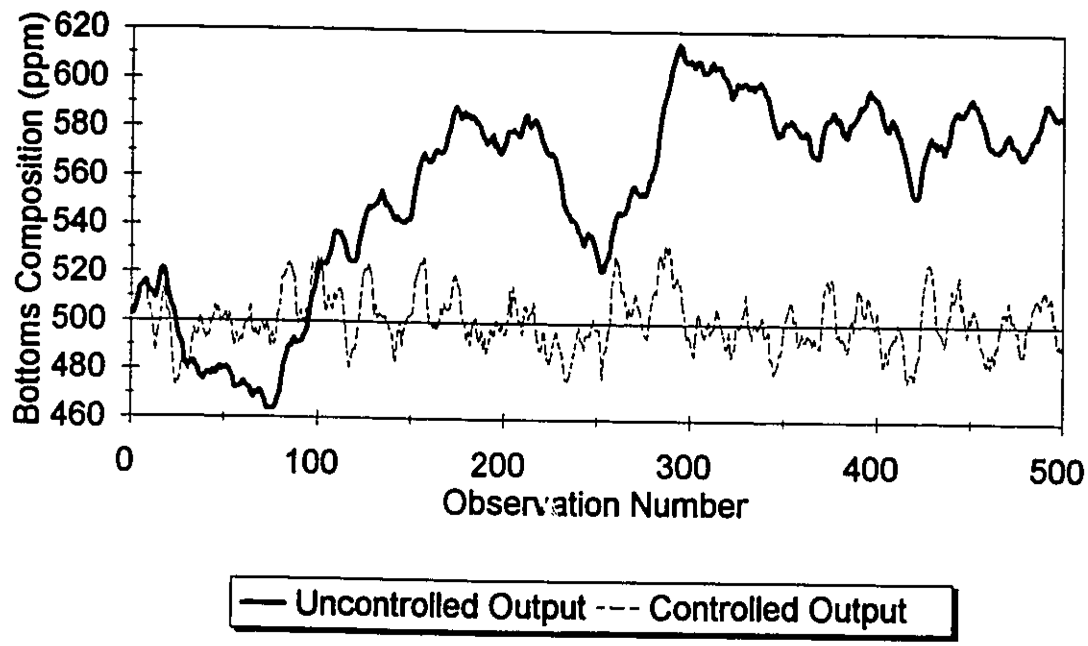


Figure 46: Bottoms composition without automatic control and with MV control.

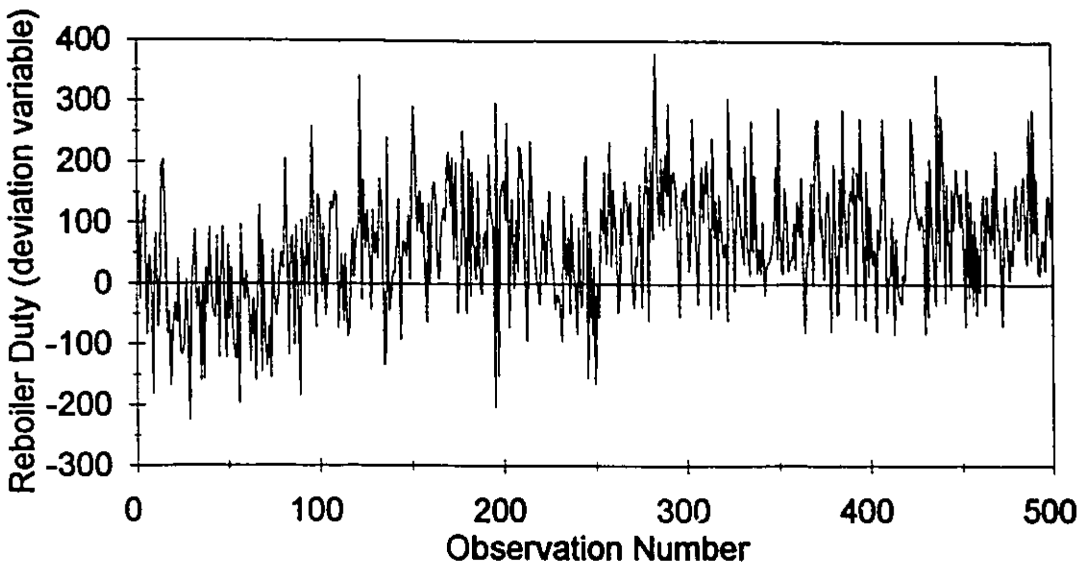


Figure 47: Reboiler duty required to achieve MV control.

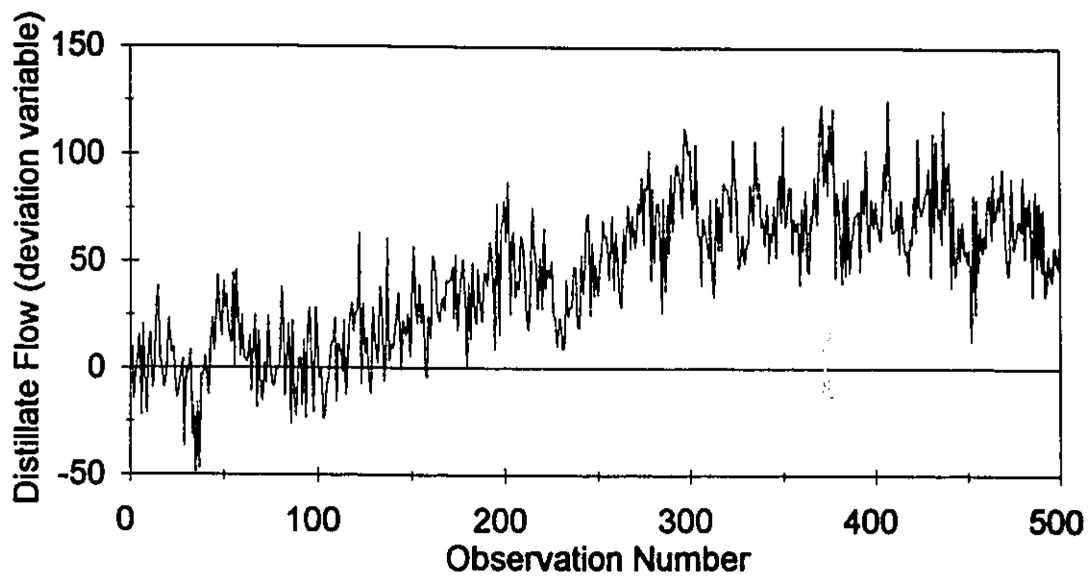


Figure 48: Distillate flow required to achieve MV control.

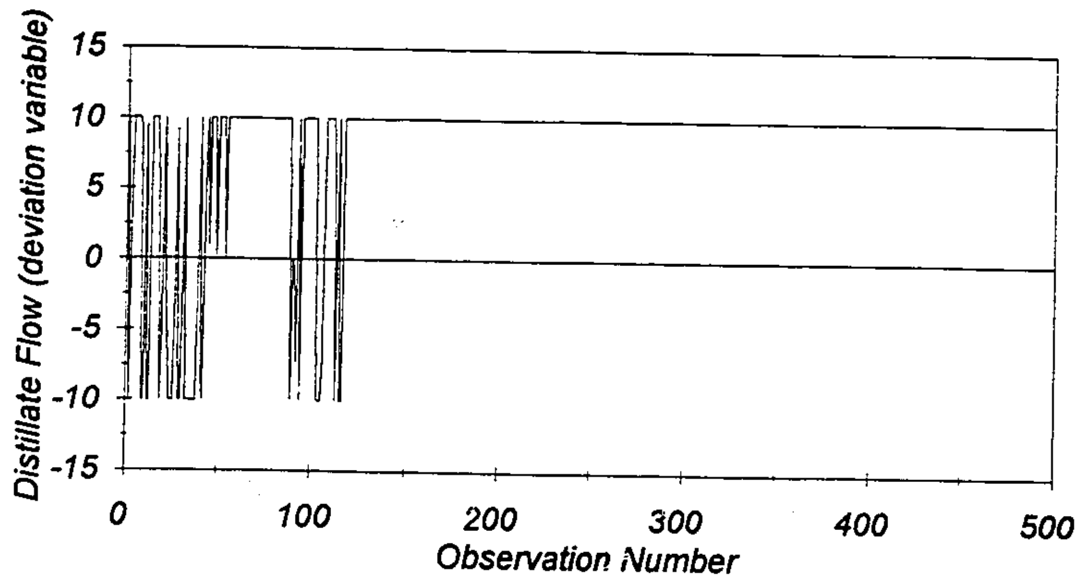


Figure 49: Distillate flow when operational constraints are imposed.

It should be noted that a great deal of the control action required to control the column pressure is due to the excessive control action needed to maintain bottoms composition, since changes in reboiler duty affects both column pressure and bottoms composition. If one could reduce the amount of manipulation of the reboiler duty, then more effective control of the column pressure would result. To demonstrate this point, the interaction between the reboiler duty and column pressure is removed (from the simulation) and the resulting control is shown in Figure 50. One can see that much better control results when the interaction term is removed, however, the output is still not stationary and therefore the manipulated variable, D_t, is still being saturated. Thus, the source of the nonstationarity must ultimately be removed to enable efficient APC.

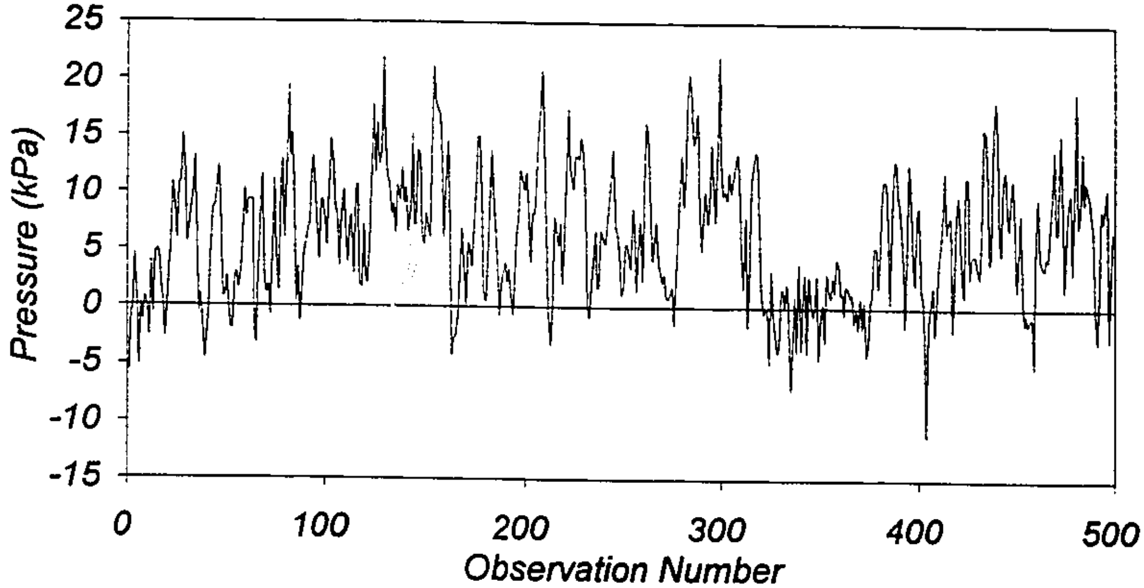


Figure 50: Automatic control of column pressure when reboiler interaction is absent

STEP 5: Choice of SPC Charting Procedure and Variable(s)

Once the automatic process control has been determined, it is time for statistical process control to be introduced. The next logical step to take at this point is to determine which variable(s) are suitable for process monitoring, and what type(s) of charting procedure(s) are going to be used. It was indicated in step 2 that perhaps a re-evaluation of the process is required before successful integration can be achieved for the C_3 splitter used in the case study. However, we did not have the luxury of being able to make the necessary changes to the process required to yield stationary, chartable data. Therefore, some of the problems that may be encountered if step 2 is not given the consideration it deserves will be demonstrated.

One of the obvious drawbacks to using the available data for identification of assignable cause was that the disturbances were highly nonstationary. The ARIMA(1,1,0) disturbances have already been shown to exhibit a great degree of nonstationarity, therefore one is limited to identification of only very large (catastrophic) assignable causes. Additionally, the constraints placed on the distillate flow excluded it as a suitable choice for a charting variable (see Figure 47). The only charting variables available were the deviations from target of the controlled variables, P and x. However, due to the constraints placed on the distillate flow, the deviation from target of the column pressure was still nonstationary and therefore not suitable for charting (see Figure 45). Thus, we were limited to identification of assignable cause in the bottoms composition. There are even problems associated with trying to identify assignable cause in the controlled bottoms composition. The first is due to the correlation between the output measurements. Secondly, the deviation from target of the output variable, x, is equivalent to the residual when MV control is used. It has been shown, by several authors, that residual plots are not effective at identifying step changes in the mean value of the disturbance model (Harris and Ross, 1990; MacGregor, 1991). The only way in which these problems could be alleviated would be to identify and remove the cause of the nonstationarity (i.e., increase the cooling capacity of the overhead condenser).

STEP 6: Continuous Process Improvement

As with all process improvement schemes, just having them in place does not mean that our work is finished. For a process improvement scheme, such as an integrated APC/SPC control system, to work effectively one must constantly be pushing the limits of the process looking for ways in which further improvements can be made.

The ultimate goal, no matter how unreasonable it may seem, is to achieve a process whose disturbances follow the SPC model shown in equation 1 with a small variance. These process improvements may arise through the use of designed experiments, evolutionary operation or simply by accident. Many new discoveries happen when a process inadvertently moves into an operating region not previously tried, or when a temporary change in suppliers yields a better product. Additionally, each time an assignable cause is identified and removed from the process one should be gaining valuable information about how the process operates.

The need for the removal of the cause of nonstationarity has become very evident in the discussion of implementing the automatic control scheme (Step 4) as well as the statistical monitoring scheme (Step 5). Therefore the COLMSIM software was revised to allow simulations to be run with stationary disturbance models. The stationary models implemented were the ARMA(1,1) equivalent to the ARIMA disturbances identified in Step 1. This was achieved by simply removing the ∇ operator from the nonstationary disturbance models. Although this is an artificial method of achieving nonstationarity, it allows a comparison of the relative improvement between a stationary and nonstationary system.

By removing the ∇ operator from the disturbance model a first order autoregressive, AR(1), model is obtained (see Figures 51 and 52). One can see, in comparing the stationary AR(1) disturbances to the ARIMA(1,1,0) disturbance, that the amount of deviation of the disturbances from their respective nominal values is greatly reduced. The resulting control of bottoms composition and column pressure, with the manipulated variable constraints, are shown in Figures 53 and 54. Table 12 indicates the ARL results for Shewhart charts of the reconstructed output and residuals. Although the $1\sigma_a$ shifts are not identified quickly, the $2\sigma_a$ and 3_σ shifts are readily identified. This is a significant improvement from only being able to identify catastrophic disturbances for the nonstationary system.

Table 12: ARL results, using Shewhart charts, for the reconstructed output and residuals of column pressure, when stationarity is induced in the Shell C_3 splitter.

Size of Shift	Reconstructed Output, W_t	Residuals (P_t-$P_{t/t-1}$)
0	369.85	369.15
1σ	89.40	212.40
2σ	20.54	78.15
3σ	7.58	29.12

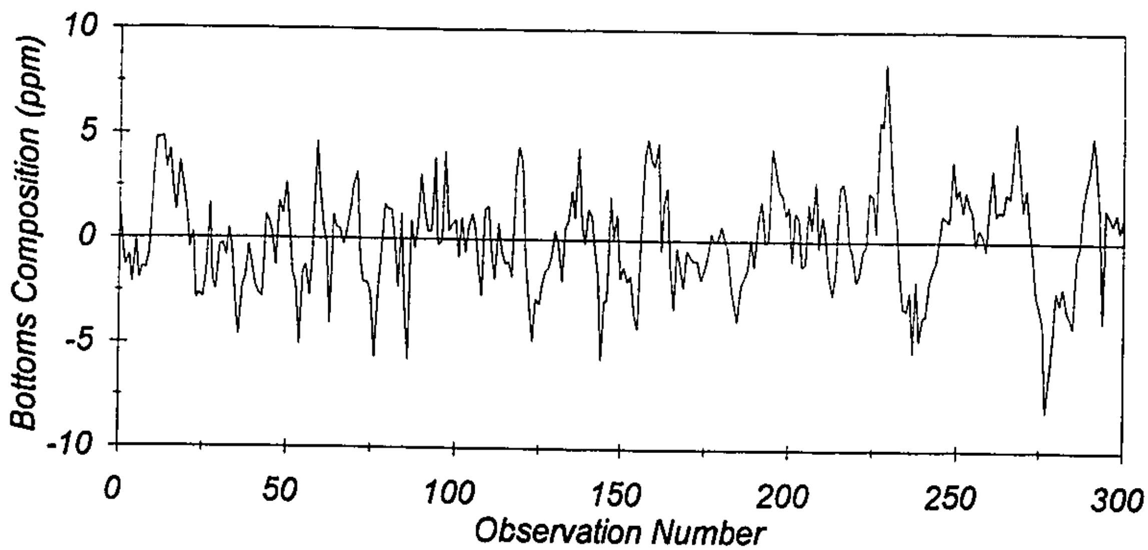


Figure 51: AR(1) model utilized to describe the disturbance affecting the bottoms composition for the stationary process example, ϕ=0.66.

