ABSTRACT

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The main objective in a chemical plant is to improve profit while assuring products meet required specifications and satisfy environmental and operational constraints. A sub-objective that directly affects profit (main objective) is to improve the control performance of key economic variables in the plant, such as production rate and quality. An optimal control-based approach is proposed to determine a set of measurements and manipulated variables (dominant variables) and to structure them to improve plant profitability. This approach is model-based, and it uses optimal control theory to find the dominant variables that affect economic variables in the plant. First, the measurements and manipulated variables that affect product flow and quality are identified. Then, a decentralized control structure is designed to pair these measurements with the manipulated variables. Finally, a model predictive control

(MPC) is built on top of the resulting control structure. This is done to manipulate the set point of these loops in order to change the production rate and product quality.

Another sub-objective that affects the profit in the plant is to improve the control of inerts. In general, the inventory of the inerts is controlled using a purge. A new methodology to optimally control inerts is presented. This methodology aims to reduce the losses that occur throughout the purge by solving an optimization problem to determine the maximum amount of inert that can be handled in the plant without having shut down of the plant due to inert accumulation. The methodology is successfully applied to the Tennessee Eastman Plant where the operating cost was reduced approximately 4%.

This methodology solves an approximation to an optimal economic problem. First, it improves the control performance of key economic variables in the plant. Therefore, tighter control of these economic variables is achieved and the plant can be operated closer to operational constraints. Second, it minimizes purge which is a variable that generally causes significant costs in the plant. This approach is applied to the Tennessee Eastman and the Vinyl Acetate Processes. Results demonstrating the effectiveness of this method are presented and compared with the results from other authors.

OPTIMAL SELECTION OF MEASUREMENTS AND MANIPULATED VARIABLES FOR PRODUCTION CONTROL

By

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Dedication

To my family whose love, support, and encouragement are always with me.

To my daughter, Sabrina, who is my strength and inspiration.

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Table of Contents

List of Tables

List of Figures

Chapter 1: Introduction

1.1. Historical Overview of Plantwide Contro1

In general, a typical chemical process has multiple units, hundreds of measurements and manipulated variables, and different control and economic objectives. For many years, engineers used the unit operation approach [Stephanopoulos, 1983] to design control structures for chemical processes. In this approach, control loops were established for each unit operation or equipment in the plant. Then, all these pieces were combined for an entire plant. This approach did not always give the expected results because, when process units are linked, they interact with one another. Also, changes in manipulated variables produce local and global effects in the process. These characteristics of the entire process create conflicts between loops. Therefore, engineers had to make adjustments either in their final control strategies or in the process to avoid these conflicts. Despite these inconveniences, the unit operation approach has worked reasonably well. However, in the late 1960's, with the objective of reduceding energy costs, operating costs, and capital investment, engineers started to increase the use of recycle streams. Also, they introduced heat integration in both existing and new plants. The use of recycle streams and heat integration improves economics in the plant. However, they introduce a feedback of material and energy among units upstream and downstream. Moreover, recycle streams and heat integration interconnect separated unit operations and create a path for disturbance propagation [Luyben et al., 1996]. The presence of recycle streams alters the dynamic behavior of the plant by introducing an integrating effect that is not localized to an isolated part of the process [Luyben et al., 1997]. These features of complex processes can only be considered from the viewpoint of the entire plant.

Over the last few decades, process control engineers have developed different methodologies to generate control structures for an entire plant, and not simply for individual units. These methodologies are called plantwide control design methodologies, and they consider the local (unit operations) and global characteristics of the process (interaction between unit operations, feedback due to recycle stream, energy integration, etc.). The plantwide control design problem is very complex because of the following: 1) The size of the problem (large number of measurements and manipulated variables, many different unit operations) is significantly larger than for single units; 2) The variables to be controlled by a plantwide control system are not as clearly and easily defined as for single units [Stephanopoulos et al., 2000]; 3) The characteristics of the process, such as several recycle streams and energy integration (may affect the entire process); and 4) The large cost involved in making a precise problem definition (the use of a detailed dynamic linear and nonlinear model and a steady state model). In order to overcome these difficulties, the plantwide control problem is decomposed into smaller subproblems. In addition, whenever the dynamic model of the process is not available, an alternative to this is to develop heuristic rules, based on experience and process insight. Therefore, plantwide control design methodologies can be divided into mathematically-oriented, process-oriented approaches, and/or a combination of both. The mathematically-oriented approaches are based on the use of mathematical models and quantitative methods to determine control structures for the process. The following researchers have presented mathematically-oriented approaches: Moore (1992), Georgiou and Floudas (1992), Narraway and Perkins (1993, 1994), Mohideen et al. (1996), Bansal and Perkins (2000) , Kookos and Perkins (2000), and Kookos (2005) among others. The process-oriented approaches are based on qualitative methods where heuristics, logic, and experience are used determine control structures for the process. Buckley (1964), McAvoy et al. (1994), Luyben et al. (1996), Skogestad (2000, 2004) were among the authors that proposed process-oriented approaches. Larsson and Skogestad (2000) presented a review on plantwide control design of process-oriented and mathematically-oriented approaches.

Several plantwide design methodologies have been presented in recent years (Details are given in Chapter 2). However, there is no systematic procedure that has been adopted by the control community, as a general procedure to solve this problem. The reason is that plantwide control design is very much open-ended which means that there is not a unique correct solution. In fact, a control structure that is good for a specific control or economic objective might not be good for another objective. Therefore, the success of the control design is measured by the extent to which it can achieve the desired control, operating, and economic objectives. Proposed control strategies can be compared and evaluated, using different criteria, such as control performance and analysis of key economic variables in the plant such as production rate, variability of product quality and amount of purge.

1.2. <u>Rationale of Research</u>

The main objective in a chemical plant is to improve profit while satisfying product specifications, environmental, and operational constraints. This can be translated into the following objectives: increase product throughput (if the market requires more product), increase yield of higher valued products, decrease energy consumption, decrease purge, decrease off-specification products, decrease pollution, improve safety, extend life of equipment, improve operability, and decrease production labor [Edgar, 2004].

In general, in complex processes, more than one variable should be controlled to satisfy the operating economic objectives in the plant. However, it is not simple to identify a direct relationship between each type of economic benefit (profitability) and how controllers are designed and operated. The key questions to answer are the following: 1) which variables (dominant variables) should be controlled? 2) which measurements and manipulated variables should be used for this purpose? Different techniques have been used for the problem of measurement selection and manipulated variable selection. Chapter 3 presents a review of current measurement and manipulated variables selection methodologies. However, in the majority of these techniques the effects of measurement and manipulated variable selection on the economic objectives in the plant is not considered. To demonstrate the importance of measurement selection and its effect on the economic objectives in the plant, two examples are presented. One case involves the feedback regulation of the temperature in a chemical reactor. The control of this loop affects the productivity, selectivity, yield, and reactor stability. Another case concerns the purity control in a distillation column, in which the control of the temperature on the right tray affects the purity and, therefore, the economics of the plant.