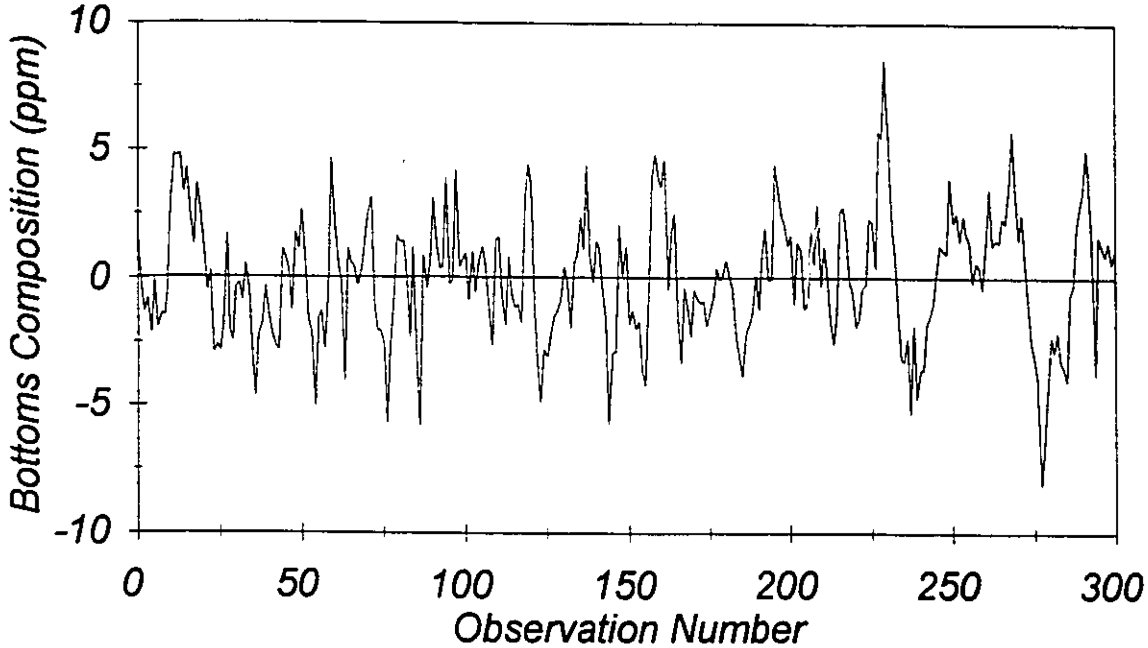


Figure 52: AR(1) model utilized to describe the disturbance affecting the column pressure for the stationary process example, $\phi=0.60$.

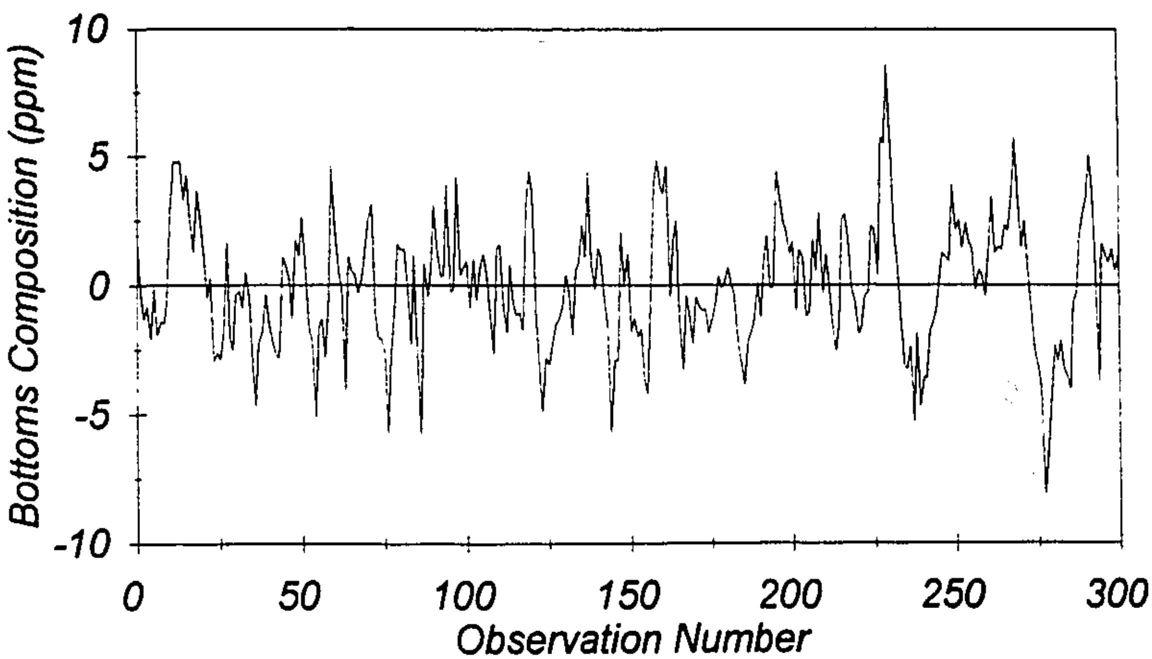


Figure 53: Bottoms composition for stationary system, when MV control is utilized.

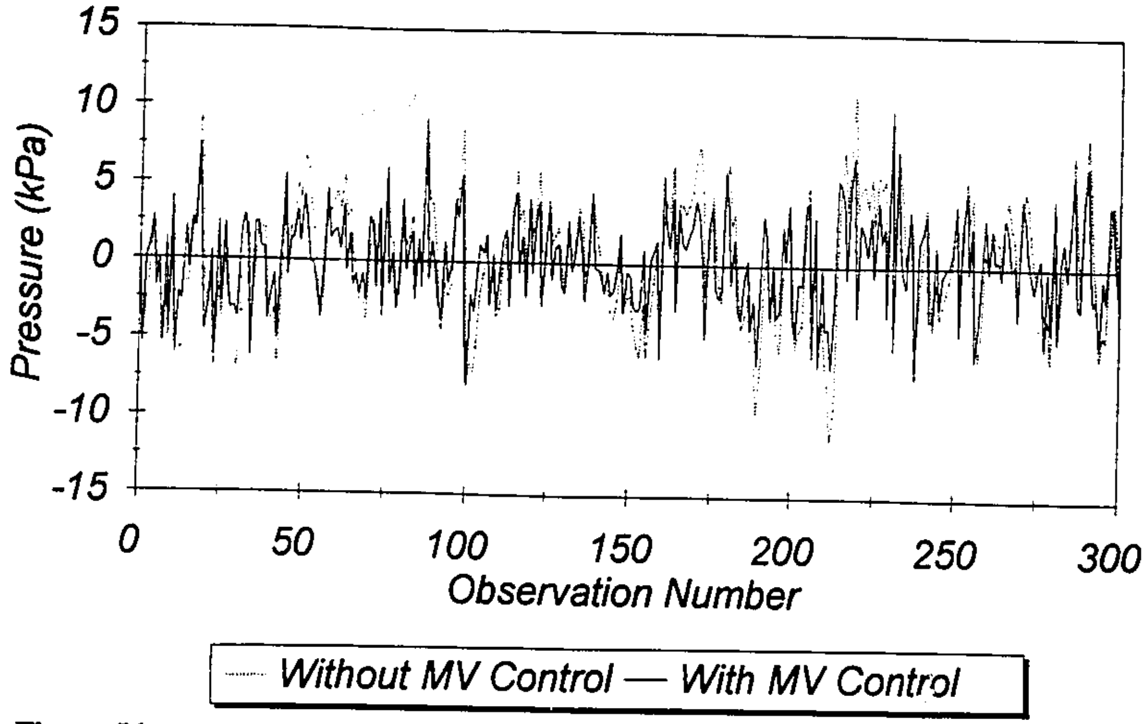


Figure 54: Column pressure for stationary system, when MV control is utilized.

Not only were the improvements in APC and SPC identified, but also the potential savings from reduced reboiler fluctuations were investigated. Taguchi's loss function (Ryan, 1989) was utilized to determine the relative cost savings resulting from removing the nonstationarity. A linear gain function was used for negative deviations of the reboiler duty from target and a quadratic loss function was used for positive deviations. Consequently, you are rewarded for having lower than target values of the reboiler duty and penalized for having reboiler duties higher than target (see Figure 55). These two functions are given by

$$\textit{Linear Loss Function:} \quad L = k_L(Y-\tau) \tag{57a}$$

$$\textit{Quadratic Loss Function:} \quad L = k_L\,(Y-\tau)^2 \tag{57b}$$

where τ is the reboiler duty set point and k is a model parameter which was set arbitrarily to unity. Although one might expect the loss functions to be linear for both the positive and negative reboiler changes, a skewed loss function was chosen to reflect two unique conditions of this example. The first condition arises when the maximum steam flowrate is encountered, resulting in a need for higher temperature steam. The second condition arises from the interaction between the reboiler duty and the column pressure. When the reboiler duty becomes too high, the column pressure rises to a level for which the distillate flow cannot make appropriate compensation, resulting in the column contents being dumped to flare. Since these are both undesirable and more costly situations a larger penalty was imposed upon positive shifts in the reboiler duty.

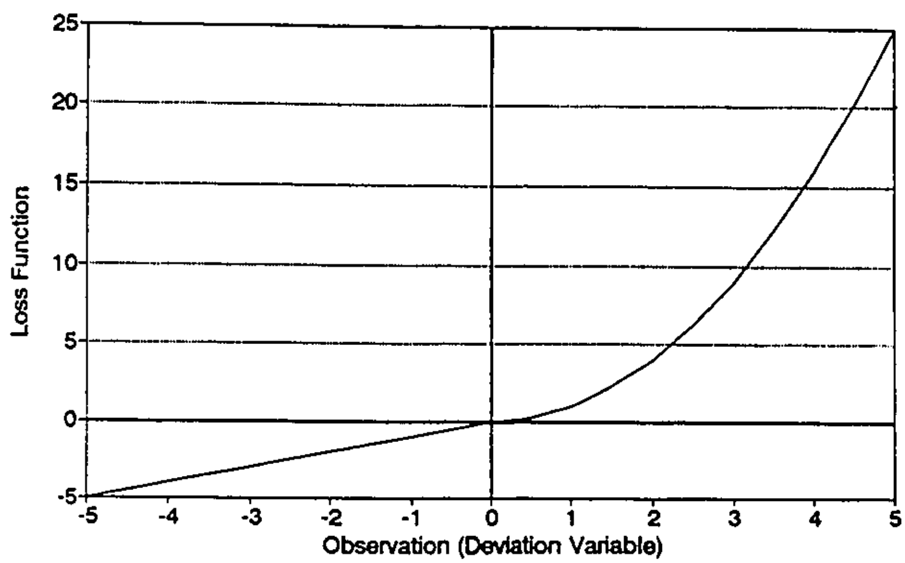


Figure 55: Loss Function Employed to Determine Relative Reboiler Cost Savings Resulting from Introducing Stationarity.

Figure 56 shows a typical plot of the reboiler duty versus time, for the nonstationary system. If it were possible to fix the mean value of the reboiler duty, while

Figure 56 shows a typical plot of the reboiler duty versus time, for the nonstationary system. If it were possible to fix the mean value of the reboiler duty, while keeping the same amount of variation, we would have a plot similar to that shown in Figure 57. Thus, it would be interesting to determine the relative improvements obtained by simply keeping the process at a fixed mean value. Using the loss functions shown in equations 57a and 57b, 4000 simulations were run to determine the relative difference between the two situations indicated in Figures 56 and 57. The loss function for the stationary process was 2935.0 while the nonstationary process yielded a value of 17,103.0. This is more than a six-fold improvement for the stationary process. Again, this gives further support to the need to remove the cause of nonstationarity in any process subject to either form of process control, SPC or APC.

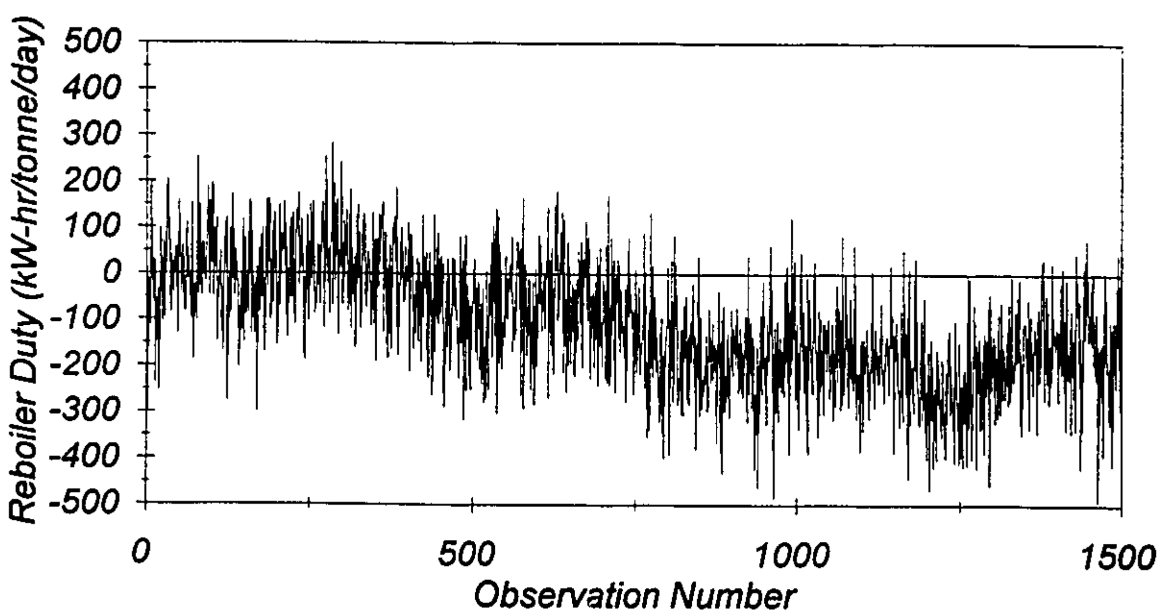


Figure 56: Example of a nonstationary reboiler duty.

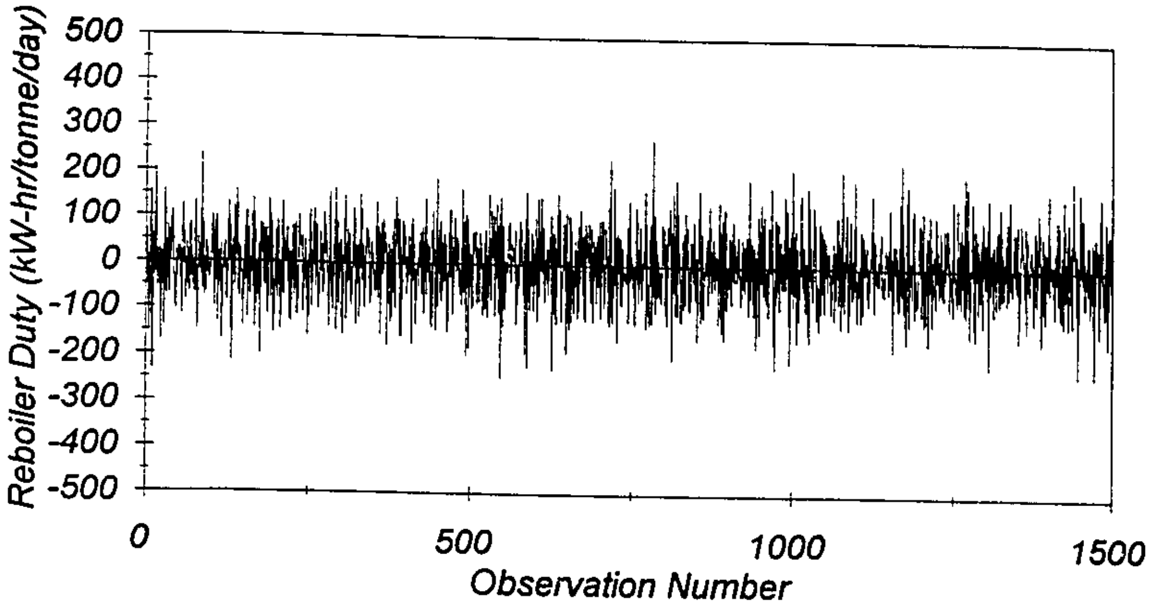


Figure 57: Example of a stationary reboiler duty.

5.3 Summary

This chapter has shown, through use of an example, an efficient six-step procedure for integrating SPC with APC. The C_3 splitter was a very useful example, as it not only highlighted the six-steps for achieving an integrated control system but also indicated some of the pitfalls that may be encountered. These pitfalls included: the presence of nonstationary disturbances, saturation of the manipulated variable and the charting of correlated data. This example also showed explicitly that setting-up an integrated system of process control is not as easy as following a recipe. Every process is different and has its own unique problems for the control engineer to deal with. Furthermore, this example has demonstrated that significant process improvements can result, through integration, if it is carried out in a careful and systematic manner.

There are many similarities between the six-step procedure outlined above and the four step procedure presented by Vander Wiel *et al.* (1993). Both strategies contain the essential steps needed to achieve an integrated system of APC and SPC; process and disturbance identification, modelling and estimation, control-rule design and process monitoring. Nevertheless, for model identification, Vander Wiel *et al.* (1993) favours constantly exciting the process with a PRBS while feedback control is being employed. Additionally, he considers an ARMAX model to describe both the transfer function of the process dynamics and the disturbance. Whereas in this work the process dynamics and disturbance are modelled separately. However, these differences are not of considerable concern. The biggest difference is in control-rule design and process monitoring.

The MV control algorithm derived by Vander Wiel *et al.* (1992) can only be used on their specific process or processes of a similar nature. FOPDT models can be used to represent the process dynamics of a large number of situations in the CPI and a first-order ARMA model is quite often representative of process disturbances. Therefore the generalized MV controllers derived in Section 3.3 are applicable in more situations than Vander Wiel's.

With respect to process monitoring, Vander Wiel *et al.* (1993) does an excellent job at identifying the function of process monitoring in ASPC but does not indicate how it should be carried out. As Vander Wiel *et al.* (1993) points out, the manner in which a specified process upset manifests itself in a particular data stream is a function of the control method employed. Nevertheless, one needs to identify a control method (i.e., MV feedback control) and begin compiling how changes manifest themselves in various data streams, as done in this body of work.

Chapter 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

6.1.1 N^{th}-Difference Charts To monitor nonstationary processes, n^{th}-difference charts were developed and guidelines for their use established, specifically:

1) The manipulated variable is the best process variable for identifying assignable cause using n^{th}-difference charts.

2) N^{th}-difference charts are effective at identifying step shifts in the mean value of IMA(1,1) disturbances when $\theta < 0.7$.

3) The efficiency of n^{th}-difference charts is significantly reduced upon the introduction of mild positive autocorrelation, $\phi > 0.2$.

4) The optimal degree of differencing is greatly influenced by the size of disturbance one wishes to detect and the amount of nonstationarity in the disturbance. Tables and Figures of ARL data that have been compiled can serve as useful guidelines for the design of n^{th}-difference control charts.

6.1.2 Disturbance Propagation Based on the study of the propagation of disturbances through the process to potential charting variables, the following conclusions can be drawn:

1) For a first-order process subject to an ARMA(1,1) disturbance and under the influence of MV feedback control the charting variables should be chosen as follows:

   the residuals should be used when θ is larger than ϕ, regardless of the extent of the process inertia, δ,

   the reconstructed outputs should be used when ϕ is larger than θ and δ is large,

   otherwise, the manipulated variable should be chosen.

2) ARIMA(1,1,0) models display the greatest amount of nonstationarity of all first-order disturbance models.

3) For all ARIMA(1,1,1) models, as ϕ increases and θ decreases, the natural drift of the disturbance model can exceed the underlying shift caused by process upsets that are considered significant. In these situations, looking for assignable causes of magnitude 1,2 or $3\sigma_a$ is pointless.

6.1.3 Effect of Sampling Interval on Disturbance Detection A study of the effect of the size of the sampling interval on the effectiveness of a charting procedure to detect disturbances lead to the following conclusions:

1) Increasing the sampling interval, and thus reducing the correlation between

successive data points, does not improve one's ability to identify assignable cause on Shewhart charts when the process disturbance is characterized by an ARMA(1,1) model.

2) Only when there are significant costs associated with sampling is an investigation into optimal sampling schemes required.

3) Sampling all of the available data has the advantage of providing a more complete picture of the process. A less frequently sampled process may go out of control before the next data point becomes available.

6.1.4 SPC/APC Integration Strategy The case study of the Shell Canada C_3 splitter provided a framework in which the overall problem of integrating SPC with APC could be addressed and evaluated. The following are conclusions reached while setting up an integrated SPC/APC system on the C_3 splitter:

1) The six-step procedure:

   i) disturbance identification and modelling,

   ii) process evaluation,

   iii) identification and modelling of process dynamics,

   iv) choice of APC algorithm,

   v) choice of SPC charting procedure and variable(s),

   vi) continuous process improvement

   not only provides a useful basis for the integration of SPC with APC in the continuous processing industry but also provides some insight into the potential pitfalls along the way.

2) The detection capabilities of all of the potential monitored variables were not very effective for processes under the influence of nonstationary disturbances. Thus, the need for removal of nonstationarity in process disturbances is imperative if successful integration of SPC with APC is to be achieved.

3) The ability of the APC algorithm to adequately maintain a process on target is greatly hindered by the presence of nonstationary disturbances. For extreme cases of nonstationarity the manipulated variables are likely to become saturated.

4) Using Taguchi's loss function, simulations identified the potential for a large savings in reboiler duty by removal of disturbance nonstationarity.

6.2 RECOMMENDATIONS FOR FURTHER WORK

1) Evaluation of optimal EWMA parameters for correlated data is needed. Since EWMA control charts are more efficient than Shewhart charts at detecting small process upsets it would be beneficial to construct tables of optimal parameter values (λ and L) for EWMA charts when applied to correlated data.

2) Use of the six-step procedure to set-up an integrated control system on a real industrial process should be attempted. The resulting experience on

a real process could potentially yield an improved, more efficient procedure for integrating SPC with APC.

3) Evaluation of the effectiveness of constrained MV control for keeping the process outputs, P and x, on target should be investigated. The nonstationary disturbances affecting the C_3 splitter resulted in saturation of the manipulated variables. If less stringent constraints were placed on the allowable variation in the output variables then perhaps more efficient control could be realized (i.e., eliminate saturation of the manipulated variables).

4) Even though the detection capabilities of many of the SPC charts are satisfactory, the usefulness of such charts as diagnostic tools is limited (perhaps non-existent). Usually when an alarm is signalled in a processing plant a search is carried out for the root cause of the process upset. Traditionally, such a search has been based on judgement, there is no scientific method for identifying the location of an assignable cause. However, one method that might reduce the degrees of freedom associated with such a search would be to monitor all of the important process inputs while implementing feedforward control.

Chapter 7

REFERENCES

Box, G.E.P. and G.M. Jenkins, "Time Series Analysis: Forecasting and Control", Holden Day, San Francisco (1970).

Box, G.E.P. and T. Kramer, "Statistical Process Monitoring and Feedback Adjustment - A Discussion", Technometrics, **34**, 251-267 (1992).

Box, G.E.P. and T. Kramer, "Statistical Process Control and Automatic Process Control - A Discussion", Report No. 41, University of Wisconsin-Madison, 1- 29 (1990).

Box, G.E.P. and T. Kramer, "Process Control From an Economic Point of View - Chapter 1: Industrial Process Control", Report No. 42, University of Wisconsin-Madison, 1-24 (1990).

Cott, B., "The Development of a Nonlinear Adaptive Generic Model Controller for Chemical Reaction Quality Control", submitted to Advances in Process Control (1993).

Cott, B, "Systems and Control Symposium IV Process Identification Workshop" 42nd Canadian Chemical Engineering Conference Proceedings, 337-340 (1992).

Deshpande, P.B., R.E. Hannula, M.A. Bhalodia and C.W. Hansen, "Achieve Total Quality Control of Continuous Processes", Chem. Eng. Prog., **89**, 59-66 (1993).

Deshpande, P.B., "Process Control Education: A Quality Control Perspective", Chem. Eng. Educ., **27** (3), 170-175(1993).

English, J.R. and K.E. Case, "Control Charts Applied as Filtering Devices Within a Feedback Control Loop", IIE Trans., **22**, 255-269 (1990).

English, J.R., M. Krishnamurthi and T. Sastri, "Quality Monitoring of Continuous Flow Processes", unpublished paper (1990).

Goldsmith, P.L. and H. Whitfield, "Average Run Lengths in Cumulative Chart Quality Control Schemes", Technometrics, **13**, 221-230 (1971).

Harris, T.J. and W.H. Ross, "Statistical Process Control Procedures for Correlated Observations", Can. J. Chem. Eng., **69**, 48-57 (1991).

Harris, T.J., "Interfaces Between Statistical Process Control and Engineering Process Control", Course Notes, Queens University (1987).

Hoerl, R.W. and A.C. Palm, "Discussion: Integrating SPC and APC", Technometrics, **34**, 268-272 (1992).

Hunter, J.S., "The Exponentially Weighted Moving Average", J. Qual. Tech., **18**, 203-210 (1986).

Ledolter, J. and B. Abraham, Notes from short course presented at the 1984 ASA annual meeting in Philadelphia, Pennsylvania.

Lucas, J.M. and R.B. Crosier, "Robust CUSUM", Commun. in Statist. Part A - Theory and Methods, **11**, 2669-2687 (1982).

Lucas, J,M. and M.S. Saccucci, "Exponentially Weighted Moving Average Control Schemes: Properties and Enhancements", Technometrics, **32**, 1-16 (1990).

Lucas, J.M., "The Design and Use of V-Mask Control Schemes", J. Qual. Tech., **8**, 1-12 (1976).

MacGregor, J.F., "On-Line Statistical Process Control", Chem. Eng. Prog., **84**(10), 21-31 (1988).

MacGregor, J.F., "Discussion: Integrating SPC and APC", Technometrics, **34**, 273-275 (1992).

Montgomery, D.C. and C.M. Mastrangelo, "Some Statistical Process Control Methods for Autocorrelated Data", J. Qual. Tech., **23**, 179-193 (1991).

Nelson, L.S., "The Shewhart Control Chart - Tests for Special Causes", J. Qual. Tech., **17**, 114-116 (1984).

Page, E.S., "Continuous Inspection Schemes", Biometrika, **41**, 101-115 (1954).

Palm, A.C., "SPC Versus Automatic Process Control", ASQC Qual. Cong. Trans., 694-699 (1990).

Roberts, S.W., "Control Chart Tests Based on Geometric Moving Averages", Technometrics, **1**, 239-250 (1959).

Ryan, T.P., "Statistical Methods for Quality Improvements", John Wiley and Sons, New York (1989).

Shewhart, W.A., "Economic Control of Quality of Manufactured Product", McMillan, New York (1931).

Slocomb, R.A.W., "Determining Assignable Cause in Continuous Processes", B.A.Sc. Thesis, University of Ottawa (1991).

Stephanopoulos, G., "Chemical Process Control", Prentice-Hall, New Jersey (1984).

Vander Wiel, S.A., T.T. Tucker, W.F. Faltin and N. Doganaksoy, "Algorithmic Statistical Process Control: Concepts and an Application", Technometrics, **34**, 286-297 (1992).

Vander Wiel, S.A., T.T. Tucker, W.F. Faltin, "Algorithmic Statistical Process Control: An Elaboration", Technometrics, **35**, 363-375 (1993)

Wardrop, D.M. and C.E. Garcia, "Discussion: Integrating SPC and APC", Technometrics, **34**, 281-282 (1992).

Western Electric Co. Inc., "Statistical Quality Control Handbook", Delmar Printing Co., North Carolina (1956).

Appendix A

Derivation of the Variance of the 5^{th}-Difference of an IMA(1,1) Disturbance

In order to set up SPC control charts for the purpose of monitoring, one must be able to determine suitable control limits for such charts. One way in which this can be done is by calculating the variance of the variable being monitored. Since the n^{th}-difference chart is new it is worthwhile calculating the variance of such a variable being charted.

Therefore, starting with the equation of the MV controller used to regulate a first-order process subject to an IMA(1,1) disturbance,

$$X_t = X_{t-1} - \frac{1}{\omega_0}\{(1-\theta)y_t + (\delta\theta-\delta)y_{t-1}\} \qquad \textbf{(58)}$$

where X_t is the value of the manipulated variable at time,t, y_t is the output variable deviations from target θ is the moving average parameter and δ is the process inertia. Differencing at time t and t-5 one obtains the 5^{th}-difference. The 5^{th}-difference is thus,

$$\begin{aligned} D_{5th} &= X_t - X_{t-5} \\ &= X_{t-1} - X_{t-6} - \frac{(1-\theta)}{\omega_0}\{[y_t - \delta y_{t-1}] - [y_{t-5} - \delta y_{t-6}]\} \end{aligned} \qquad \textbf{(59)}$$

Taking the conditional expectation of the square of the 5^{th}-difference minus its mean value will give the variance of D_{5th}. However, one must first express equation 59 in terms of past values of a_t's otherwise the expression for the variance of D_{5th} will require variances of the X_t's, which for nonstationary processes are undefined. Thus if we expand equation 58, for X_{t-1}, we obtain

$$X_{t-1} = X_{t-6} - \frac{(1-\theta)}{\omega_0}\{(y_{t-1} - \delta y_{t-2}) + (y_{t-2} - \delta y_{t-3}) + (y_{t-3} - \delta y_{t-4}) + (y_{t-4} - \delta y_{t-5}) + (y_{t-5} - \delta y_{t-6})\} \quad (60)$$

which when substituted into equation 59 yields,

$$D_{5th} = -\frac{(1-\theta)}{\omega_0}\{y_t + (1-\delta)y_{t-1} + (1-\delta)y_{t-2} + (1-\delta)y_{t-3} + (1-\delta)y_{t-4} - \delta y_{t-5}\}. \quad (61)$$

Taking the conditional expectation of the square of equation 61, since the mean value, μ, of a difference is 0, gives the variance of D_{5th}

$$E[(D_{5th}-\mu)(D_{5th}-\mu)] = [\frac{(1-\theta)}{\omega_0}]^2\{E[y_t^2] + (1-\delta)^2E[y_{t-1}^2] + (1-\delta)^2E[y_{t-2}^2] + (1-\delta)^2E[y_{t-3}^2] + (1-\delta)^2E[y_{t-4}^2] + \delta^2E[a_{t-5}] + cross\ terms\} \quad (62)$$

where all of the cross terms are set to zero, since the y_t's are independent (for MV control) and therefore not correlated. All of the $E[y_i^2]$, $i=0,1,\ldots,5$, are simply the variance of the white noise, σ_a^2. Therefore, substituting σ_a^2 in the appropriate places gives the final expression for the variance of D_{5th},

$$Var[D_{5th}] = [\frac{(1-\theta)}{\omega_0}]^2\{4(1-\delta)^2+\delta^2+1\}\sigma_a^2. \quad (63)$$

Therefore, one can see that the variance of the n^{th}-difference of an IMA(1,1) disturbance is simply,

$$Var[D_{5th}] = [\frac{(1-\theta)}{\omega_0}]^2\{(n-1)(1-\delta)^2+\delta^2+1\}\sigma_a^2 \quad (64)$$

where n is the degree of differencing.

Appendix B

SPCSIM FORTRAN PROGRAM

This appendix contains a listing of the SPCSIM FORTRAN code and a sample data file. This program allows simulations of first-order plus dead time processes, with minimum variance feedback control when subject to an ARMA(1,1) disturbance or first-order processes when subject to ARIMA(1,1,1) disturbances. PID controllers can also be used but controller tuning is required. The three traditional SPC charting techniques - EWMA, CUSUM and Shewhart charts - are available for process monitoring purposes. When the disturbance model is represented by an ARIMA(1,1,1) disturbance then n^{th}-difference charts may also be utilized. The reconstructed output, controlled variable deviations from target and manipulated variable are all available as process monitoring variables. A trial and error method is required for setting the control limits in the data file for the SPC charts. All of the process parameters can be set to specified values and the simulation time and the number of simulations to be carried out can also be set as needed.