It is important to point out that the majority of current plantwide control design methodologies do not focus on the main economic objective in the plant (to improve profit). The reasons for this are the following: 1) These methodologies put more emphasis on the control and operation of the plant and 2) It is not an easy task to quantify profitability at this stage (when control strategies for the plant are going to be determined) because the key economic considerations are not easily formulated, using a single objective function. Among, the limited number of researchers who consider economics for control structure design are Nishida (1981), Narraway and Perkins (1993), and Bansal and Perkins (2000), and Kookos (2005). Their approaches are rigorous and produce control structures that are optimal within the limitations imposed by the model, and the mathematical methods used [Bansal and Perkins, 2000]. However, they involve a detailed evaluation which can be translated into engineering effort and computational time.

The motivation of this research work is to develop a systematic methodology for plantwide control design that focuses on improving profit in the plant. A sub-objective that directly affects the profit in the plant is to improve the control performance of key economic variables in the plant, such as production rate and product quality.

In this work, an optimal control-based approach is proposed to determine the set of measurements and manipulated variables (dominant variables) and to structure them to improve profit in a plant. This approach uses a linear dynamic model of the process (linear time invariant, LTI, state space model) and optimal control theory to identify the dominant variables that affect production rate and product quality. The original idea of using a LTI model and optimal control theory for control structure design was presented by Schnelle (1989). More recent research on this subject has been presented by Chen and McAvoy (2003, 2004) and Chen (2002).

Another objective that is considered in this dissertation is to improve the control of inerts in a plant. In general, the inventory of the inerts is controlled using the purge. Sometimes the loss that occurs through the purge is very significant because not only the inerts leave the process through the purge but also the reactants and products leave. A new methodology to improve the control of inerts in a plant is proposed. This methodology uses the amount of inerts that enters in the plant to solve an optimization problem to determine the maximum amount of inerts that can be handled in the plant without having to shut down the plant due to inert accumulation. This methodology uses a Kalman filter to estimate the amount of inerts that enters the plant if there is no analyzer to measure it. Then the setpoint of the purge controller is modified according to the results of the optimization problem.

This methodology solves an approximation to an optimal economic problem. First, it improves the control performance of key economic variables in the plant (production rate and product quality). Therefore, tighter control of these economic variables is achieved and the plant can be operated closer to operational constraints. Second, it minimizes purge which is a variable that generally causes significant costs in the plant. For example, by looking at the cost function of the Tennessee Eastman plant it is obvious that the purge represents a significant cost (approximately 67% of the total operational cost).

1.3. Introduction to Optimal Control

The plantwide control design methodology presented in this work is based on optimal control theory, therefore a brief introduction to some basic definitions in optimal control theory is presented in this section. Optimal control theory describes the application of different forcing to a dynamic system for the purpose of maximizing some measurement of performance or minimizing a cost function [Stengel, 1993]. In other words, the optimal control problem consists in finding the control which attains the desired objective while maximizing or minimizing a given criterion (performance index). Optimal control theory has a large number of applications such as determining optimal flight path, maximizing the range of a rocket, minimizing the error in estimation of the position of a vehicle. Specifically, in process control, optimal control theory has been used as follows: 1) to regulate a system to remain near a desired condition in the presence of disturbances, and 2) to follow a nominal path with minimum error, even though system parameters have uncertain values.

In general, the majority of chemical processes are considered nonlinear. Even though there is an optimal control design approach for general nonlinear systems [Lewis, 1992], no systematic design approach has been suggested at the present time. In fact, experience is always needed for solving each particular nonlinear problem. By contrast, optimal control theory and linear quadratic regulator (LQR) are firmly established for linear and time-invariant (LTI) systems. The optimal controller design for linear time invariant (LTI) systems with quadratic performance indices is called the linear quadratic regulator (LQR) problem. In the optimal control theory, LQR is the basic controller design for LTI systems. The general formulation for an optimal LQR, using state feedback, is given as follows [Lewis, 1992]:

Process

$$\dot{x} = Ax + Bu \qquad t \geq t_o \qquad x(t_o) = x_o \tag{1.1}$$

Performance Index or cost function:

$$J(t_0) = \frac{1}{2}x^T(T)S(T)x(T) + \frac{1}{2}\int_{t_0}^{T}(x^TQx + u^TRu)dt \qquad S(t) \geq 0 \qquad Q \geq 0 \qquad R > 0 \tag{1.2}$$

with $\quad S(T) \geq 0 \qquad Q \geq 0 \qquad R > 0$

The optimal LQR is determined by solving a Riccati Equation (Equation 1.3).

$$-\dot{S} = A^TS + SA - SBR^{-1}B^TS + Q \tag{1.3}$$

where the optimal feedback gain is given by the Kalman gain *K(t)* as follows:

$$K = R^{-1}B^{T}S \tag{1.4}$$

The control strategy that minimizes the value of a quadratic performance index or cost function is described by a state feedback control law. Then the optimal control *u(t)* is a time varying state feedback given by Equation 1.5

$$u = -K(t)x \tag{1.5}$$

Optimal Cost:

$$J(t_0) = \frac{1}{2}x_0^{\,T}S(t_0)x_0 \tag{1.6}$$

This formulation assumes that the state of the plant is known; therefore, the cost function can be calculated before the control action is applied to the plant, if the initial state is known in advance. More details of this formulation can be found in [Lewis, 1992].

1.4. Topics of the Dissertation

The organization of this disseration is as follows: Chapter 2 provides a background on plantwide control design and a review of current relevant research in this area. Chapter 3 provides a background, review, and comparison of current measurements and manipulated variable selection methods. In Chapter 4, the optimal control-based measurement and manipulated variable selection methodology is presented. In Chapters 5 and 6, the proposed methodology is applied to two well-known process models, the Tenessee Eastman Process and the Vinyl Acetate Process, respectively. In Chapter 7 the optimal control of inerts methodology is presented. Finally, in Chapter 8, conclusions and future research are presented.