The listing for SPCSIM follows:

```
      PARAMETER (N=5000)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),
     &  RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),
     &  RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),
     &  SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,
     &  ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N)
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP,
     &        SCL,EWCL,DFCL,XSTD
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH,IRUN1,IRUN2
C      REAL R(N)
      EXTERNAL DRNNOA,DSCAL,DADD,RNSET
      CALL READER
C ********************************************************************
```

```
C    RANDOM NUMBER GENERATOR                                          SPC00150
C ******************************************************************* SPC00160
     DO 626 JJ=1,NSIM                                                 SPC00170
     ISEED=JJ*675                                                     SPC00180
     NR=ISIM                                                          SPC00190
     XSTD=1.0D0                                                       SPC00200
     XM=0.0D0                                                         SPC00210
     IRUN1=0                                                          SPC00220
     IRUN2=0                                                          SPC00230
     CALL RNSET(ISEED)                                                SPC00240
     CALL DRNNOA (NR, R)                                              SPC00250
     CALL DSCAL (NR, XSTD, R, 1)                                      SPC00260
     CALL DADD (NR, XM, R, 1)                                         SPC00270
C ******************************************************************* SPC00280
C    FOR PID CONTROLLER MUST FIRST TUNE IT (IE: ZIEGLER NICHOLS)      SPC00290
C ******************************************************************* SPC00300
C                                                                     SPC00310
     TD=0.0D0                                                         SPC00320
     EKP=(1.0D0-THETA)*DELTA/(G*(1.0D0-DELTA))                        SPC00330
     EKI=(1.0D0-THETA)/G                                              SPC00340
C                                                                     SPC00350
C                                                                     SPC00360
     DO 10 K=1,IB+1                                                   SPC00370
       TIME(K)=FLOAT(K)                                               SPC00380
       TIME1(K)=FLOAT(K)+0.5D0                                        SPC00390
       ZT(K)=0.0D0                                                    SPC00400
       UT(K)=0.0D0                                                    SPC00410
       YT(K)=0.0D0                                                    SPC00420
10   CONTINUE                                                         SPC00430
C******************************************************************** SPC00440
C    CALL TO APPROPRIATE SIMULATION SUBROUTINE                        SPC00450
C******************************************************************** SPC00460
     RUNSH(JJ)=0.0D0                                                  SPC00470
     RUNEW(JJ)=0.0D0                                                  SPC00480
     RUNCU(JJ)=0.0D0                                                  SPC00490
     RUNDF(JJ)=0.0D0                                                  SPC00500
     IF (ID .EQ. 0) CALL ARMA11                                       SPC00510
     IF (ID .NE. 0) CALL ARIMA1                                       SPC00520
     CALL PTVAR                                                       SPC00530
     CALL CHARTS                                                      SPC00540
626  CONTINUE                                                         SPC00550
     CALL ARLS                                                        SPC00560
     STOP                                                             SPC00570
     END                                                              SPC00580
C******************************************************************** SPC00590
C******************************************************************** SPC00600
C    READ DATA IN FROM DATA FILE                                      SPC00610
C******************************************************************** SPC00620
C******************************************************************** SPC00630
     SUBROUTINE READER                                                SPC00640
     PARAMETER (N=5000)                                               SPC00650
     IMPLICIT DOUBLE PRECISION (A-H,O-Z)                              SPC00660
     COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),     SPC00670
    &     RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),    SPC00680
    &     RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),  SPC00690
    &     SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,     SPC00700
    &     ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N)          SPC00710
     COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP, SPC00720
    &        SCL,EWCL,DFCL,XSTD                                       SPC00730
     COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH,IRUN1,IRUN2      SPC00740
     CHARACTER*80 TITLE                                               SPC00750
     READ (15,394) TITLE                                              SPC00760
```

```
      READ (15,*) ISIM,IPVAR,ICONT,NSIM
      READ (15,394) TITLE
      READ (15,*) IB, DELTA, G, PHI, THETA, ID
      READ (15,394) TITLE
      READ (15,*) DLAMB,EH,EL,STEP,TSTEP
      READ (15,394) TITLE
      READ (15,394) TITLE
      READ (15,*) IPH
      READ (15,394) TITLE
      READ (15,*) DFCL,EWCL,SCL
      IF(THETA .EQ. 0) THEN
        ITHET=0
      ELSE
        ITHET=1
      ENDIF
      IF(PHI .EQ. 0) THEN
        IPHI=0
      ELSE
        IPHI=1
      ENDIF
      IF (ID .EQ. 0) THEN
        WRITE (16,395) IPHI,ITHET
      ELSE
        WRITE (16,396) IPHI,ID,ITHET
      ENDIF
      WRITE(16,397) PHI,THETA,ID
      WRITE(16,399) DELTA,G
      WRITE (16,398) STEP
      WRITE (16,392)
      WRITE (16,392)
  392 FORMAT ('********************************************************',
     &'*********')
  394 FORMAT (A80)
  395 FORMAT ('THIS IS AN ARMA(',I1,',',I1,') PROCESS'/)
  396 FORMAT ('THIS IS AN ARIMA(',I1,',',I1,',',I1,') PROCESS'/)
  397 FORMAT ('PHI= ',F6.3,', THETA= ',F6.3,' AND D= ',I2)
  398 FORMAT ('FOR A ',F6.3,' SIGMA STEP SHIFT IN DISTURBANCE MEAN')
  399 FORMAT ('PROCESS INERTIA= ',F6.3,' AND GAIN= ', F6.3)
      RETURN
      END
C
C*******************************************************************
C*******************************************************************
C   SUBROUTINE TO DETERMINE CONTROL LIMITS FOR CHARTING TECHNIQUES
C*******************************************************************
C*******************************************************************
C
      SUBROUTINE PTVAR
      PARAMETER (N=5000)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),
     &    RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),
     &    RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),
     &    SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,
     &    ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N)
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP,
     &          SCL,EWCL,DFCL,XSTD
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH,IRUN1,IRUN2
C
      DO 223 I=IB+2,ISIM
        IF (IPVAR .EQ. 1) PLTVAR(I)=ZT(I)
```

```
      IF (IPVAR .EQ. 2) PLTVAR(I)=YT(I)                    SPC01390
      IF (IPVAR .EQ. 3) PLTVAR(I)=UT(I)                    SPC01400
      IF (IPVAR .EQ. 4) PLTVAR(I)=RES(I)                   SPC01410
 223  CONTINUE                                             SPC01420
C                                                          SPC01430
      STDZ=(((1.D0-2.D0*(THETA*PHI)+THETA**2)/(1.D0-PHI**2))**0.5D0)    SPC01440
C     STDZ=(1.0/(1.0-PHI**2.0))**0.5                       SPC01450
      IF (IPVAR .EQ. 1) STDVAR=STDZ                        SPC01460
      IF (IPVAR .EQ. 2 .OR. IPVAR .EQ. 4) STDVAR=XSTD      SPC01470
      IF (IPVAR .EQ. 3 .AND. ID .EQ. 0) THEN               SPC01480
      STDVAR=((PHI**(2*IB))/((G*(1-DELTA))**2))*((1-DELTA**2)*((PHI**2)*SPC01490
     & STDZ**2+(THETA**2)*(XSTD**2))-2*THETA*PHI*(DELTA**2)*(XSTD**2)-  SPC01500
     & 2*(PHI**2)*DELTA*(PHI*(STDZ**2)+(1-THETA)*(STD**2))-2*THETA*     SPC01510
     & PHI*(XSTD**2)+2*PHI*THETA*DELTA*(PHI-THETA)*(XSTD**2))           SPC01520
      ELSEIF (IPVAR .EQ. 3 .AND. ID .EQ. 1) THEN           SPC01530
      STDVAR=1.0D0                                         SPC01540
      ENDIF                                                SPC01550
      RETURN                                               SPC01560
      END                                                  SPC01570
C                                                          SPC01580
C                                                          SPC01590
C****************************************************************** SPC01600
C****************************************************************** SPC01610
C     SIMULATES A CHEMICAL PROCESS WITH FIRST ORDER PLUS DEAD TIME OR  SPC01620
C     PURE GAIN PROCESS DYNAMICS WHOSE DISTURBANCE MODEL IS DESCRIBED  SPC01630
C     BY ANY FIRST ORDER AUTOREGRESSIVE MOVING AVERAGE MODEL.          SPC01640
C****************************************************************** SPC01650
C****************************************************************** SPC01660
C                                                          SPC01670
      SUBROUTINE ARMA11                                    SPC01680
      PARAMETER (N=5000)                                   SPC01690
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                  SPC01700
C                                                          SPC01710
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),      SPC01720
     &     RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),     SPC01730
     &     RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),   SPC01740
     &     SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,      SPC01750
     &     ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N)           SPC01760
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP, SPC01770
     &          SCL,EWCL,DFCL,XSTD                         SPC01780
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH,IRUN1,IRUN2       SPC01790
C                                                          SPC01800
      DO 40 I=IB+2,ISIM                                    SPC01810
      TIME(I)=FLOAT(I)                                     SPC01820
      TIME1(I)=FLOAT(I)+0.5D0                              SPC01830
      RR(I)=0.0D0                                          SPC01840
      IF (TIME(I) .GE. TSTEP) THEN                         SPC01850
        RR(I)=(1.0D0-PHI)*STEP*XSTD                        SPC01860
      ENDIF                                                SPC01870
C                                                          SPC01880
C                                                          SPC01890
      R(IB+1)=0.0D0                                        SPC01900
      ZT(I)=PHI*ZT(I-1) +R(I) - THETA*R(I-1) +RR(I)        SPC01910
C                                                          SPC01920
C                                                          SPC01930
      IF (ICONT .EQ. 1) THEN                               SPC01940
C                                                          SPC01950
C     *****************************                        SPC01960
C      MINIMUM VARIANCE CONTROLLER                         SPC01970
C     *****************************                        SPC01980
C                                                          SPC01990
      YT(I)=DELTA*YT(I-1) +G*(1.0D0-DELTA)*UT(I-1) +ZT(I) -DELTA*ZT(I-1)SPC02000
```

```
      SUM(I)=PHI*SUM(I-1)+YT(I)                                         SPC02010
C      UT(I)=-((PHI**IB)/(G*(1.D0-DELTA)))*(((1.D0-THETA)*(1.D0-DELTA)  SPC02020
C     & *PHI*SUM(I))+(((1.D0-THETA)*DELTA*PHI)-THETA+PHI*THETA)*YT(I)+  SPC02030
C     &     ((THETA*DELTA)-(PHI*THETA*DELTA))*YT(I-1))                  SPC02040
      UT(I)=-(((PHI**IB)*(PHI-THETA))/(G*(1.D0-DELTA)))*(YT(I)-         SPC02050
     &     DELTA*YT(I-1))+THETA*UT(I-1)+(PHI-THETA)*(PHI**IB)*          SPC02060
     &     UT(I-IB-1)                                                   SPC02070
      ELSE                                                              SPC02080
C                                                                       SPC02090
C     ****************                                                  SPC02100
C      PID CONTROLLER                                                   SPC02110
C     ****************                                                  SPC02120
C                                                                       SPC02130
      YT(I)=DELTA*YT(I-1) +G*(1.0D0-DELTA)*UT(I-1) +ZT(I) -DELTA*ZT(I-1)SPC02140
      SUM1(I)=SUM1(I-1)+YT(I)                                           SPC02150
      UT(I)=-(EKP*YT(I)+EKI*(SUM1(I))+TD*(YT(I)-YT(I-1)))               SPC02160
      ENDIF                                                             SPC02170
C                                                                       SPC02180
C     ***********************                                           SPC02190
C      RESIDUAL CALCULATIONS                                            SPC02200
C     ***********************                                           SPC02210
C                                                                       SPC02220
C      ZHAT(I)=(PHI**(IB))*(PHI*ZT(I)-THETA*R(I))                       SPC02230
      ZHAT(I)=(PHI**(IB))*(PHI*(SUM(I)-THETA*SUM(I-1))-THETA*YT(I))     SPC02240
      RES(I)=ZT(I)-ZHAT(I-IB-1)                                         SPC02250
C      WRITE (16,*) ZT(I),UT(I),YT(I)                                   SPC02260
   40 CONTINUE                                                          SPC02270
      RETURN                                                            SPC02280
      END                                                               SPC02290
C*********************************************************************** SPC02300
C*********************************************************************** SPC02310
C      SIMULATES A CHEMICAL PROCESS WITH FIRST ORDER PLUS DEAD TIME OR  SPC02320
C      PURE GAIN PROCESS DYNAMICS WHOSE DISTURBANCE MODEL IS DESCRIBED  SPC02330
C      BY ANY FIRST ORDER AUTOREGRESSIVE INTEGRATED MOVING AVERAGE MODEL.SPC02340
C*********************************************************************** SPC02350
C*********************************************************************** SPC02360
C                                                                       SPC02370
      SUBROUTINE ARIMA1                                                 SPC02380
      PARAMETER (N=5000)                                                SPC02390
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                               SPC02400
C                                                                       SPC02410
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),      SPC02420
     &     RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),     SPC02430
     &     RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),   SPC02440
     &     SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,      SPC02450
     &     ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N)           SPC02460
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP, SPC02470
     &          SCL,EWCL,DFCL,XSTD                                      SPC02480
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH,IRUN1,IRUN2       SPC02490
C                                                                       SPC02500
C                                                                       SPC02510
      DO 60  I=IB+2,ISIM                                                SPC02520
C                                                                       SPC02530
      TIME(I)=FLOAT(I)                                                  SPC02540
      TIME1(I)=FLOAT(I)+0.5D0                                           SPC02550
      RR(I)=0.0D0                                                       SPC02560
      IF (TIME(I) .EQ. TSTEP) RR(I)=STEP*(1.0D0-PHI)*XSTD               SPC02570
      R(IB+1)=0.0D0                                                     SPC02580
      ZT(I)=(1.0D0+PHI)*ZT(I-1) -PHI*ZT(I-2)+R(I)-THETA*R(I-1) +RR(I)   SPC02590
C                                                                       SPC02600
C                                                                       SPC02610
      IF (ICONT .EQ. 1) THEN                                            SPC02620
```

```
C
C  ****************************
C   MINIMUM VARIANCE CONTROLLER
C  ****************************
C
      YT(I)=DELTA*YT(I-1) +G*(1.D0-DELTA)*UT(I-1) +ZT(I) -DELTA*ZT(I-1)
      SUM2(I)=SUM2(I-1)+YT(I)
      SUM3(I)=PHI*SUM3(I) +SUM2(I)
C      UT(I)=-((1.D0-THETA)*(1.D0-DELTA)/(G*(1.D0-DELTA)))*(SUM2(I)+(PHI
C     & *THETA)/((1.D0-THETA)*(1.D0-DELTA))+(DELTA/(1.D0-DELTA))+
C     & ((PHI*DELTA/(1.D0-DELTA)))*YT(I)+PHI*(SUM3(I)))
      IF (IB .EQ. 0) THEN
      UT(I)=-(1.D0/(G*(1.D0-DELTA)))*(((1.D0+PHI-THETA)*YT(I))-((DELTA+
     & (PHI*DELTA)+PHI-(DELTA*THETA))*YT(I-1))+(PHI*DELTA*YT(I-2)))+
     & (1.D0+PHI)*UT(I-1)-PHI*UT(I-2)
      ELSEIF (IB .EQ. 1) THEN
      UT(I)=-(1.D0/(G*(1.D0-DELTA)))*(((1.D0+PHI+(PHI**2)-(THETA*(1.D0
     &   +PHI)))*YT(I))-((DELTA+PHI*DELTA+(DELTA*(PHI**2))+PHI+(PHI**2)
     &   -(PHI*THETA)-(DELTA*THETA)-(DELTA*THETA*PHI))*YT(I-1))+
     &   (((DELTA*PHI)+(DELTA*(PHI**2))-(DELTA*THETA*PHI))*YT(I-2)))+
     &   (1.D0+PHI)*UT(I-1)-PHI*UT(I-2)
      ENDIF
      ELSE
C
C  ***************
C   PID CONTROLLER
C  ***************
C
      YT(I)=DELTA*YT(I-1) +G*(1.D0-DELTA)*UT(I-1) +ZT(I) -DELTA*ZT(I-1)
      SUMYT(I)=SUMYT(I-1)+YT(I)
      UT(I)=-(EKP*YT(I)+EKI*(SUMYT(I))+TD*(YT(I)-YT(I-1)))
      ENDIF
C
C  **********************
C   RESIDUAL CALCULATIONS
C  **********************
C
      ZHAT(1)=(1.D0+PHI)*ZT(I)-PHI*ZT(I-1)-THETA*YT(I)
      IF(IB .EQ. 0) GOTO 301
      ZHAT(2)=(1.D0+PHI)*ZHAT(1)-PHI*ZT(I)
      IF(IB .EQ. 1) GOTO 301
      DO 222 J=3,IB+1
        ZHAT(J)=(1.D0+PHI)*ZHAT(J-1)-PHI*ZHAT(J-2)
 222  CONTINUE
 301  RES(I)=-(ZT(I)-ZHAT(IB+1))
  60  CONTINUE
      RETURN
      END
C
C*******************************************************************
C*******************************************************************
C     SUBROUTINE FOR CALCULATING RUN LENGTHS FOR VARIOUS
C     CHARTING TECHNIQUES.
C*******************************************************************
C*******************************************************************
C
      SUBROUTINE CHARTS
      PARAMETER (N=5000)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),
     &     RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),
```

```
     &      RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),  SPC03250
     &      SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,     SPC03260
     &      ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N)          SPC03270
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP, SPC03280
     &           SCL,EWCL,DFCL,XSTD                                     SPC03290
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH,IRUN1,IRUN2       SPC03300
C                                                                       SPC03310
C****************************                                          SPC03320
C   SHEWHART CHART       *                                              SPC03330
C****************************                                          SPC03340
      DO 124 I=IB+2,ISIM                                                SPC03350
C                                                                       SPC03360
      SHEW(I)=PLTVAR(I)                                                 SPC03370
C                                                                       SPC03380
C*****************************************                             SPC03390
C   CUMULATIVE SUM CHARTING TECHNIQUE  *                                SPC03400
C*****************************************                             SPC03410
C                                                                       SPC03420
      CUSUM1(I)=DMAX1((CUSUM1(I-1)-((PLTVAR(I))+0.5D0)),0.0D0)          SPC03430
      CUSUM2(I)=DMAX1((CUSUM2(I-1)+((PLTVAR(I))-0.5D0)),0.0D0)          SPC03440
      IF (CUSUM2(I) .GT. CUSUM1(I)) THEN                                SPC03450
      CUSUM3(I)=CUSUM2(I)                                               SPC03460
      ELSE                                                              SPC03470
      CUSUM3(I)=CUSUM1(I)                                               SPC03480
      ENDIF                                                             SPC03490
C*************************************************                     SPC03500
C   EXPONENTIALLY WEIGHTED MOVING AVERAGE (EWMA) *                      SPC03510
C*************************************************                     SPC03520
C                                                                       SPC03530
      EWMA(I)=DLAMB*(PLTVAR(I))+(1.0D0-DLAMB)*EWMA(I-1)                 SPC03540
C                                                                       SPC03550
C**********************************************                        SPC03560
C   NTH ORDER DIFFERENCING TECHNIQUE.        *                          SPC03570
C   -FOR USE ON INTEGRATED DISTURBANCES ONLY-  *                        SPC03580
C**********************************************                        SPC03590
C                                                                       SPC03600
      IF(ID .EQ. 0) GOTO 120                                            SPC03610
C                                                                       SPC03620
      IF (I .LE. IPH+IB+1) THEN                                         SPC03630
       DIFF(I)=0.0D0                                                    SPC03640
      ELSE                                                              SPC03650
       DIFF(I)=PLTVAR(I)-PLTVAR(I-IPH)                                  SPC03660
      ENDIF                                                             SPC03670
C      WRITE (16,727) ZT(I),UT(I),YT(I),DIFF(I)                         SPC03680
C727  FORMAT (4(F9.3,4X))                                               SPC03690
C      WRITE (16,727) DIFF(I)                                           SPC03700
C727  FORMAT ((F9.3,4X))                                                SPC03710
 120  IF(RUNSH(JJ) .GT. 0.0D0 .OR. TIME(I).LE. TSTEP) GOTO 121          SPC03720
C       IF ((SHEW(I)) .LE. 0.0) THEN                                    SPC03730
C         IRUN2=0                                                       SPC03740
C         IRUN1=IRUN1+1                                                 SPC03750
C       ELSE                                                            SPC03760
C         IRUN1=0                                                       SPC03770
C         IRUN2=IRUN2+1                                                 SPC03780
C       ENDIF                                                           SPC03790
C       IF(IRUN1 .EQ. 35 .OR. IRUN2 .EQ. 35) RUNSH(JJ)=TIME(I)          SPC03800
      IF(ABS(SHEW(I)) .GE. SCL) RUNSH(JJ)=TIME(I)                       SPC03810
 121  IF(RUNEW(JJ) .GT. 0.0D0 .OR. TIME(I) .LE. TSTEP) GOTO 122         SPC03820
      IF(ABS(EWMA(I)) .GE. EWCL) RUNEW(JJ)=TIME(I)                      SPC03830
 122  IF(RUNCU(JJ) .GT. 0.0D0 .OR. TIME(I) .LE. TSTEP) GOTO 123         SPC03840
      IF(CUSUM3(I) .GE. EH) RUNCU(JJ)=TIME(I)                           SPC03850
      IF(ID .EQ. 0) GOTO 124                                            SPC03860
```

```
 123  IF(RUNDF(JJ) .GT. 0.0D0 .OR. TIME(I) .LE. TSTEP) GOTO 124
      IF(ABS(DIFF(I)) .GE. DFCL) RUNDF(JJ)=TIME(I)
 124  CONTINUE
      RETURN
      END
C
C*****************************************************************
C*****************************************************************
C     SUBROUTINE FOR CALCULATING RUN LENGTHS FOR VARIOUS
C     CHARTING TECHNIQUES.
C*****************************************************************
C*****************************************************************
C
      SUBROUTINE ARLS
      PARAMETER (N=5000)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),
     &     RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),
     &     RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),
     &     SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,
     &     ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N)
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP,
     &          SCL,EWCL,DFCL,XSTD
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH,IRUN1,IRUN2
C
      DO 678 I=IB+2,NSIM
        IF(RUNSH(I) .EQ. 0.0D0) RUNSH(I)=TIME(ISIM)
        IF(RUNEW(I) .EQ. 0.0D0) RUNEW(I)=TIME(ISIM)
        IF(RUNCU(I) .EQ. 0.0D0) RUNCU(I)=TIME(ISIM)
        IF(RUNDF(I) .EQ. 0.0D0) RUNDF(I)=TIME(ISIM)
C
        RNLTH1(I)=RNLTH1(I-1)+RUNSH(I)
        RNLTH2(I)=RNLTH2(I-1)+RUNEW(I)
        RNLTH3(I)=RNLTH3(I-1)+RUNCU(I)
        RNLTH4(I)=RNLTH4(I-1)+RUNDF(I)
 678  CONTINUE
      ARL1=(RNLTH1(NSIM)/(FLOAT(NSIM)))-(TSTEP)
      ARL2=(RNLTH2(NSIM)/(FLOAT(NSIM)))-(TSTEP)
      ARL3=(RNLTH3(NSIM)/(FLOAT(NSIM)))-(TSTEP)
      ARL4=(RNLTH4(NSIM)/(FLOAT(NSIM)))-(TSTEP)
      WRITE (16,*) ARL1,ARL2,ARL3,ARL4
      WRITE (16,*) XSTD
      RETURN
      END
```

SPCSIM DATA FILE:

```
sim. time   choice of var. to chart   choice of controller   # of sim.
  1503            3                        1                  2000
dead time   inertia (delta)   gain cnst   phi   theta   d
  0          0.75d0            1.0d0      0.0d0  0.95d0  1
lambda   h   control limits   step dist.   time of step dist.
 0.15d0  56.1d0   15.0d0       1.0d0        113.0d0
amount of differencing (nth order differencing) only for integrated
disturbances (choose 1,4,5,6,10 or 20)
   8
control limits   difference   ewma      shewhart
                 0.8475d0     2.695d0   4.805d0
```

Appendix C

Quattro Program

phi	0	theta	0.9
shift	1		
gain	1		
inertia	0.5		

ARIMA(1,1,1) Model

Time	zt	zhat	Res zt	xt	yt	R(i)	zt1	zhat1	res1	xt1	yt1
0	0	0	0	0	0	-0.8269	-0.8269	-0.0827	-0.8269	0.16539	-0.8269
1	0	0	0	0	0	1.09995	1.01726	0.0273	1.09995	-0.1373	1.09995
2	0	0	0	0	0	0.19461	0.22191	0.04676	0.19461	-0.0662	0.19461
3	0	0	0	0	0	1.1338	1.18056	0.16014	1.1338	-0.2735	1.1338
4	0	0	0	0	0	1.29248	1.45262	0.28939	1.29248	-0.4186	1.29248
5	0	0	0	0	0	-0.4282	-0.1388	0.24657	-0.4282	-0.2038	-0.4282
6	0	0	0	0	0	-0.7861	-0.5395	0.16797	-0.7861	-0.0894	-0.7861
7	0	0	0	0	0	0.06111	0.22908	0.17408	0.06111	-0.1802	0.06111
8	0	0	0	0	0	-0.1394	0.03465	0.16013	-0.1394	-0.1462	-0.1394
9	0	0	0	0	0	0.45599	0.61612	0.20573	0.45599	-0.2513	0.45599
10	0	0	0	0	0	-1.7437	-1.538	0.03136	-1.7437	0.14301	-1.7437
11	0	0	0	0	0	-0.3502	-0.3188	-0.0037	-0.3502	0.03867	-0.3502
12	0	0	0	0	0	0.5467	0.54305	0.05102	0.5467	-0.1057	0.5467
13	0	0	0	0	0	-0.421	-0.37	0.00892	-0.421	0.03318	-0.421
14	0	0	0	0	0	-0.6584	-0.6495	-0.0569	-0.6584	0.12277	-0.6584
15	0	0	0	0	0	-0.2241	-0.281	-0.0793	-0.2241	0.10175	-0.2241
16	0	0	0	0	0	-0.7483	-0.8276	-0.1542	-0.7483	0.229	-0.7483
17	0	0	0	0	0	1.33624	1.18207	-0.0205	1.33624	-0.1131	1.33624
18	0	0	0	0	0	0.96176	0.94122	0.07563	0.96176	-0.1718	0.96176
19	0	0	0	0	0	0.1025	0.17813	0.08588	0.1025	-0.0961	0.1025
20	0	0	0	0	0	0.79286	0.87875	0.16517	0.79286	-0.2445	0.79286
21	0	0	0	0	0	-1.275	-1.1098	0.03767	-1.275	0.08982	-1.275
22	0	0	0	0	0	-1.596	-1.5583	-0.1219	-1.596	0.28153	-1.596
23	0	0	0	0	0	0.08294	-0.039	-0.1136	0.08294	0.10534	0.08294
24	0	0	0	0	0	0.06244	-0.0512	-0.1074	0.06244	0.10115	0.06244
25	0	0	0	0	0	0.30956	0.20217	-0.0764	0.30956	0.04548	0.30956
26	0	0	0	0	0	-0.3478	-0.4243	-0.1112	-0.3478	0.146	-0.3478
27	0	0	0	0	0	-1.091	-1.2022	-0.2203	-1.091	0.32942	-1.091
28	0	0	0	0	0	-0.2006	-0.4209	-0.2404	-0.2006	0.26043	-0.2006
29	0	0	0	0	0	2.40415	2.16378	4.3E-05	2.40415	-0.2405	2.40415
30	0	0	0	0	0	0.03914	0.03918	0.00396	0.03914	-0.0079	0.03914
31	0	0	0	0	0	1.90641	1.91037	0.1946	1.90641	-0.3852	1.90641
32	0	0	0	0	0	-1.4072	-1.2126	0.05387	-1.4072	0.08685	-1.4072
33	0	0	0	0	0	1.14055	1.19442	0.16793	1.14055	-0.282	1.14055
34	0	0	0	0	0	-0.6026	-0.4346	0.10767	-0.6026	-0.0474	-0.6026
35	0	0	0	0	0	-0.1449	-0.0373	0.09318	-0.1449	-0.0787	-0.1449

36	0	0	0	0	0	-0.1095	-0.0164	0.08222	-0.1095	-0.0713	-0.1095
37	0	0	0	0	0	1.13289	1.21511	0.19551	1.13289	-0.3088	1.13289
38	0	0	0	0	0	0.03852	0.23403	0.19936	0.03852	-0.2032	0.03852
39	0	0	0	0	0	-1.1807	-0.9813	0.0813	-1.1807	0.03677	-1.1807
40	0	0	0	0	0	0.6557	0.737	0.14687	0.6557	-0.2124	0.6557
41	0	0	0	0	0	1.77978	1.92665	0.32485	1.77978	-0.5028	1.77978
42	0	0	0	0	0	-1.0599	-0.7351	0.21885	-1.0599	-0.1129	-1.0599
43	0	0	0	0	0	-1.7795	-1.5606	0.04091	-1.7795	0.13704	-1.7795
44	0	0	0	0	0	-0.4179	-0.377	-0.0009	-0.4179	0.04267	-0.4179
45	0	0	0	0	0	0.27228	0.2714	0.02634	0.27228	-0.0536	0.27228
46	0	0	0	0	0	1.82442	1.85076	0.20879	1.82442	-0.3912	1.82442
47	0	0	0	0	0	0.40079	0.60958	0.24887	0.40079	-0.2889	0.40079
48	0	0	0	0	0	1.33971	1.58858	0.38284	1.33971	-0.5168	1.33971
49	0	0	0	0	0	0.23434	0.61717	0.40627	0.23434	-0.4297	0.23434
50	0	0	0	0	0	0.89696	1.30323	0.49597	0.89696	-0.5857	0.89696
51	0	0	0	0	0	-1.209	-0.713	0.37507	-1.209	-0.2542	-1.209
52	0	0	0	0	0	0.1187	0.49377	0.38694	0.1187	-0.3988	0.1187
53	0	0	0	0	0	0.5966	0.98353	0.4466	0.5966	-0.5063	0.5966
54	0	0	0	0	0	0.25736	0.70395	0.47233	0.25736	-0.4981	0.25736
55	0	0	0	0	0	-1.1924	-0.7201	0.35309	-1.1924	-0.2338	-1.1924
56	0	0	0	0	0	-1.2914	-0.9383	0.22395	-1.2914	-0.0948	-1.2914
57	0	0	0	0	0	-0.2783	-0.0544	0.19612	-0.2783	-0.1683	-0.2783
58	0	0	0	0	0	-1.7158	-1.5197	0.02453	-1.7158	0.14705	-1.7158
59	0	0	0	0	0	0.59551	0.62005	0.08408	0.59551	-0.1436	0.59551
60	0	0	0	0	0	-0.1051	-0.0211	0.07357	-0.1051	-0.0631	-0.1051
61	0	0	0	0	0	0.99123	1.0648	0.17269	0.99123	-0.2718	0.99123
62	0	0	0	0	0	0.43268	0.60537	0.21596	0.43268	-0.2592	0.43268
63	0	0	0	0	0	-0.105	0.11096	0.20546	-0.105	-0.195	-0.105
64	0	0	0	0	0	0.35582	0.56128	0.24104	0.35582	-0.2766	0.35582
65	0	0	0	0	0	0.59094	0.83198	0.30014	0.59094	-0.3592	0.59094
66	0	0	0	0	0	-1.2117	-0.9115	0.17897	-1.2117	-0.0578	-1.2117
67	0	0	0	0	0	1.64941	1.82838	0.34391	1.64941	-0.5089	1.64941
68	0	0	0	0	0	0.28911	0.63302	0.37282	0.28911	-0.4017	0.28911
69	0	0	0	0	0	-0.0954	0.27741	0.36328	-0.0954	-0.3537	-0.0954
70	0	0	0	0	0	-0.0249	0.33836	0.36079	-0.0249	-0.3583	-0.0249
71	0	0	0	0	0	-0.1857	0.17506	0.34222	-0.1857	-0.3236	-0.1857
72	0	0	0	0	0	0.69789	1.04011	0.412	0.69789	-0.4818	0.69789
73	0	0	0	0	0	0.43562	0.84762	0.45557	0.43562	-0.4991	0.43562
74	0	0	0	0	0	-0.54	-0.0845	0.40156	-0.54	-0.3476	-0.54
75	0	0	0	0	0	-0.1704	0.23115	0.38452	-0.1704	-0.3675	-0.1704
76	0	0	0	0	0	0.1867	0.57122	0.40319	0.1867	-0.4219	0.1867
77	0	0	0	0	0	-0.4367	-0.0335	0.35953	-0.4367	-0.3159	-0.4367
78	0	0	0	0	0	-0.1501	0.20946	0.34452	-0.1501	-0.3295	-0.1501
79	0	0	0	0	0	2.07902	2.42354	0.55242	2.07902	-0.7603	2.07902
80	0	0	0	0	0	2.09061	2.64303	0.76148	2.09061	-0.9705	2.09061
81	0	0	0	0	0	0.67546	1.43694	0.82903	0.67546	-0.8966	0.67546
82	0	0	0	0	0	-1.3742	-0.5452	0.69161	-1.3742	-0.5542	-1.3742
83	0	0	0	0	0	1.89855	2.59016	0.88147	1.89855	-1.0713	1.89855
84	0	0	0	0	0	0.12384	1.00531	0.89385	0.12384	-0.9062	0.12384
85	0	0	0	0	0	0.943	1.83685	0.98815	0.943	-1.0824	0.943
86	0	0	0	0	0	-1.7883	-0.8002	0.80932	-1.7883	-0.6305	-1.7883
87	0	0	0	0	0	-0.3231	0.48623	0.77701	-0.3231	-0.7447	-0.3231
88	0	0	0	0	0	0.35539	1.1324	0.81255	0.35539	-0.8481	0.35539