Chapter 2: Plantwide Control Design

*2.1. **Background***

Over the last few decades, process control engineers started to consider the entire plant, for addressing the control design problem for chemical plants instead of individual units of the process. Numerous authors have proposed plantwide control methodologies that consider the local (unit operations) and global characteristics of the process (interaction between unit operations, feedback because of recycle streams, energy integration, etc). Today's chemical plants contain several recycle streams, energy integration, many different unit operations, and a large number of measurements and manipulated variables which make the plantwide control design problem more complex. Several methodologies have been proposed to solve this problem. The majority of them decompose the problem into smaller sub-problems that are easily handled. In addition, these methodologies can be categorized into heuristic-based methodologies, mathematically based-methodologies, and a combination of both. The heuristic-based methodologies are based on qualitative methods that use experience and logical rules to generate plantwide control structures. The main advantage of these methodologies is that they do not involve any detailed evaluation; therefore, the engineering effort and computational time is relatively small, compared to mathematically-based methodologies, even for large problems. On the other hand, the mathematically-based methodologies use quantitative methods in which mathematical models are formulated and solved, using mathematical programming methods. These methodologies are rigorous and produce control structures that are optimal within the limitations imposed by the methods and models used; however, they involve more engineering effort and computational time.

In this chapter, a number of plantwide control methodologies, proposed by researchers in recent years, are reviewed to give a background to the methodology presented in this thesis. In Section 2.2, the terms and definitions used in the plantwide control area are defined. In Section 2.3, control structure design is explained. In Section 2.4, current methodologies for plantwide control design are reviewed. In Section 2.5, partial control is explained. Finally, in Section 2.6, simulation techniques used to evaluate plantwide control performance are discussed.

2.2. Plantwide Control Design Terms and Definitions

The term plantwide refers to an entire chemical plant consisting of recycle streams, energy integration, and many different interconnected unit operations (distillation columns, reactors, heat exchangers, pumps, compressors, absorbers, tanks, etc.). Plantwide control involves the systems and strategies to control an entire chemical plant. Therefore, plantwide control tries to address the following question: which variables should be controlled, which variables should be measured, which inputs should be manipulated and how should they be linked together [Foss, 1973]. The main objective of a plantwide control system is to satisfy the desired economic and operational objectives, reject disturbances, and handle safety, operational, and environmental constraints. In general, the design of a plantwide control system can be an overwhelming task, considering the following:

1) The size of the design problem is always related to the difficulty of solving the problem. Often in a complex process, the number of measurements is large and exceeds the number of manipulated variables. Therefore, a large number of control schemes can be generated by pairing the manipulated variables with measurements (process outputs) in different ways. It is not always obvious, even to experienced process control engineers, which of these structures would be the best to accomplish the desired objectives.

2) In some cases, it is relatively easy to determine the variable or set of variables that should be controlled to achieve a specific objective. However, when global objectives are being considered (e.g. maximize profit, minimize process variations), it is not an easy task to find the set of variables that define the behavior represented by the global objective.

3) Features of the entire plant, such as recycle streams, energy integration, interaction between units, and a large number of variables can make the size of the mathematical problem too large and difficult to handle. Therefore, plantwide control design methodologies divide the overall problem into sub-problems through a hierarchical design procedure.

Hierarchical decomposition

Buckley [Buckley, 1964] was the first researcher to use the idea of decomposing the plantwide design control problem into sub-problems. Buckley, proposed a procedure that consisted of two stages: 1) Determine the material balance control structure to handle vessel inventories for low-frequency disturbances; 2) Establish product quality control structure to regulate high frequency disturbances. This procedure has been used for plantwide control design and as a conceptual framework for developing later procedures. The main disadvantage of this methodology is that it does not explicitly consider the energy management and recycle streams. Also, by selecting the material balance control structure before the product quality controls, the procedure can significantly limit flexibility in chosing the control structure for product quality [Luyben, 1997]. Another pioneer in the use of a hierarchical solution for the plantwide control design problem was Umeda [Umeda, 1978]. His procedure is a unit-based approach that consists of four stages: 1) Decompose the plant into individual unit operations; 2) Generate the best control structure for each unit; 3) Combine all these structures to form a complete design for the entire plant; and 4) Eliminate conflicts through manual adjustment. Although this approach has been widely used in industry, it becomes impractical for today's chemical plants (recycle stream, energy integration, etc.). The reason is that there are too many conflicts when individual unit operation control structures are linked together. In 1980, Morari presented a review on plantwide control methodologies. He also discussed two hierarchical ways of decomposing the plantwide problem:

1) Multi-Layer (Vertical) Decomposition. The decomposition can be based on either the priorities of the control objectives or the time scale (the frequency of adjustment of the input). Authors that use the vertical decomposition based on time scale in their plantwide control methodologies are: [Buckley, 1964], [McAvoy and Ye, 1994], and [Ng and Stephanopoulos, 1998], [Chen, 2002], among other. Ng and Stephanopoulos

(1998), combine vertical decomposition with horizontal decomposition, discussed below. On the other hand, plantwide control methodologies that use vertical decomposition based on the priority of control objectives were presented by [Luyben, 1997], [McAvoy, 1999], [Ng and Stephanopoulos, 1998], and [Chen, 2002] among others. The control objectives used by these authors are basically the same: stability, energy balance, production rate, product quality, safety control, material balance, unit operation, optimize economics. However, they were prioritized in a different way. Chen (2002) compared the way that [Luyben, 1997], [McAvoy, 1999] and [Ng, Stephanopoulos, 1998] prioritized these control objectives. Also, Chen pointed out that McAvoy's vertical decomposition can be explained from both points of views (time scale and priority of the control objective).

2) Horizontal Decomposition. The system is divided into non-interacting parts. Douglas (1988), Ng and Stephanopoulos (1998), and Vasbinder and Hoo et al. (2003) are some of the authors that have used horizontal decomposition to solve the plantwide design problem. Table 2.1 shows how these authors decompose the problem.

Table 2.1 Horizontal Decomposition-Based Plantwide Design Methods

Level	**Douglas**	**Hoo**	**Ng, Stephanopoulos**
1	Batch/Continuous Operation	Batch/Continuous Operation	Preliminary Analysis to Collect Plant Operation Information
2	Definition of Input/Output Structure	Definition of Input/Output Structure	Definition of Input/Output Structure
3	Design of Recycle Subsystem	Design of the Chemical Reactor Subsystem	Design of Recycle Subsystem a) Reaction b)Separation
4	Design of Separator Subsystem	Design of Separator Subsystem	Define Objectives/Constrains for Unit Operations
5	Energy Integration	Unit Operation: a)Recycle b) Energy Integration	Unit Operation

Almost all the available hierarchical design procedures have been consistent with these ideas [Chen, 2002].