89	0	0	0	0	0	-1.7941	-0.9815	0.63314	-1.7941	-0.4537	-1.7941
90	0	0	0	0	0	-0.7545	-0.1214	0.55769	-0.7545	-0.4822	-0.7545
91	0	0	0	0	0	-0.3971	0.16059	0.51798	-0.3971	-0.4783	-0.3971
92	0	0	0	0	0	-2.8017	-2.2837	0.2378	-2.8017	0.04237	-2.8017
93	0	0	0	0	0	-0.0553	0.18254	0.23228	-0.0553	-0.2268	-0.0553
94	0	0	0	0	0	0.23434	0.46662	0.25571	0.23434	-0.2791	0.23434
95	0	0	0	0	0	0.87396	1.12967	0.34311	0.87396	-0.4305	0.87396
96	0	0	0	0	0	0.0062	0.34931	0.34373	0.0062	-0.3443	0.0062
97	0	0	0	0	0	-0.866	-0.5223	0.25713	-0.866	-0.1705	-0.866
98	0	0	0	0	0	-0.1987	0.05844	0.23726	-0.1987	-0.2174	-0.1987
99	0	0	0	0	0	1.02253	1.25979	0.33951	1.02253	-0.4418	1.02253
100	1	0.1	1	-0.2	1	1.40035	2.73986	0.57955	2.40035	-0.8196	2.40035
101	1	0.19	0.9	-0.28	0.9	-1.2259	0.25367	0.54696	-0.3259	-0.5144	-0.3259
102	1	0.271	0.81	-0.352	0.81	-0.341	1.01596	0.59386	0.469	-0.6408	0.469
103	1	0.3439	0.729	-0.4168	0.729	-0.731	0.59188	0.59366	-0.002	-0.5935	-0.002
104	1	0.40951	0.6561	-0.4751	0.6561	0.346	1.59576	0.69387	1.0021	-0.7941	1.0021
105	1	0.46856	0.59049	-0.5276	0.59049	1.15024	2.4346	0.86794	1.74073	-1.042	1.74073
106	1	0.5217	0.53144	-0.5748	0.53144	0.65406	2.05344	0.98649	1.1855	-1.105	1.1855
107	1	0.56953	0.4783	-0.6174	0.4783	0.31774	1.78253	1.0661	0.79604	-1.1457	0.79604
108	1	0.61258	0.43047	-0.6556	0.43047	2.52226	4.01882	1.36137	2.95273	-1.6566	2.95273
109	1	0.65132	0.38742	-0.6901	0.38742	-1.7865	-0.0377	1.22146	-1.3991	-1.0815	-1.3991
110	1	0.68619	0.34868	-0.7211	0.34868	-1.1917	0.37842	1.13716	-0.843	-1.0529	-0.843
111	1	0.71757	0.31381	-0.749	0.31381	1.12031	2.57128	1.28057	1.43412	-1.424	1.43412
112	1	0.74581	0.28243	-0.7741	0.28243	0.07638	1.63938	1.31645	0.35881	-1.3523	0.35881
113	1	0.77123	0.25419	-0.7967	0.25419	0.62205	2.19268	1.40407	0.87624	-1.4917	0.87624
114	1	0.79411	0.22877	-0.817	0.22877	0.78043	2.41327	1.50499	1.00919	-1.6059	1.00919
115	1	0.8147	0.20589	-0.8353	0.20589	-1.2345	0.47641	1.40213	-1.0286	-1.2993	-1.0286
116	1	0.83323	0.1853	-0.8518	0.1853	-0.7008	0.88659	1.35058	-0.5155	-1.299	-0.5155
117	1	0.84991	0.16677	-0.8666	0.16677	-0.8991	0.61827	1.27735	-0.7323	-1.2041	-0.7323
118	1	0.86491	0.15009	-0.8799	0.15009	0.45992	1.88736	1.33835	0.61002	-1.3994	0.61002
119	1	0.87842	0.13509	-0.8919	0.13509	-0.0717	1.40175	1.34469	0.0634	-1.351	0.0634
120	1	0.89058	0.12158	-0.9027	0.12158	0.22363	1.6899	1.37921	0.34521	-1.4137	0.34521
121	1	0.90152	0.10942	-0.9125	0.10942	1.6764	3.16503	1.55779	1.78582	-1.7364	1.78582
122	1	0.91137	0.09848	-0.9212	0.09848	-1.0189	0.63741	1.46576	-0.9204	-1.3737	-0.9204
123	1	0.92023	0.08863	-0.9291	0.08863	0.58862	2.14301	1.53348	0.67725	-1.6012	0.67725
124	1	0.92821	0.07977	-0.9362	0.07977	0.87202	2.48527	1.62866	0.95179	-1.7238	0.95179
125	1	0.93539	0.07179	-0.9426	0.07179	-0.2417	1.45878	1.61167	-0.1699	-1.5947	-0.1699
126	1	0.94185	0.06461	-0.9483	0.06461	-0.0758	1.60045	1.61055	-0.0112	-1.6094	-0.0112
127	1	0.94767	0.05815	-0.9535	0.05815	-1.0108	0.65786	1.51528	-0.9527	-1.42	-0.9527
128	1	0.9529	0.05233	-0.9581	0.05233	-0.8052	0.76237	1.43999	-0.7529	-1.3647	-0.7529
129	1	0.95761	0.0471	-0.9623	0.0471	-1.0116	0.47553	1.34354	-0.9645	-1.2471	-0.9645
130	1	0.96185	0.04239	-0.9661	0.04239	1.13128	2.51721	1.46091	1.17367	-1.5783	1.17367
131	1	0.96566	0.03815	-0.9695	0.03815	-1.1889	0.3102	1.34584	-1.1507	-1.2308	-1.1507
132	1	0.9691	0.03434	-0.9725	0.03434	1.16734	2.54751	1.46601	1.20167	-1.5862	1.20167
133	1	0.97219	0.0309	-0.9753	0.0309	-0.9188	0.5781	1.37722	-0.8879	-1.2884	-0.8879
134	1	0.97497	0.02781	-0.9777	0.02781	0.85863	2.26366	1.46586	0.88644	-1.5545	0.88644
135	1	0.97747	0.02503	-0.98	0.02503	0.76567	2.25656	1.54493	0.7907	-1.624	0.7907

136	1	0.97972	0.02253	-0.982	0.02253	-0.4725	1.09496	1.49993	-0.45	-1.4549	-0.45
137	1	0.98175	0.02028	-0.9838	0.02028	0.65628	2.17649	1.56759	0.67655	-1.6352	0.67655
138	1	0.98358	0.01825	-0.9854	0.01825	1.09717	2.68301	1.67913	1.11542	-1.7907	1.11542
139	1	0.98522	0.01642	-0.9869	0.01642	0.42548	2.12103	1.72332	0.4419	-1.7675	0.4419
140	1	0.9867	0.01478	-0.9882	0.01478	-0.5834	1.15473	1.66646	-0.5686	-1.6096	-0.5686
141	1	0.98803	0.0133	-0.9894	0.0133	0.28997	1.96974	1.69679	0.30328	-1.7271	0.30328
142	1	0.98922	0.01197	-0.9904	0.01197	-0.9168	0.79193	1.6063	-0.9049	-1.5158	-0.9049
143	1	0.9903	0.01078	-0.9914	0.01078	0.08989	1.70697	1.61637	0.10067	-1.6264	0.10067
144	1	0.99127	0.0097	-0.9922	0.0097	0.0905	1.71657	1.62639	0.1002	-1.6364	0.1002
145	1	0.99214	0.00873	-0.993	0.00873	-0.1713	1.46378	1.61013	-0.1626	-1.5939	-0.1626
146	1	0.99293	0.00786	-0.9937	0.00786	-0.515	1.10299	1.55941	-0.5071	-1.5087	-0.5071
147	1	0.99364	0.00707	-0.9943	0.00707	0.71976	2.28624	1.6321	0.72683	-1.7048	0.72683
148	1	0.99427	0.00636	-0.9949	0.00636	-1.3892	0.24925	1.49381	-1.3829	-1.3555	-1.3829
149	1	0.99485	0.00573	-0.9954	0.00573	-0.6777	0.82185	1.42662	-0.672	-1.3594	-0.672
150	1	0.99536	0.00515	-0.9959	0.00515	1.37349	2.80526	1.56448	1.37865	-1.7023	1.37865
151	1	0.99583	0.00464	-0.9963	0.00464	2.30265	3.87177	1.79521	2.30729	-2.0259	2.30729
152	1	0.99624	0.00417	-0.9967	0.00417	1.58638	3.38576	1.95426	1.59055	-2.1133	1.59055
153	1	0.99662	0.00376	-0.997	0.00376	-0.0908	1.86719	1.94556	-0.0871	-1.9368	-0.0871
154	1	0.99696	0.00338	-0.9973	0.00338	0.10233	2.05127	1.95613	0.10571	-1.9667	0.10571
155	1	0.99726	0.00304	-0.9976	0.00304	0.92859	2.88776	2.04929	0.93163	-2.1425	0.93163
156	1	0.99753	0.00274	-0.9978	0.00274	0.10838	2.16041	2.0604	0.11112	-2.0715	0.11112
157	1	0.99778	0.00247	-0.998	0.00247	-0.0581	2.0048	2.05484	-0.0556	-2.0493	-0.0556
158	1	0.998	0.00222	-0.9982	0.00222	-0.1711	1.88597	2.03796	-0.1689	-2.0211	-0.1689
159	1	0.9982	0.002	-0.9984	0.002	1.71016	3.75011	2.20917	1.71216	-2.3804	1.71216
160	1	0.99838	0.0018	-0.9986	0.0018	-0.5691	1.64183	2.15244	-0.5673	-2.0957	-0.5673
161	1	0.99854	0.00162	-0.9987	0.00162	-0.0661	2.08791	2.14598	-0.0645	-2.1395	-0.0645
162	1	0.99869	0.00146	-0.9988	0.00146	-0.6502	1.49722	2.08111	-0.6488	-2.0162	-0.6488
163	1	0.99882	0.00131	-0.999	0.00131	1.77704	3.85946	2.25894	1.77835	-2.4368	1.77835
164	1	0.99894	0.00118	-0.9991	0.00118	-0.2217	2.03839	2.23689	-0.2206	-2.2148	-0.2206
165	1	0.99904	0.00106	-0.9992	0.00106	-0.5733	1.66465	2.17966	-0.5722	-2.1224	-0.5722
166	1	0.99914	0.00096	-0.9992	0.00096	-0.4252	1.75546	2.13724	-0.4242	-2.0948	-0.4242
167	1	0.99923	0.00086	-0.9993	0.00086	-1.9627	0.17542	1.94106	-1.9618	-1.7449	-1.9618
168	1	0.9993	0.00077	-0.9994	0.00077	0.60637	2.54821	2.00178	0.60715	-2.0625	0.60715
169	1	0.99937	0.0007	-0.9994	0.0007	-1.9221	0.08039	1.80964	-1.9214	-1.6175	-1.9214
170	1	0.99944	0.00063	-0.9995	0.00063	0.57317	2.38343	1.86702	0.57379	-1.9244	0.57379
171	1	0.99949	0.00056	-0.9995	0.00056	-0.3659	1.50172	1.83049	-0.3653	-1.794	-0.3653
172	1	0.99954	0.00051	-0.9996	0.00051	1.36585	3.19685	1.96712	1.36636	-2.1038	1.36636
173	1	0.99959	0.00046	-0.9996	0.00046	-0.9835	0.98404	1.86882	-0.9831	-1.7705	-0.9831
174	1	0.99963	0.00041	-0.9997	0.00041	-0.2093	1.65997	1.84793	-0.2088	-1.827	-0.2088
175	1	0.99967	0.00037	-0.9997	0.00037	1.3644	3.2127	1.98441	1.36477	-2.1209	1.36477
176	1	0.9997	0.00033	-0.9997	0.00033	1.08307	3.06781	2.09275	1.08341	-2.2011	1.08341
177	1	0.99973	0.0003	-0.9998	0.0003	1.35829	3.45133	2.22861	1.35859	-2.3645	1.35859
178	1	0.99976	0.00027	-0.9998	0.00027	-0.4023	1.82659	2.1884	-0.402	-2.1482	-0.402
179	1	0.99978	0.00024	-0.9998	0.00024	-0.8949	1.29374	2.09894	-0.8947	-2.0095	-0.8947
180	1	0.9998	0.00022	-0.9998	0.00022	-0.1219	1.97725	2.08677	-0.1217	-2.0746	-0.1217
181	1	0.99982	0.0002	-0.9998	0.0002	1.77327	3.86024	2.26412	1.77347	-2.4415	1.77347
182	1	0.99984	0.00018	-0.9999	0.00018	-1.4291	0.83524	2.12123	-1.4289	-1.9783	-1.4289

183	1	0.99986	0.00016	-0.9999	0.00016	-0.5314	1.58996	2.0681	-0.5313	-2.015	-0.5313
184	1	0.99987	0.00014	-0.9999	0.00014	-0.9363	1.13198	1.97449	-0.9361	-1.8809	-0.9361
185	1	0.99988	0.00013	-0.9999	0.00013	1.69482	3.66944	2.14398	1.69495	-2.3135	1.69495
186	1	0.9999	0.00012	-0.9999	0.00012	-0.289	1.85512	2.1151	-0.2889	-2.0862	-0.2889
187	1	0.99991	0.0001	-0.9999	0.0001	-0.239	1.87621	2.09121	-0.2389	-2.0673	-0.2389
188	1	0.99992	9.4E-05	-0.9999	9.4E-05	-1.112	0.97927	1.98002	-1.1119	-1.8688	-1.1119
189	1	0.99992	8.5E-05	-0.9999	8.5E-05	-1.3001	0.68004	1.85002	-1.3	-1.72	-1.3
190	1	0.99993	7.6E-05	-0.9999	7.6E-05	1.0022	2.85229	1.95025	1.00227	-2.0505	1.00227
191	1	0.99994	6.9E-05	-0.9999	6.9E-05	2.01847	3.96878	2.1521	2.01854	-2.354	2.01854
192	1	0.99994	6.2E-05	-1	6.2E-05	-0.5548	1.5974	2.09663	-0.5547	-2.0412	-0.5547
193	1	0.99995	5.6E-05	-1	5.6E-05	-0.6406	1.45607	2.03257	-0.6406	-1.9685	-0.6406
194	1	0.99996	5E-05	-1	5E-05	0.37697	2.40959	2.07028	0.37702	-2.108	0.37702
195	1	0.99996	4.5E-05	-1	4.5E-05	-2.5422	-0.4719	1.81606	-2.5421	-1.5618	-2.5421
196	1	0.99996	4E-05	-1	4E-05	-0.5584	1.25768	1.76022	-0.5584	-1.7044	-0.5584
197	1	0.99997	3.6E-05	-1	3.6E-05	1.38913	3.14939	1.89914	1.38916	-2.0381	1.38916
198	1	0.99997	3.3E-05	-1	3.3E-05	0.95773	2.8569	1.99492	0.95776	-2.0907	0.95776
199	1	0.99997	3E-05	-1	3E-05	0.10234	2.09729	2.00515	0.10237	-2.0154	0.10237
200	1	0.99998	2.7E-05	-1	2.7E-05	-1.6637	0.34152	1.83879	-1.6636	-1.6724	-1.6636
201	1	0.99998	2.4E-05	-1	2.4E-05	1.38063	3.21945	1.97686	1.38066	-2.1149	1.38066
202	1	0.99998	2.2E-05	-1	2.2E-05	1.10617	3.08305	2.08747	1.1062	-2.1981	1.1062
203	1	0.99998	1.9E-05	-1	1.9E-05	0.99922	3.08672	2.1874	0.99924	-2.2873	0.99924
204	1	0.99998	1.7E-05	-1	1.7E-05	2.37628	4.5637	2.42503	2.3763	-2.6627	2.3763
205	1	0.99999	1.6E-05	-1	1.6E-05	-1.9873	0.43769	2.2263	-1.9873	-2.0276	-1.9873
206	1	0.99999	1.4E-05	-1	1.4E-05	-0.6798	1.54655	2.15832	-0.6797	-2.0903	-0.6797
207	1	0.99999	1.3E-05	-1	1.3E-05	-1.8605	0.29787	1.97228	-1.8605	-1.7862	-1.8605
208	1	0.99999	1.1E-05	-1	1.1E-05	0.38789	2.36018	2.01107	0.38791	-2.0499	0.38791
209	1	0.99999	1E-05	-1	1E-05	-1.1655	0.84559	1.89452	-1.1655	-1.778	-1.1655
210	1	0.99999	9.3E-06	-1	9.3E-06	1.60695	3.50148	2.05522	1.60696	-2.2159	1.60696
211	1	0.99999	8.3E-06	-1	8.3E-06	0.64282	2.69805	2.1195	0.64283	-2.1838	0.64283
212	1	0.99999	7.5E-06	-1	7.5E-06	-1.7731	0.34643	1.94219	-1.7731	-1.7649	-1.7731
213	1	0.99999	6.8E-06	-1	6.8E-06	-1.1094	0.83284	1.83126	-1.1093	-1.7203	-1.1093
214	1	0.99999	6.1E-06	-1	6.1E-06	-2.5471	-0.7158	1.57655	-2.5471	-1.3218	-2.5471
215	1	1	5.5E-06	-1	5.5E-06	0.07747	1.65402	1.5843	0.07748	-1.592	0.07748
216	1	1	4.9E-06	-1	4.9E-06	-0.2221	1.36221	1.56209	-0.2221	-1.5399	-0.2221
217	1	1	4.4E-06	-1	4.4E-06	0.39899	1.96108	1.60199	0.39899	-1.6419	0.39899
218	1	1	4E-06	-1	4E-06	-0.4711	1.13092	1.55488	-0.4711	-1.5078	-0.4711
219	1	1	3.6E-06	-1	3.6E-06	-0.4043	1.15058	1.51445	-0.4043	-1.474	-0.4043
220	1	1	3.2E-06	-1	3.2E-06	-1.0557	0.45875	1.40888	-1.0557	-1.3033	-1.0557
221	1	1	2.9E-06	-1	2.9E-06	-1.6783	-0.2694	1.24105	-1.6783	-1.0732	-1.6783
222	1	1	2.6E-06	-1	2.6E-06	0.14629	1.38735	1.25568	0.1463	-1.2703	0.1463
223	1	1	2.4E-06	-1	2.4E-06	0.85779	2.11347	1.34146	0.85779	-1.4272	0.85779
224	1	1	2.1E-06	-1	2.1E-06	0.04846	1.38992	1.34631	0.04846	-1.3512	0.04846
225	1	1	1.9E-06	-1	1.9E-06	0.61229	1.9586	1.40754	0.6123	-1.4688	0.6123
226	1	1	1.7E-06	-1	1.7E-06	-0.5997	0.80783	1.34757	-0.5997	-1.2876	-0.5997
227	1	1	1.5E-06	-1	1.5E-06	1.05378	2.40134	1.45294	1.05378	-1.5583	1.05378
228	1	1	1.4E-06	-1	1.4E-06	0.76423	2.21718	1.52937	0.76423	-1.6058	0.76423
229	1	1	1.3E-06	-1	1.3E-06	0.83182	2.36119	1.61255	0.83182	-1.6957	0.83182

APPENDIX D

Autocorrelation and Partial Autocorrelation Functions

The covariance between two observations, z_t, separated in time by k measurement intervals is called the *autocovariance* at lag k and is defined by

$$\gamma_k = cov[z_t, z_{t+k}] = E[(z_t-\mu)(z_{t+k}-\mu)] . \tag{65}$$

Therefore, if γ_0 is the process variance then the autocorrelation function (ACF) is defined by

$$\rho_k = \frac{\gamma_k}{\gamma_0} \tag{66}$$

which implies $\rho_0=1$. However, this is the theoretical definition of the autocorrelation function; one is more interested in the estimated ACF. If the data set of interest consists of N observations generated by a stationary stochastic process, then the most satisfactory estimate of the k^{th} lag autocorrelation ρ_k is

$$r_k = \frac{c_k}{c_0} \tag{67}$$

where

$$c_k = \frac{1}{N}\sum_{t=1}^{N-k} (z_t-\bar{z})(z_{t+k}-\bar{z}) , \quad k=0,1,2,\ldots,K \tag{68}$$

is the estimate of the autocovariance γ_k, and $\bar{z}$ is the data mean.