2.3. ***Control Structure Design***

The control structure design consists of five tasks: 1) selection of controlled variables, 2) selection of manipulated variables, 3) selection of measurements, 4) selection of control configuration, and 5) selection of controller law. These tasks are performed for each sub-problem or stage in the hierarchical plantwide control design procedure. The control structures designed for each sub-problem or stage are used in the next sub-problem or stage. Control structure design approaches can be divided into mathematically-oriented, process-oriented approaches, and/or a combination of both. The mathematically-oriented approaches are based on quantitative models, optimization, and the use of mathematical tools. In general, the control structure design problem is difficult to define mathematically because of the size of the problem and the effort involved in making a precise problem definition -- for example, a detailed dynamic and steady-state model [Skogestad et al., 1998]. The process oriented approaches consist of heuristic rules that are based on experience and process understanding

2.3.1. Selection of Controlled Variables

The selection of controlled variables is probably the least studied of the five tasks in the control structure design problem. The decision about which variables should be controlled has mostly been based on engineering insight and experience. According to Skogestad (1998), the reason for this is that it is a structural decision for which there has not been much theory. In addition, the majority of researchers believe that the decision about which variables should be controlled is directly related to the operational control objectives in the plant. These objectives can be categorized as follows:

1) Maintain process stability.

2) Regulate material and energy balances.

3) Satisfy operational, equipment and environmental constraints.

4) Satisfy production rate and quality specification.

5) Maintain normal unit operations.

6) Optimize economics.

In 2002, Chen explained that the controlled variable selection procedure consists of four steps: Step 1) Define control objectives by analyzing plant design and operation specifications. Step 2) Determine controlled variables for each control objective and check the correlation among these variables. Step 3) Rank control objectives by applying engineering judgment. Step 4) Assign controlled variables for each sub-problem or stage in the hierarchical plantwide control design procedure. Chen pointed out that, in most cases, it is not difficult to assign specific controlled variables for these control objectives. However, when there are more controlled variables than manipulated variables, or if the controlled variables need to be kept at exact setpoints, then the process needs to be modified to provide enough degrees of freedom. On the other hand, if the controlled variables can be kept within prescribed bounds, the idea of partial control can be used for this purpose [Arbel, 1996]. To explain the concept of partial control, it is important to point out that there are some variables (dominant variables) that have a strong influence on other variables of interest. Therefore, by controlling the dominant variables, the variables of interest (associated with a specific control objective) can be kept within the desired limits. This is known as partial control. Research done in the partial control area can be found in Arbel, (1996), (1997), and (1999).

Skogestad et al. (1998) addressed the problem of the selection of controlled variables for which the setpoints are determined by an optimization layer. They pointed out that some people think that it does not really matter which variables are specified for controlled variables, as long as all degrees of freedom are used. The reason is because the remaining variables are then uniquely determined. This is true only when there is no uncertainty (signal uncertainty or model uncertainty). In the presence of uncertainty, it does make a difference which variables are selected to be controlled at their setpoint (when these setpoints are determined by an optimization layer). Therefore, Skogestad stated that when selecting controlled variables for the optimization layer, one should try to find a set of variables that achieves self-optimizing control. A process (with its control structure) is self-optimizing if, by keeping the setpoints of the optimized variables constants, it is possible to keep the loss within an acceptable bound, and within a specific time period . In other words, the sensitivity of the economic objective to uncertainty is less than the accepted limit [Skogestad, 1998]. A few researchers [Morari et al., 1980], [Skogestad et al. 1996], [Skogestad et al. 1998] have done work to address the problem of the selection of controlled variables to minimize the sensitivity to uncertainty. Skogestad (1996) presented two optimization-based methods to select controlled variables in the presence of uncertainty. In 2003, Skogestad [Skogestad et al. 2003] proposed a methodology to find an optimal linear combination of measurements to use as controlled variables. This methodology considers the selection of controlled variables that when kept constant, lead to minimum economic loss (self-optimizaing control). Skogestad defined self optimizing control as the acceptable economical loss that is achieved by keeping the setpoint values of the controlled variables constant, in the presence of disturbances. A requirement to be a good candidate controlled variable is that its optimal value is insensitive to disturbances. More recently, Araujo and Skogestad [Araujo et al., 2007] and Kariwala [Kariwala, 2007] presented their research work using the idea of self-optimizing control. In his work, Araujo (2007) applied the self-optimizing control to a HAD plant. The main limitation with this methodology is that it finds a good set of controlled variables for the steady state conditions (not set point changes). However, it does not consider cases, such as change of production rate or product quality and/or changes in operating conditions.

The minimum singular value (MSV) has been used for selecting control structure and manipulated variables. Morari (1983) showed that the MSV is related to input saturation. Yu and Luyben (1986) propose using MSV to select between input sets. They claim that the MSV is a measure of the plant's inherent ability to handle disturbances, model plant mismatches, changes in operating conditions, etc. [Skogestad et al. 1998]. However, this claim seems to be based on experience or intuition since no further justification is given. In 1990, Chang and Yu proposed a related idea that uses the columns' sum for non-square plants for selecting controlled outputs. The set of outputs with the largest row sum will lead to small steady-state sum of square error. Once the controlled variables are selected, Chen, (2002) used Singular Value Decomposition (SVD) to check for linear correlation between them. The SVD is applied to the steady state gain matrix to obtain $K=USV^T$. Then the correlation matrix, called C, is calculated, as explained in Appendix I, for the following matrix $z = SV^T$. If any two rows in the C are linearly correlated, controlled variables related with these two rows cannot be used in the same design.

2.3.2. Selection of Manipulated Variables

Manipulated variables are the physical degrees of freedom which typically are valve positions or electric power inputs. Skogestad (1998) pointed out that the selection of manipulated variables is not a difficult task at the stage of control structure design, since these variables generally are a direct consequence of the design of the process itself. However, there are still interesting issues to address, such as: the need to add more valves, the removal or relocation of the available ones, and the selection of the strongest (dominant) manipulated variables for specific control objectives. A detailed review of current approaches for selecting manipulated variables is given in Chapter 3.

2.3.3. Selection of Measurements

Measurement selection involves the task of determining the number and the best set of measurements for controlling a variable or a set of variables. This should not be confused with the sensor allocation problem which determines the position where the sensor should be installed. Sometimes measurement selection can be a difficult task because there are often many possible measurements that can be used to control a variable. For example, if only one of the pressures in two process units should be controlled, the measurement selection method determines which unit should be used to measure the pressure [Chen, 2002]. Therefore, the number, location, and accuracy of the measurement selected is a tradeoff between cost of measurement and benefits of improved control [Skogestad1998]. Since the selection of dominant measurements and manipulated variables to control production rate and product quality is the main focus of this work, an entire chapter (Chapter 3) is devoted to reviewing current approaches for measurement/manipulated variables (input/output) selection.

2.3.4. Selection of Control Configuration

After the measurements and manipulated variables are determined, the next step is to interconnect or structure them. This task is known as control configuration, and it is one of the most important tasks in control structure design. The way in which the controllers are structured can be centralized (multivariable control structure), decentralized (multi-loops control structure), or a combination of both. When a hierarchical decomposition is used to solve the plantwide control design problem, then control configuration is performed in each stage or sub-problem. The control structures designed for each sub-problem or stage are kept for the next sub-problem or stage.

There are several approaches that address the control configuration problem. These approaches can be categorized as mathematically-based approaches and heuristic-based approaches. Within the mathematically-based approaches can be found approaches that used steady-state information, such as relative gain array, SVD, etc., and approaches based on optimization.

Mathematically Based Approaches

In general, the mathematically based approaches use quantitative methods where mathematical models are formulated to solve control problems. Mathematical-based approaches for the control configuration problem generate control structures that are optimal, within the limitations imposed by the mathematical methods and models used. The main limitations with mathematical-based approaches are the size and complexity of the models that can be attempted within a mathematical programming method [Kookos and Perkins, 2000]. The approaches reviewed in this section are not only based on the use of mathematical models and optimization-based approaches, but also based on mathematical techniques (SVD, eigenvalue analysis, etc.). More detail is given for the most relevant approaches and the ones that serve as theoretical background for the methodology proposed in this work.

Relative Gain Array

Originally, the relative gain array (RGA) was defined and applied at steady state by Bristol (1966). Many researchers have studied and extended the RGA [McAvoy, 1983], [Shinskey, 1988], and [Hovd and Skogestad, 1992]. The RGA is a matrix composed of elements defined as ratios of open-loop to closed-loop gains [Marlin, 1995]. The procedure to calculate the RGA is to evaluate the open-loop gain matrix K; calculate its inverse transposed $(K^{-1})^T$; and multiply them, element by element (Hadamard product) [McAvoy, 1983].

$$\lambda = K.*(K^{-1})^T \tag{2.1}$$

The closer λ_{ij} is to one the less difference closing other loops makes on the loop being considered. Therefore, the difference between λ_{ij} and the value 1.0 is related to the deviation from single loop behavior. In other words, the amount that λ_{ij} deviates from 1.0 indicates, in some sense, the extent of transmission of interaction (in a quantitative manner) [Marlin, 1995]. From the control configuration point of view, the desired pairings are those whose values of λ_{ij} are close to 1.0. Also, pairing with λ_{ij} values of 0 and/or negative numbers are avoided. The main advantages of the RGA are: 1) it is very simple to use; 2) it only uses steady state information (K); and 3) the RGA is independent of scaling, which means that the rules for interpretation do not change when the units of a variable change. The main limitations with the RGA are: 1) it does not consider the dynamic character of the system; 2) it does not consider disturbance rejection.

Linear Quadratic Regulator (LQR) Design Based Approach

The LQR design-based approach was originally proposed by Schnelle (1989) and later extended by the works of Schnelle et al. (1997), Chen et al. (2002) and (2004). This is an optimization-based approach that uses a linear state space model of the process, a linear quadratic regulator design, and process knowledge to generate control structures for an entire plant. The key idea in Schnelle's approach is to extract information from the dynamic model about how the plant should be controlled. In 1997, Schnelle presented an approach that addressed the control configuration problem by using the LQR design approach. This approach can be described as follows: Given a linearized state space model, a state feedback LQR is used to calculate the optimal static state feedback controller *K* as follows:

$$\min_{K} J = \frac{1}{2} E\left[\int_{0}^{\infty} (x^T Q x + u^T R u) dt\right] \tag{2.2}$$

$$\begin{cases} \dot{x} = Ax + Bu \\ y = Cx \\ u = -Kx \end{cases} \tag{2.3}$$

In this approach, two sensitivity matrices (S_{FB} and S_{FF}), representing the dominant feedback and feed-forward paths of a process, are obtained from the optimal static state feedback controller (*K*). Then, based on these sensitivity matrices, heuristics are used to determine feasible control structures. Also, information about the way in which these control structures should be implemented (using a centralized or decentralized control structure) is obtained. More details on this approach can be found in Schnelle (1997). Although this was an innovative approach, it had the following main limitations: 1) the assumption that all states are measurable is generally not feasible in practice; 2) setpoint tracking and disturbance rejection were not considered in the control structure design. In order to overcome these limitations Chen et. al. (2002) extended Schnelle's approach by using an output feedback controller. Also, Chen et al. reformulate the problem to consider setpoint tracking and disturbance rejection. More details on the Chen et al. approach can be found in section 2.3.

Singular Value Decomposition

Singular values and singular vectors of the process gain matrix are used in Lau et al. (1985) to determine control configurations that are preferable for control. These control configurations are the ones in which the associated loops have minimal interactions with other loops. An interaction measurement is developed that quantifies the difference between the control configuration candidates. The main limitations with this approach are: 1) it does not consider dynamic information; and 2) it does not consider setpoint tracking and disturbance rejection. In order to consider both static and dynamic effects, the analysis should be carried out over the frequency range of interest.

Other Mathematical-Based Approaches:

A mathematically-oriented approach based on optimization was presented by Kookos and Perkins (2000). In this approach, the control objectives are posed in terms of economic penalties associated with the effect of disturbances on key process variables. These control objectives are then related to a subset of potential measured variables, and a suitable set of control variables is selected among the potential manipulated variables so that the dynamic economics are as favorable as possible. Integer variables are used to model these control algorithms in an Mixed Integer Linear Programming (MINLP) formulation of special structure [Perkins, 2000]. The main advantage with this approach is that global optimality is guaranteed. Another author that uses a mathematical approach for control structure selection is Kookos [Kookos 2005]. His approach consists of a set of linear constraints that determine the set of manipulated and controlled variables and the steady-state operating policy that minimizes the effect of disturbances on process economics.

Another optimization-based control configuration that uses MILP is proposed by McAvoy and Wang (2001). In this approach the control configuration for the base control system (safety loops and product variables) is obtained by using a steady state model or a linear dynamic model in terms of valve movement and specific disturbances. The main idea in the MILP formulation is that a set of manipulated variables is selected if it minimizes the total valve movement when a specific disturbance is present. This approach is performed automatically and it was successfully applied to the Tennessee Eastman model.