The partial autocorrelation function (PACF) is a tool which allows one to determine the order of autoregressive process to fit to a particular data set generated by a stochastic disturbance model. An AR(p) process can by nature be described in terms of p non-zero functions of the autocorrelations. The Yule-Walker equations, which can be found in Box and Jenkins (1970), expressed in matrix notation

$$\mathbf{P}_k \boldsymbol{\phi}_k = \boldsymbol{\rho}_k \qquad (69)$$

can be solved for k=1,2,3,... successively to obtain the partial autocorrelation function, ϕ_{kk}, at lag k. For an autoregressive process of order p, the PACF ϕ_{kk} will be non-zero for k less than or equal to p and zero for k greater than p. The PACF may be estimated by successively fitting AR processes of orders 1,2,3,... by least squares, as described in Box and Jenkins (1970) Chapter 7.

Appendix E

Detailed Derivation of Minimum Variance Controller for Maintaining Bottoms Composition in C_3 Splitter

The process dynamics relating bottoms composition to reboiler duty are first-order plus dead-time and represented by

$$x_{t+8} = -\frac{0.05}{(1-0.945B)}Q_t + z_{x_{t+8}} \tag{70}$$

One can minimize the variance of the control variable deviation from target by setting x_{t+8} to zero, yielding

$$Q_t = \frac{(1-0.945B)}{0.05}z_{x_{t+8}} \tag{71}$$

This equation indicates that we need a future value of the disturbance; thus the eight step ahead prediction of the disturbance is substituted for z_{x+8} in the above equation giving

$$Q_t = -\frac{(1-0.945B)}{0.05}\hat{z}_{x_{t+8/t}} \tag{72}$$

The disturbance affecting the bottoms composition is given by

$$z_{x_{t+8}} = \frac{a_{t+8}}{\nabla(1-0.66B)} \tag{73}$$

Expanding yields

$$z_{x_{t+8}} = 1.66z_{x_{t+7}} - 0.66z_{x_{t+6}} + a_{t+8} \tag{74}$$

Taking the conditional expectation of both sides of the above equation and through repeated substitution one obtains

$$
\begin{aligned}
\hat{z}_{x_{t+8/t}} &= 1.66E[z_{x_{t+7}}] - 0.66E[z_{x_{t+6}}] + E[a_{t+8}] \\
&= 1.66E[1.66z_{x_{t+6}}-0.66z_{x_{t+5}}+a_{t+7}]-0.66E[1.66z_{x_{t+5}}-0.66z_{x_{t+4}}+a_{t+6}]+0 \\
&= \ldots \\
&= 2.8713\ z_{x_t}-1.8713\ z_{x_{t-1}}
\end{aligned}
\tag{75}
$$

Substituting the last expression in equation 75 into equation 72 yields

$$
Q_t = \frac{(1-0.945B)}{0.05}\ (2.8713\ -1.8713B)\, z_{x_t} \tag{76}
$$

Substituting equation 73 into equation 76 and premultiplying both sides by $\nabla(1\text{-}0.66B)$ gives

$$
\nabla(1-0.66B)\, Q_t = \frac{(1-0.945B)}{0.05}\ (2.8713\ -1.8713B)\, a_t \tag{77}
$$

It is preferable to have equation 77 in terms of deviations from target of the control variable, x_t, therefore we must derive a relationship between x_t and a_t. The aforementioned relationship is obtained by substituting equation 76 and the expression for z_{t+8}, in terms of known values of the disturbance,

$$
\begin{aligned}
z_{x_{t+8}} = 2.8713z_t -1.8713z_{t-1} +\{&1+1.66B+2.0956B^2+2.3831B^3 \\
&+2.5728B^4+2.6981B^5+2.7807B^6+2.8353B^7\}\, a_{t+8}
\end{aligned}
\tag{78}
$$

into equation 70 yielding

$$
\begin{aligned}
x_t = \{1+1.66B+2.0956B^2+2.3831B^3+2.5728B^4+2.6981B^5 \\
+2.7807B^6+2.8353B^7\}\, a_t
\end{aligned}
\tag{79}
$$

Rearranging yields

$$
a_t = \frac{x_t}{(1+1.66B+2.0956B^2+2.3831B^3+\ldots+2.7807B^6+2.8353B^7)} \tag{80}
$$

Substituting equation 80 into equation 77 yields the minimum variance controller in terms of the deviation from target of the control variable shown in equation 56, that is

$$
\begin{aligned}
Q_t^* = 2.8713Q_{t-8}^* -1.8713Q_{t-9}^* +20.0\{2.8713x_t^* -4.5847x_{t-1}^* \\
+1.7684x_{t-2}^*\}
\end{aligned}
\tag{81}
$$