Other Mathematical-based approaches for the control configuration problem were categorized and reviewed by Van der Wal and Jager (1995). Among these approaches are: Structured Singular Value, Combined Nominal Performance and Performance Degradation, Relative Gain Array and Related Concepts, Nominal Stability and Integrity, Direct Nyquist Array, Relative Degree, Interaction Potential, Numerical Invertibility, and Decentrally Fixed Eigenvalues. Van der Wal and Jager compared these approaches based on some desirable properties, such as: efficiency, robust performance and stability, effectiveness, general applicability, practical applicability, etc. After the comparison they concluded that there is no control configuration selection method that satisfies all the desired properties. The main problem seems to be with robust performance and stability, since the majority of these methods do not tackle the setpoint tracking problems and disturbance rejection problems. Also, effectiveness was a key factor since in many of these methodologies it is not easy to eliminate nonviable candidates and maintain the viable ones. Van der Wal and Jager (1995) proposed some future research to overcome some of the limitations with the reviewed methodologies.

Heuristic Based Approaches

Heuristic approaches are based on the use of process insight and experience to determine plantwide control structures. Buckley (1964) was the first researcher in considering plantwide control. He discussed important issues, such as material balance control (in the direction of flow and in the direction opposite of flow), production rate control, indirect control, buffer tanks as low pass filters, predictive optimization, recycle, and the need to purge inerts. Although Buckley presented a number of useful engineering insights that are still used in the industry, he did not present an overall plantwide control design procedure. Wolff and Skogestad (1994) presented a review of previous work on plantwide control, with emphasis in process oriented decomposition approaches. In their paper, they suggested that plantwide control systems should start with a "top-down" selection of controlled and manipulated variables and a "bottom-up" design of control systems. They also listed ten heuristic guidelines for plantwide control [Skogestad and Larson, 1998]. Among the authors that consider heuristic rules for plantwide control are Luyben et al (1998), McAvoy et al. (1994), Tyreus (1999)

The design of a plantwide control system is a difficult task; therefore, the majority of the proposed methodologies decompose the problem into manageable parts. The most common ways of decomposing the problem are:

1) Decomposition based on process units.
2) Decomposition based on process structure.

3) Decomposition based on control objective (material balance, energy balance, quality, etc.)
4) Decomposition based on time scale.

2.3.5. Selection of Control Law

After the control configuration is determined, the next step is to choose the type of controller that will be used. Basically the controller types included single-input single-output (SISO) controllers (e.g. PID) and multi-input-multi-output (MIMO) controllers (e.g. Model Predictive Controller (MPC) and Modular Multivariable Controller (MCC)).

2.4. Review of Plantwide Control Design Methodology

In this section several Plantwide control design methodologies that are relevant for this work are presented. The majority of this section is devoted to Chen's plantwide control design procedure because the methodology proposed in this work is based on Chen's methodology.

Luyben's Approach

A systematic design procedure is presented for plantwide design control structures based on heuristics that were presented by Luyben [Luyben et al., 1997]. This procedure consists of 9 steps that deal with plantwide control issues (not being addressed by simply combining the control systems for individual unit operations): **Step 1**) Establish the objectives of the control system. This is the most important step because different objectives lead to different control structures. **Step 2)**

Determine the available degrees of freedom. **Step 3)** Establish the energy management system. The objective in this stage is to obtain a control system that prevents the propagation of thermal disturbances and ensures that the exothermic reactor heat is dissipated and not recycled. **Step 4)** Set production rate. The main goal in this stage is to select a manipulated variable that provides smooth and stable production-rate transitions and rejects disturbances. Based on previous experience and research, Luyben [Luyben et al., 1997] explained that the selected variable should have a rapid and direct effect on the reaction rate in the reactor, while having the least effect on the separation section. Luyben et al. pointed out the importance of this selection because of the implications for component balances examined in Step 7. **Step 5)** Control product quality and handle safety, operational, and environmental constraints. In general, tight control of these variables is required for economic and operational reasons. Therefore, the manipulated variables selected should have a dynamic relationship with the controlled variables that feature small time constants and dead times, and large steady-state gains. Also, the magnitude of the various flow rates is considered in this stage. **Step 6)** Involves inventory control (pressures and levels) and fixing a flow in every recycle loop. Luyben pointed out that an inventory variable should typically be controlled with the manipulated variable that has the largest effect on it within that unit. Inventory may also be controlled with fresh reactant makeup streams. **Step 7)** Check component balances. In this stage component balances are evaluated for each chemical element. The objective is to determine whether they are consumed, generated, or leave the system in an exit stream (purge or product). Fresh reactant makeup feed streams can be manipulated to control reactor feed or recycle compositions (or to hold pressure or level). **Step 8)** Control individual unit operations. In this step, the required loops to control each individual unit operation in the plant are selected. **Step 9**) Optimize economics or improve dynamic controllability. In this stage, alternatives to improve steady-state economic and dynamic performance are evaluated by using the available degrees of freedom or the setpoint of some controllers that can be adjusted.

McAvoy and Ye's Approach

They presented a systemathic plantwide design control procedure based upon relative loop speed. This procedure consists of four stages that are described as follows: **Stage 1)** Inner cascade loops are closed. This reduces the effect of disturbances associated with these loops. **Stage 2)** The basic decentralized PID system is designed. This stage involves all the loops except those associated with the process analyzer and product rate. Tools, such as relative gain [Bristol, 1966], Niederlinski Index, linear saturation analysis, nonlinear disturbance and saturation analysis, and dynamic simulation are used for this purpose. **Stage 3)** Analyzer and product rate loops are closed. To do so, they use overall mass balance of the plant. **Stage 4)** Higher level controls, such as model predictive control and/or optimization can be added. From stages 1 to 3, the speed of loops involve decreases.

Optimal Control-Based Plantwide Control Design Methodology (Chen's Approach)

Chen's approach is explained in more detail because the methodology presented in this work is based on his approach. Chen's plantwide control design methodology is based on output optimal control and uses a linear dynamic process model of the plant for designing plantwide control systems. This approach consists of four stages, and the results from one stage are used as the inputs to the next. For each stage, the following tasks are carried out: 1) An optimal static output feedback controller (OSOFC) is designed for the available measurements and manipulated variables. 2) Control structure candidates are determined, using mathematical analysis and engineering judgment. 3) For each control structure candidate, centralized or decentralized controllers are automatically tuned. 4) Process transients are generated, based on linearized models in order to compare the control performance of the different candidates.

Basic Optimal control output Feedback Problem

Given a linear time invariant (LTI) state space model, an OSOFC is designed to stabilized the system and bring the states from arbitrary initial values to zero, following a trajectory that minimizes a linear quadratic objective function (LQR) [Chen and McAvoy, 2003]. The basic formulation of the OSOF LQR design problem is presented by Lewis as follows:

The LTI Process Model is given as:

$$\begin{cases} \dot{x} = Ax + Bu \\ y = Cx \\ x(0) = x_0 \end{cases} \tag{2.4}$$

This is a linearized state space model where x is the vector of the system states, u is the vector of control inputs (manipulated variables), and y is the vector of measured outputs (controlled variables). A, B and C are matrices whose elements describe the system dynamics. The state space model can represent MIMO and SISO systems. Output feedback control Equation is given as:

$$u = -Ky \tag{2.5}$$

where K is a mxp matrix of constant feedback coefficients. The problem to be solved is to find the K that minimizes a quadratic time domain performance index function given by:

$$\min_K \quad J = \frac{1}{2}\int_0^{\infty} (y^T Q y + u^T R u)dt + \frac{1}{2}\sum_i \sum_j g_{ij} k_{ij}{}^2 \tag{2.6}$$

where Q and R are weighting matrices for y and u respectively, while g_{ij} is a weight on element k_{ij} in K. In general, g_{ij}'s are zero. However, when a single input single output (SISO) structure is used, the g_{ij}'s elements are used to force the off-diagonal elements of K to be zero; then the resulting K has only diagonal elements. In order to make the k_{ij}'s elements small, large values of the corresponding g_{ij}'s elements should be used.

The design equations needed to calculate K that minimize the performance index (2.6) are:

$$A_C^T P + PA_C + C^T K^T RKC + C^T QC = 0 \tag{2.7}$$

$$A_C S + SA_C^T + X = 0 \tag{2.8}$$

$$RKCSC^T - B^T PSC^T + g * K = 0 \tag{2.9}$$

$$A_C = A - BKC \qquad X = x(0)x(0)^T \tag{2.10}$$

where $g*K$ is a matrix with elements $g_{ij*}\, k_{ij}$. These equations result from the first-order necessary condition for optimality given by Lewis (1992). Because there is no explicit analytical solution for the OSOF controller (K) numerical optimization is used to solve Equations (2.7), (2.8) and (2.8) simultaneously. In solving these equations the following conditions are required:

1) R should be positive definite, and Q should be positive semidefinite to ensure CQC is positive semidefinite

2) P is positive definite or positive semidefinite as long as A_C is stable and ($CKRKC+CQC$) is positive definite or positive semidefinite

3) S is positive definite or positive semidefinite as long as A_C is stable and X is positive definite or positive semidefinite.

The OSOFC K solution depends on:

1) The initial states x_0, and in most of the cases, x_0 is unknown. This problem can be solved by minimizing the expected value of J [Levine, 1970]:

$$\min_K \quad E\{J\} = E\left\{\frac{1}{2}\int_0^\infty (y^T Q y + u^T R u)dt\right\} + \frac{1}{2}\sum_i \sum_j g_{ij} {k_{ij}}^2 \tag{2.11}$$

Then, Equation 2.10 is replaced by:

$$A_C = A - BKC \qquad\qquad X = E\left\{x(0)x(0)^T\right\} \tag{2.12}$$

where X is the initial autocorrelation of the states. Assuming that the initial states are uniformly distributed on the unit sphere, then, X=I, the identity matrix. Chen (2002), presented alternative OSOF LQR design methods for specific setpoint tracking and/or disturbance rejection. Details on the calculation of the optimal gain matrix can be found in Appendix II.

2) How the *x*, *y* and *u* are scaled. The scaling options evaluated in this work are presented in the next section.

Numerical Considerations for the OSOF Problem.

The algorithms used to solve the OSOF problem are shown in Appendix II. These algorithms are based on Chen's (2003) numerical considerations. In order to solve for the OSOFC the following issues need to be considered:

1) Whether the system can be stabilized by static output feedback (SOF). The Even Parity-Interlacing-Property necessary condition on Wei (1990) is used to check whether a given system can be stabilized by a SOF. If the system does not violate this necessary condition, then, it is assumed that at least a SOF, which stabilizes the system, exists [Chen 2003].

2) Selection of the algorithms. The Moerder and Calise algorithm algorithm is used because of its conditionally global convergence, simplicity and

efficiency. This algorithm iteratively calculates a solution that satisfies the first-order necessary conditions for optimality.

3) Convergence properties. Moerder and Calise's algorithm converges to a local optimum. If the set of stabilizing static output feedback gains is convex and the solution of K, P, and S is unique, then the global optimum is obtained. However these two conditions are not testable, and therefore it is necessary to compare different solutions to determine the global optimum.

4) Calculation of the initial stabilizing SOF Controller K. The calculation of the initial SOF controller is done by generating random numbers (ranging between $\pm\alpha$) for the elements of K until $A\text{-}BKC$ is asymptotically stable. α is a design parameter and its value is given by the users. The default value of α is 1. This is not necessary if the uncontrolled plant is stable.

5) Computational load. An important issue related to the computational load is the order of the model (number of state variables), because the larger the order of the model, the slower the calculation of the OSOFC. In order to speed up calculations, it is recommended to reduce the order of the model. Because the optimal-based measurement selection approach studies the interaction between inputs and outputs, the reduced model should retain the major characteristics of the process dynamics and interactions as well as inputs and outputs. It is important to mention that model reduction techniques always introduce some model error. Therefore, they should only be used when is absolutely necessary to reduce the computational load. The model reduction method used in this work is the balance and truncate approximation method

without coprime factorization [Moore, 1981]. The Matlab program used is called sysred() (system reduction) and is provided in the SLICOT package [Varga, 1999].

The **inputs** for this design procedure include the following information: 1) a state space linear time-invariant process model; 2) process flowsheet and steady-state process data for state variables, manipulated variables, and measurements; 3) operating range for measurements and manipulated variables used for scaling the model; 4) control objectives, used to define controlled variables (specifications of production rate and product quality); 5) process constraints, used to define controlled variables, involve hard constraints related to safety issues in the process; and 6) process insight and engineering judgment.

Stage 1) Preparation. The objectives in this stage are as follows:

1) Scale the process model. The reason for this is that the elements in the OSOFC should be dimensionless and have values in a relatively small range, to be compared with one another.

2) Identify measurements and manipulated variables to be used in the next stage. This consists of three operations: a) Identify controlled variables, based on control objectives and process constraints; b) Select the best measurement location whenever there is more than one measurement that can be used to control the variables from Step a; 3) Identify unstable and slow-responding variables than can make the process unstable. If the process is open-loop unstable, it is necessary to determine which

measurements are best to detect instability. To do so, an eigenvalue analysis is used. More details on this can be found in Chen (2002).