Appendix F

COLMSIM FORTRAN PROGRAM

The COLMSIM FORTRAN program is the same as the SPCSIM program, except that the process models, disturbances and minimum variance controllers have been specified as a result of the modelling done in Chapter 5. Control limits, simulation time and the number of simulations to be run are the only factors that can be changed in this program.

```
      PARAMETER (N=5000)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),
     &  RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),
     &  RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),
     &  SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,
     &  ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N),PN(N),
     &  XT(N),QT(N),PT(N),DT(N),ZTP(N),ZTX(N),R1(N),RR1(N),DNEW(N),
     &  PACT(N),QLF(N)
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP,
     &          SCL,EWCL,DFCL,XSTD,XSTD1
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH
C     REAL R(N)
      EXTERNAL DRNNOA,DSCAL,DADD,RNSET
      CALL READER
C *****************************************************************
C     RANDOM NUMBER GENERATOR
C *****************************************************************
      DO 626 JJ=1,NSIM
      ISEED=JJ*836
      ISEED1=JJ*99
      NR=ISIM
      XSTD=3.05D0
      XSTD1=1.73D0
      XM=0.0D0
      CALL RNSET(ISEED)
      CALL DRNNOA (NR, R)
      CALL DSCAL (NR, XSTD, R, 1)
      CALL DADD (NR, XM, R, 1)
      CALL RNSET(ISEED1)
      CALL DRNNOA (NR, R1)
      CALL DSCAL (NR, XSTD1, R1, 1)
      CALL DADD (NR, XM, R1, 1)
C *****************************************************************
C     FOR PID CONTROLLER MUST FIRST TUNE IT (IE: ZIEGLER NICHOLS)
C *****************************************************************
C
```

```
      TD=0.0D0                                              COL00380
      EKP=(1.0D0-THETA)*DELTA/(G*(1.0D0-DELTA))             COL00390
      EKI=(1.0D0-THETA)/G                                   COL00400
C                                                           COL00410
C                                                           COL00420
      DO 10 K=1,IB+1                                        COL00430
        TIME(K)=FLOAT(K)                                    COL00440
        TIME1(K)=FLOAT(K)+0.5D0                             COL00450
        ZT(K)=0.0D0                                         COL00460
        UT(K)=0.0D0                                         COL00470
        YT(K)=0.0D0                                         COL00480
 10   CONTINUE                                              COL00490
C******************************************************************* COL00500
C     CALL TO APPROPRIATE SIMULATION SUBROUTINE             COL00510
C******************************************************************* COL00520
      RUNSH(JJ)=0.0D0                                       COL00530
      RUNEW(JJ)=0.0D0                                       COL00540
      RUNCU(JJ)=0.0D0                                       COL00550
      RUNDF(JJ)=0.0D0                                       COL00560
      IF (ID .EQ. 0) CALL ARMA11                            COL00570
      IF (ID .NE. 0) CALL ARIMA1                            COL00580
      QLF(JJ)=QLF(JJ-1)+SUMYT(ISIM)                         COL00590
      CALL PTVAR                                            COL00600
      CALL CHARTS                                           COL00610
 626  CONTINUE                                              COL00620
      CALL ARLS                                             COL00630
      STOP                                                  COL00640
      END                                                   COL00650
C******************************************************************* COL00660
C******************************************************************* COL00670
C     READ DATA IN FROM DATA FILE                           COL00680
C******************************************************************* COL00690
C******************************************************************* COL00700
      SUBROUTINE READER                                     COL00710
      PARAMETER (N=5000)                                    COL00720
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                   COL00730
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),     COL00740
     &     RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),    COL00750
     &     RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),  COL00760
     &     SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,     COL00770
     &     ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N),PN(N),   COL00780
     &   XT(N),QT(N),PT(N),DT(N),ZTP(N),ZTX(N),R1(N),RR1(N),DNEW(N),   COL00790
     &   PACT(N),QLF(N)                                     COL00800
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP, COL00810
     &        SCL,EWCL,DFCL,XSTD,XSTD1                      COL00820
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH       COL00830
      CHARACTER*80 TITLE                                    COL00840
      READ (15,394) TITLE                                   COL00850
      READ (15,*) ISIM,IPVAR,ICONT,NSIM                     COL00860
      READ (15,394) TITLE                                   COL00870
      READ (15,*) IB, DELTA, G, PHI, THETA, ID              COL00880
      READ (15,394) TITLE                                   COL00890
      READ (15,*) DLAMB,EH,EL,STEP,TSTEP                    COL00900
      READ (15,394) TITLE                                   COL00910
      READ (15,394) TITLE                                   COL00920
      READ (15,*) IPH                                       COL00930
      READ (15,394) TITLE                                   COL00940
      READ (15,*) SCL,EWCL                                  COL00950
      IF(THETA .EQ. 0) THEN                                 COL00960
        ITHET=0                                             COL00970
      ELSE                                                  COL00980
        ITHET=1                                             COL00990
```

```
      ENDIF
      IF(PHI .EQ. 0) THEN
        IPHI=0
      ELSE
        IPHI=1
      ENDIF
C      IF (ID .EQ. 0) THEN
C        WRITE (16,395) IPHI,ITHET
C      ELSE
C        WRITE (16,396) IPHI,ID,ITHET
C      ENDIF
C      WRITE(16,397) PHI,THETA,ID
C      WRITE(16,399) DELTA,G
C      WRITE (16,398) STEP
C      WRITE (16,392)
C      WRITE (16,392)
C      WRITE (16,727)
C 392 FORMAT ('********************************************************',
C    &'*********')
  394 FORMAT (A80)
C 395 FORMAT ('THIS IS AN ARMA(',I1,',',I1,') PROCESS'/)
C 396 FORMAT ('THIS IS AN ARIMA(',I1,',',I1,',',I1,') PROCESS'/)
C 397 FORMAT ('PHI= ',F6.3,', THETA= ',F6.3,' AND D= ',I2)
C 398 FORMAT ('FOR A ',F6.3,' SIGMA STEP SHIFT IN DISTURBANCE MEAN')
C 399 FORMAT ('PROCESS INERTIA= ',F6.3,' AND GAIN= ', F6.3)
C727  FORMAT (5X,'XT',6X,'QT',7X,'DCON',5X,'PCON',6X,'DT',6X,'PT',6X,
C    &'PNC',6X,'PACT')
      RETURN
      END
C
C*********************************************************************
C*********************************************************************
C     SUBROUTINE TO DETERMINE CONTROL LIMITS FOR CHARTING TECHNIQUES
C*********************************************************************
C*********************************************************************
C
      SUBROUTINE PTVAR
      PARAMETER (N=5000)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),
     &      RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),
     &      RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),
     &      SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,
     &      ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N),PN(N),
     &   XT(N),QT(N),PT(N),DT(N),ZTP(N),ZTX(N),R1(N),RR1(N),DNEW(N),
     &   PACT(N),QLF(N)
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP,
     &          SCL,EWCL,DFCL,XSTD,XSTD1
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH
C
      DO 223 I=IB+2,ISIM
        IF (IPVAR .EQ. 1) PLTVAR(I)=QT(I)
        IF (IPVAR .EQ. 2) PLTVAR(I)=DT(I)
        IF (IPVAR .EQ. 3) PLTVAR(I)=XT(I)
        IF (IPVAR .EQ. 4) PLTVAR(I)=DT(I)
  223 CONTINUE
C
      STDZ=(((1.D0-2.D0*(THETA*PHI)+THETA**2)/(1.D0-PHI**2))**0.5D0)
C      STDZ=(1.0/(1.0-PHI**2.0))**0.5
      IF (IPVAR .EQ. 1) STDVAR=STDZ
      IF (IPVAR .EQ. 2 .OR. IPVAR .EQ. 4) STDVAR=XSTD
```

```
      IF (IPVAR .EQ. 3 .AND. ID .EQ. 0) THEN
      STDVAR=((PHI**(2*IB))/((G*(1-DELTA))**2))*((1-DELTA**2)*((PHI**2)*
     & STDZ**2+(THETA**2)*(XSTD**2))-2*THETA*PHI*(DELTA**2)*(XSTD**2)-
     & 2*(PHI**2)*DELTA*(PHI*(STDZ**2)+(1-THETA)*(STD**2))-2*THETA*
     & PHI*(XSTD**2)+2*PHI*THETA*DELTA*(PHI-THETA)*(XSTD**2))
      ELSEIF (IPVAR .EQ. 3 .AND. ID .EQ. 1) THEN
      STDVAR=1.0D0
      ENDIF
C      EWCL=147.9D0
C      SCL=347.2D0
      RETURN
      END
C
C
C*****************************************************************
C*****************************************************************
C     SIMULATES A CHEMICAL PROCESS WITH FIRST ORDER PLUS DEAD TIME OR
C     PURE GAIN PROCESS DYNAMICS WHOSE DISTURBANCE MODEL IS DESCRIBED
C     BY ANY FIRST ORDER AUTOREGRESSIVE MOVING AVERAGE MODEL.
C*****************************************************************
C*****************************************************************
C
      SUBROUTINE ARMA11
      PARAMETER (N=5000)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),
     &     RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),
     &     RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),
     &     SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,
     &     ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N),PN(N),
     &   XT(N),QT(N),PT(N),DT(N),ZTP(N),ZTX(N),R1(N),RR1(N),DNEW(N),
     &   PACT(N),QLF(N)
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP,
     &         SCL,EWCL,DFCL,XSTD,XSTD1
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH
C
      DO 40  I=IB+2,ISIM
      TIME(I)=FLOAT(I)
      TIME1(I)=FLOAT(I)+0.5D0
      RR(I)=0.0D0
      IF (TIME(I) .GE. TSTEP) THEN
        RR(I)=(1.0D0-PHI)*STEP*XSTD
      ENDIF
C
C
      ZTP(I)=(1.6D0)*ZTP(I-1) -0.6D0*ZTP(I-2)+R(I) +RR(I)
      ZTX(I)=(0.66D0)*ZTX(I-1) +R1(I) +RR1(I)
C      R(IB+1)=0.0D0
C      ZT(I)=PHI*ZT(I-1) +R(I) - THETA*R(I-1) +RR(I)
C
C
      IF (ICONT .EQ. 1) THEN
C
C     ****************************
C      MINIMUM VARIANCE CONTROLLER
C     ****************************
C
      XT(I)=0.945D0*XT(I-1)-(0.05D0*QT(I-8)) +ZTX(I) - 0.945D0*ZTX(I-1)
      QT(I)=(0.66D0**8)*QT(I-8)+((0.66D0**8)*20.0D0*(XT(I)-0.945D0
     &  *XT(I-1)))
      PT(I)=1.61D0*PT(I-1) -0.67D0*DT(I-1) +ZTP(I) -1.61D0*ZTP(I-1)
```

```
     & +0.1D0*(QT(I-1)-0.85D0*QT(I-2))-0.646D0*PT(I-2)+0.646D0*ZTP(I-2) COL02240
     & +0.67D0*0.76D0*DT(I-2)                                            COL02250
C     PT(I)=0.85D0*PT(I-1)+ZTP(I)-0.85D0*ZTP(I-1)-0.67D0*DT(I-1)         COL02260
C     PN(I)=0.85D0*PT(I-1)+ZTP(I)-0.85D0*ZTP(I-1)-0.67D0*DNEW(I-1)       COL02270
      PN(I)=1.61D0*PN(I-1) -0.67D0*DNEW(I-1) +ZTP(I) -1.61D0*ZTP(I-1)    COL02280
     & +0.1D0*(QT(I-1)-0.85D0*QT(I-2))-0.646D0*PN(I-2)+0.646D0*ZTP(I-2) COL02290
     & +0.67D0*0.76D0*DNEW(I-2)                                          COL02300
C     DT(I)=1.6D0*DT(I-1)-0.6*DT(I-2)+1.5D0*(1.6D0*PT(I)-1.96D0*PT(I-1) COL02310
C    & +0.51D0*PT(I-2))                                                  COL02320
      DT(I)=2.36D0*DT(I-1)-1.816D0*DT(I-2)+0.456D0*DT(I-3)+1.5D0         COL02330
     & *(1.6D0*PT(I)-3.176D0*PT(I-1)+1.9996D0*PT(I-2)-0.3876D0*PT(I-3))COL02340
     & +0.15D0*(QT(I)-2.45D0*QT(I-1)+1.96D0*QT(I-2)-0.51D0*QT(I-3))     COL02350
C     YT(I)=DELTA*YT(I-1) +G*(1.0D0-DELTA)*UT(I-1) +ZT(I) -DELTA*ZT(I-1)COL02360
C     SUM(I)=PHI*SUM(I-1)+YT(I)                                          COL02370
C     UT(I)=-((PHI**IB)/(G*(1.D0-DELTA)))*(((1.D0-THETA)*(1.D0-DELTA)   COL02380
C    & *PHI*SUM(I))+(((1.D0-THETA)*DELTA*PHI)-THETA+PHI*THETA)*YT(I)+  COL02390
C    &     ((THETA*DELTA)-(PHI*THETA*DELTA))*YT(I-1))                    COL02400
C     UT(I)=-(((PHI**IB)*(PHI-THETA))/(G*(1.D0-DELTA)))*(YT(I)-         COL02410
C    &     DELTA*YT(I-1))+THETA*UT(I-1)+(PHI-THETA)*(PHI**IB)*          COL02420
C    &     UT(I-IB-1)                                                    COL02430
      SUMYT(I)=SUMYT(I-1)+(XT(I)**2)                                     COL02440
      ELSE                                                               COL02450
C                                                                        COL02460
C     ****************                                                   COL02470
C      PID CONTROLLER                                                    COL02480
C     ****************                                                   COL02490
C                                                                        COL02500
      YT(I)=DELTA*YT(I-1) +G*(1.0D0-DELTA)*UT(I-1) +ZT(I) -DELTA*ZT(I-1)COL02510
      SUM1(I)=SUM1(I-1)+YT(I)                                            COL02520
      UT(I)=-(EKP*YT(I)+EKI*(SUM1(I))+TD*(YT(I)-YT(I-1)))                COL02530
      ENDIF                                                              COL02540
C                                                                        COL02550
C     **********************                                             COL02560
C     RESIDUAL CALCULATIONS                                              COL02570
C     **********************                                             COL02580
C                                                                        COL02590
C     ZHAT(I)=(PHI**(IB))*(PHI*ZT(I)-THETA*R(I))                         COL02600
      ZHAT(I)=(PHI**(IB))*(PHI*(SUM(I)-THETA*SUM(I-1))-THETA*YT(I))      COL02610
      RES(I)=ZT(I)-ZHAT(I-IB-1)                                          COL02620
C     WRITE (16,4) QT(I),XT(I) DT(I),PT(I)                               COL02630
C 4   FORMAT (4(F9.3))                                                   COL02640
 40   CONTINUE                                                           COL02650
      RETURN                                                             COL02660
      END                                                                COL02670
C******************************************************************** COL02680
C******************************************************************** COL02690
C     SIMULATES A CHEMICAL PROCESS WITH FIRST ORDER PLUS DEAD TIME OR    COL02700
C     PURE GAIN PROCESS DYNAMICS WHOSE DISTURBANCE MODEL IS DESCRIBED    COL02710
C     BY ANY FIRST ORDER AUTOREGRESSIVE INTEGRATED MOVING AVERAGE MODEL.COL02720
C******************************************************************** COL02730
C******************************************************************** COL02740
C                                                                        COL02750
      SUBROUTINE ARIMA1                                                  COL02760
      PARAMETER (N=5000)                                                 COL02770
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                                COL02780
C                                                                        COL02790
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),       COL02800
     &    RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),       COL02810
     &    RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),     COL02820
     &    SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,        COL02830
     &    ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N),PN(N),      COL02840
     &  XT(N),QT(N),PT(N),DT(N),ZTP(N),ZTX(N),R1(N),RR1(N),DNEW(N),      COL02850
```

```
     &   PACT(N),QLF(N)                                             COL02860
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP, COL02870
     &        SCL,EWCL,DFCL,XSTD,XSTD1                              COL02880
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH               COL02890
C                                                                   COL02900
C                                                                   COL02910
      DO 60  I=10,ISIM                                              COL02920
C                                                                   COL02930
      TIME(I)=FLOAT(I)                                              COL02940
      TIME1(I)=FLOAT(I)+0.5D0                                       COL02950
      RR(I)=0.0D0                                                   COL02960
      RR1(I)=0.0D0                                                  COL02970
      IF (TIME(I) .EQ. TSTEP) RR1(I)=STEP*(1.0D0-0.66D0)            COL02980
C      IF (TIME(I) .EQ. TSTEP) RR(I)=STEP*(1.0D0-0.6D0)*XSTD        COL02990
C      R(IB+1)=0.0D0                                                COL03000
      ZTP(I)=(1.6D0)*ZTP(I-1) -0.6D0*ZTP(I-2)+R(I) +RR(I)           COL03010
      ZTX(I)=(1.66D0)*ZTX(I-1) -0.66D0*ZTX(I-2)+R1(I) +RR1(I)       COL03020
C                                                                   COL03030
C                                                                   COL03040
      IF (ICONT .EQ. 1) THEN                                        COL03050
C                                                                   COL03060
C     *****************************                                 COL03070
C      MINIMUM VARIANCE CONTROLLER                                  COL03080
C     *****************************                                 COL03090
C                                                                   COL03100
      XT(I)=0.945D0*XT(I-1)-(0.05D0*QT(I-8)) +ZTX(I) - 0.945D0*ZTX(I-1) COL03110
      QT(I)=2.8713D0*QT(I-8)-1.8713D0*QT(I-9)+(2.8713D0*XT(I)-      COL03120
     &        4.5847D0*XT(I-1) +1.7684D0*XT(I-2))/0.05D0            COL03130
C      QT(I)=(2.8713D0*ZTX(I)-4.5847D0*ZTX(I-1)+1.7684D0*ZTX(I-2))/0.05D0COL03140
      PT(I)=1.61D0*PT(I-1) -0.67D0*DT(I-1) +ZTP(I) -1.61D0*ZTP(I-1)   COL03150
     & +0.1D0*(QT(I-1)-0.85D0*QT(I-2))-0.646D0*PT(I-2)+0.646D0*ZTP(I-2) COL03160
     &  +0.67D0*0.76D0*DT(I-2)                                      COL03170
C      PT(I)=0.85D0*PT(I-1)+ZTP(I)-0.85D0*ZTP(I-1)-0.67D0*DT(I-1)   COL03180
C      PN(I)=0.85D0*PT(I-1)+ZTP(I)-0.85D0*ZTP(I-1)-0.67D0*DNEW(I-1) COL03190
      PN(I)=1.61D0*PN(I-1) -0.67D0*DNEW(I-1) +ZTP(I) -1.61D0*ZTP(I-1) COL03200
     & +0.1D0*(QT(I-1)-0.85D0*QT(I-2))-0.646D0*PN(I-2)+0.646D0*ZTP(I-2) COL03210
     &  +0.67D0*0.76D0*DNEW(I-2)                                    COL03220
C      DT(I)=1.6D0*DT(I-1)-0.6*DT(I-2)+1.5D0*(1.6D0*PT(I)-1.96D0*PT(I-1) COL03230
C     &  +0.51D0*PT(I-2))                                           COL03240
      DT(I)=2.36D0*DT(I-1)-1.816D0*DT(I-2)+0.456D0*DT(I-3)+1.5D0    COL03250
     &  *(1.6D0*PT(I)-3.176D0*PT(I-1)+1.9996D0*PT(I-2)-0.3876D0*PT(I-3))COL03260
     &  +0.15D0*(QT(I)-2.45D0*QT(I-1)+1.96D0*QT(I-2)-0.51D0*QT(I-3))  COL03270
      PACT(I)=ZTP(I)+0.76D0*ZTP(I-1)+0.1D0*QT(I-1)                  COL03280
      IF (DT(I) .GT. 10.0) DNEW(I)=10.0                             COL03290
      IF (DT(I) .LT. -10.0) DNEW(I)=-10.0                           COL03300
      IF (ABS(DT(I)) .LE. 10.0) DNEW(I)=DT(I)                       COL03310
      SUMYT(I)=SUMYT(I-1)+(QT(I)**2)                                COL03320
      ELSE                                                          COL03330
C                                                                   COL03340
C     ****************                                              COL03350
C      PID CONTROLLER                                               COL03360
C     ****************                                              COL03370
C                                                                   COL03380
C      YT(I)=DELTA*YT(I-1) +G*(1.D0-DELTA)*UT(I-1) +ZT(I) -DELTA*ZT(I-1) COL03390
C      SUMYT(I)=SUMYT(I-1)+YT(I)                                    COL03400
C      UT(I)=-(EKP*YT(I)+EKI*(SUMYT(I))+TD*(YT(I)-YT(I-1)))         COL03410
C      ZHAT(I)=2.8713*ZTX(I)-1.8713*ZTX(I-1)                        COL03420
      ENDIF                                                         COL03430
C                                                                   COL03440
C     ***********************                                       COL03450
C      RESIDUAL CALCULATIONS                                        COL03460
C     ***********************                                       COL03470
```

```
C
      ZHAT(1)=(1.D0+0.66D0)*ZTX(I)-0.66D0*ZTX(I-1)
C      IF(IB .EQ. 0) GOTO 301
      ZHAT(2)=(1.D0+0.66D0)*ZHAT(1)-0.66D0*ZTX(I)
C      IF(IB .EQ. 1) GOTO 301
      DO 222 J=3,8
        ZHAT(J)=(1.D0+0.66D0)*ZHAT(J-1)-0.66D0*ZHAT(J-2)
 222  CONTINUE
      SUM1(I)=ZHAT(8)
      RES(I)=ZTX(I)-2.8713*ZTX(I-1)+1.8713*ZTX(I-2)
C     WRITE (16,44) QT(I),XT(I),DT(I),PT(I)
C 44  FORMAT (4(F9.3))
C     WRITE (16,726) ZTX(I)
      WRITE (16,726) ZTP(I)
 726  FORMAT (F8.3,3X)
C726  FORMAT (F8.2)
  60  CONTINUE
      RETURN
      END
C
C*******************************************************************
C*******************************************************************
C     SUBROUTINE FOR CALCULATING RUN LENGTHS FOR VARIOUS
C     CHARTING TECHNIQUES.
C*******************************************************************
C*******************************************************************
C
      SUBROUTINE CHARTS
      PARAMETER (N=5000)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),
     &      RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),
     &      RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),
     &      SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,
     &      ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N),PN(N),
     &    XT(N),QT(N),PT(N),DT(N),ZTP(N),ZTX(N),R1(N),RR1(N),DNEW(N),
     &    PACT(N),QLF(N)
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP,
     &           SCL,EWCL,DFCL,XSTD,XSTD1
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH
C
C***************************
C     SHEWHART CHART     *
C***************************
      DO 124 I=IB+2,ISIM
C
      SHEW(I)=PLTVAR(I)
C
C*****************************************
C     CUMULATIVE SUM CHARTING TECHNIQUE  *
C*****************************************
C
      CUSUM1(I)=DMAX1((CUSUM1(I-1)-(PLTVAR(I))+0.5D0)),0.0D0)
      CUSUM2(I)=DMAX1((CUSUM2(I-1)+((PLTVAR(I))-0.5D0)),0.0D0)
      IF (CUSUM2(I) .GT. CUSUM1(I)) THEN
      CUSUM3(I)=CUSUM2(I)
      ELSE
      CUSUM3(I)=CUSUM1(I)
      ENDIF
C************************************************
C     EXPONENTIALLY WEIGHTED MOVING AVERAGE (EWMA) *
```

```
C*********************************************              COL04100
C                                                    COL04110
      EWMA(I)=DLAMB*(PLTVAR(I))+(1.0D0-DLAMB)*EWMA(I-1)          COL04120
C                                                    COL04130
C*******************************************              COL04140
C     NTH ORDER DIFFERENCING TECHNIQUE.       *             COL04150
C     -FOR USE ON INTEGRATED DISTURBANCES ONLY-  *          COL04160
C*******************************************              COL04170
C                                                    COL04180
      IF(ID .EQ. 0) GOTO 120                               COL04190
C                                                    COL04200
      IF (I .LE. IPH+IB+1) THEN                            COL04210
       DIFF(I)=0.0D0                                      COL04220
      ELSE                                              COL04230
       DIFF(I)=PLTVAR(I)-PLTVAR(I-IPH)                       COL04240
      ENDIF                                             COL04250
      IF(TIME(I) .LE. TSTEP) GOTO 124                      COL04260
  120 IF(RUNSH(JJ) .GT. 0.0D0) GOTO 121                    COL04270
      IF(ABS(SHEW(I)) .GE. SCL) RUNSH(JJ)=TIME(I)             COL04280
  121 IF(RUNEW(JJ) .GT. 0.0D0) GOTO 122                    COL04290
      IF(ABS(EWMA(I)) .GE. EWCL) RUNEW(JJ)=TIME(I)            COL04300
  122 IF(RUNCU(JJ) .GT. 0.0D0) GOTO 123                    COL04310
      IF(CUSUM3(I) .GE. EH) RUNCU(JJ)=TIME(I)               COL04320
      IF(ID .EQ. 0) GOTO 124                               COL04330
  123 IF(RUNDF(JJ) .GT. 0.0D0) GOTO 124                    COL04340
      IF(ABS(DIFF(I)) .GE. DFCL) RUNDF(JJ)=TIME(I)            COL04350
  124 CONTINUE                                          COL04360
      RETURN                                            COL04370
      END                                               COL04380
C                                                    COL04390
C***************************************************************** COL04400
C***************************************************************** COL04410
C     SUBROUTINE FOR CALCULATING RUN LENGTHS FOR VARIOUS         COL04420
C     CHARTING TECHNIQUES.                                COL04430
C***************************************************************** COL04440
C***************************************************************** COL04450
C                                                    COL04460
      SUBROUTINE ARLS                                    COL04470
      PARAMETER (N=5000)                                 COL04480
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)                  COL04490
C                                                    COL04500
      COMMON/STUFF/ YT(N), UT(N), ZT(N), TIME(N), ZHAT(N), RES(N),     COL04510
     &     RUNCU(N),RUNEW(N),RUNSH(N),RUNDF(N),RNLTH1(N),RNLTH2(N),    COL04520
     &     RNLTH3(N),RNLTH4(N),EWMA(N),CUSUM3(N),CUSUM1(N),CUSUM2(N),  COL04530
     &     SUMYT(N),SUM1(N),SUM2(N),SUM3(N),TIME1(N),DIFF(N),ARL1,     COL04540
     &     ARL2,ARL3,ARL4,RR(N),SUM(N),PLTVAR(N),SHEW(N),R(N),PN(N),   COL04550
     &   XT(N),QT(N),PT(N),DT(N),ZTP(N),ZTX(N),R1(N),RR1(N),DNEW(N),   COL04560
     &   PACT(N),QLF(N)                                  COL04570
      COMMON/VARI/ DLAMB,PHI,THETA,G,DELTA,EL,EKP,EKI,TD,EH,STEP,TSTEP, COL04580
     &          SCL,EWCL,DFCL,XSTD,XSTD1                 COL04590
      COMMON/VARI2/IPVAR,JJ,ISIM,NSIM,ICONT,ID,IB,IPH           COL04600
C                                                    COL04610
      DO 678 I=IB+2,NSIM                                 COL04620
        IF(RUNSH(I) .EQ. 0.0D0) RUNSH(I)=TIME(ISIM)           COL04630
        IF(RUNEW(I) .EQ. 0.0D0) RUNEW(I)=TIME(ISIM)           COL04640
        IF(RUNCU(I) .EQ. 0.0D0) RUNCU(I)=TIME(ISIM)           COL04650
        IF(RUNDF(I) .EQ. 0.0D0) RUNDF(I)=TIME(ISIM)           COL04660
C                                                    COL04670
        RNLTH1(I)=RNLTH1(I-1)+RUNSH(I)                    COL04680
        RNLTH2(I)=RNLTH2(I-1)+RUNEW(I)                    COL04690
        RNLTH3(I)=RNLTH3(I-1)+RUNCU(I)                    COL04700
        RNLTH4(I)=RNLTH4(I-1)+RUNDF(I)                    COL04710
```

```
678 CONTINUE                                                    COL04720
    ARL1=(RNLTH1(NSIM)/(FLOAT(NSIM)))-(TSTEP)                   COL04730
    ARL2=(RNLTH2(NSIM)/(FLOAT(NSIM)))-(TSTEP)                   COL04740
    ARL3=(RNLTH3(NSIM)/(FLOAT(NSIM)))-(TSTEP)                   COL04750
    ARL4=(RNLTH4(NSIM)/(FLOAT(NSIM)))-(TSTEP)                   COL04760
    WRITE (16,*) ARL1,ARL2,ARL3,ARL4                            COL04770
    WRITE(16,*) 'QUADRATIC LOSS FUNCTION= ',QLF(NSIM)/FLOAT(ISIM*   COL04780
   & NSIM)                                                      COL04790
C   WRITE (16,*) XSTD                                           COL04800
    RETURN                                                      COL04810
    END                                                         COL04820
```

COLMSIM DATA FILE:

```
sim. time   choice of var. to chart   choice of controller   # of sim.
 1710              3                         1                   1
dead time   inertia (delta)   gain cnst   phi   theta   d
  0            0.85d0          4.47d0    0.6d0  0.0d0   1
lambda   h   control limits   step dist.   time of step dist.
 0.15d0  200.0d0   40.0d0      0.0d0        200.0d0
amount of differencing (nth order differencing) only for integrated
disturbances (choose 1,4,5,6,10 or 20)
   5
Shewhart C.L.    EWMA C.L.
  31.950d0        18.53d0
  15.400d0        18.65d0
```