Stage 2) Decentralized control structure for safety variables. The objective in this stage is to generate decentralized control structure candidates for the variables identified in Stage 1. The control structure candidates are determined by analyzing the OSOFC, using the sensitivity matrix and applying engineering judgment. The proportional-only controllers are automatically tuned for each control structure candidate. These controllers are incorporated into the model for use in later stages. Then the control structure candidates that show good performance in tracking setpoint changes are retained for the next stage.

Stage 3) Control structure for production rate and product quality. The objective in this stage is to generate centralized or decentralized control structures for controlling production rate and product quality variables, identified from the control objectives. Stage 3 should be performed for each control structure generated in stage 2. In stage 3, the setpoint of the loops closed in stage 2 can be used as manipulated variables. Once the control structures for controlling production rate and product quality are generated, an important issue to consider is whether to implement a centralized or decentralized control structure. This issue is addressed by implementing decentralized and multivariable control structures using process simulation based on the linearized model. The decentralized control structures are implemented by generating an OSOFC that contains only diagonal elements while the multivariable control structures are implemented by generating a full OSOFC full matrix. Chen (2003) proposed comparing the transients generated from the decentralized and the multivariable control structures to estimate the benefits of using multivariable control structures.

Stage 4) Control structure for remaining variables (inventory loops and unit operation loops). The objective in this stage is to generate decentralized or multivariable control structure candidates for maintaining component balances and controlling unit operations. To identify the components that need to be controlled in this stage, Chen (2003) used a Downs Drill Analysis [Luyben, 1992]. This analysis is used for checking the component balances for each control structure generated in Stage 3. After the component balance loops are closed, the remaining degrees of freedom can be used for unit operation control and process optimization. Once the component elements and unit operation measurements have been identified, an OSOFC is obtained to generate control structures from them.

The **output** for this design procedure is a set of plantwide control structures. These structures can be decentralized or multivariable control structures. The control performance of these control structures is evaluated by using transients, based on linearized models.

Details for how to generate control structures from the OSOFC are presented:

Calculate an OSOFC. An OSOFC is analogous to a process-gain matrix. For Stages 2, 3, and 4, an OSOFC is calculated for the given set of measurements and manipulated variables. The OSOFC can be a non-square system and its formulation is given in Chapter 4 Section 4.2. Users should specify the design parameters, which are the weighting matrices to use in the objective function. The default value of the Q and R matrices are identity matrices, and the default value for g_{ij} is zero.

Calculate the sensitivity matrix. The sensitivity matrix, proposed by Chen et al. (2002), is a measure similar to the RGA that measures the dynamic process interaction between variables. Chen (2002) defined the sensitivity matrix, S, as

$$S = matrix[\sigma_{ij}] = matrix\left[\frac{(\partial MV_i / \partial CV_j)_{R=Ro}}{(\partial MV_i / \partial CV_j)_{R=Ri}}\right] \tag{2.13}$$

The sensitivity matrix is calculated as follows: 1) An OSOFC is solved with the R matrix equal to *Ro* (e.g. an identity matrix); 2) The same problem is re-solved, emphasizing each manipulated variables. To do so, first, all the diagonal entries in the R matrix are multiplied by 100, except the entry for the manipulated variable that is being emphasized. In other words, in each of these calculations, only one of the manipulated variables is not heavily penalized. Then, the sensitivity matrix is calculated by dividing the gains for the base case by the gains when a manipulated variable is emphasized. A more detailed explanation of the sensitivity matrix can be found in Chen (2002).

Generate a decentralized control structure. Decentralized control structures are generated using OSOFC, the sensitivity matrix, and engineering judgment. Chen (2002) proposed the following heuristics: 1) Only pairings with elements having an absolute value greater than 0.2 in the OSOFC are considered. 2) Only pairings with values between 0.2 and 5 in the sensitivity matrix are considered. 3) The pairings accepted by 1 and 2 are checked, using engineering judgment.

Limitation of the optimal control based plantwide control design methodology:

The main limitations with this methodology are the following:

1) This methodology does not consider specific setpoint tracking and/or disturbance rejection for designing control structures. In fact, Chen assumed that the initial states are uniformly distributed on the unit circle sphere. Therefore, the control structures obtained using this methodology might not be the most appropriate for specific disturbance rejection and setpoint changes. Even thought Chen (2003) also presented a rigorous formulation that includes setpoint changes and disturbance rejection for the calculation of the OSOFC he did not show any results using this methodology. In this work this formulation was tried but it did not converge.
2) This methodology uses a fairly simple way to control the key economic variables in the plant (production rate and product quality). These two variables are controlled using two manipulated variables respectively. In this work, it has been proven that using a more sophisticated control structure, that involves the adjustment of key dominant variables in the plant has improved the control performance of production rate and product quality and therefore the economics in the plant.

2.5. Partial Control

Partial control involves whether acceptable control can be indirectly achieved for a subset of outputs by controlling only a subset of the outputs. For instance, the outputs are divided into two sets:

y_1 (temporarily) uncontrolled outputs (for which there is an associated control objective). The use of the word temporarily means that y_1 are normally controlled outputs at some higher level in the hierarchy

y_2 (locally) measured and controlled output.

Then, by controlling only the subset y2, acceptable control can be obtained for y1 [Skogestgad and Postlethwaite, 1996]. Tyreus (1999) defined partial control as a decentralized control structure in which economic operating objectives are controlled, either at their setpoints or within a specific range by controlling a few dominant variables [Tyreus, 1999]. Research on partial control area are presented by Arbel and Shinar, [Arbel, 1995a], [Arbel, 1995b], [Arbel, 1996], [Arbel, 1997], [Arbel, 1999], and [Tyreus, 1999]. In the majority of these papers, dominant variables are determined by experience and process insight. However, Tyreus used a thermodynamic information-based methodology for identifying dominant variables. In his work, Tyreus stated that economic-related variables such as flow and production rates are almost always related to the internal process rates. He identified the dominant variables affecting these internal rates by using a thermodynamic process description that focuses on the power release expression for each process unit. Details in how this methodology works are presented in the next chapter and in Tyreus (1999a and 1999b).

Chapter 3: Measurements and Manipulated Variables (Input/Output) Selection Methods

*3.1 **Background***

The measurement and manipulated variables selection problem consists in choosing a proper set of variables (input's, u's, actuators) to be manipulated by the controller, and a proper set of measurements (outputs, y's, sensors) to be given to the controller. The selection of the appropriate measurements and manipulated variables will determine the success or failure of the control system. The reason is that this choice affects the performance, reliability, complexity, and cost of the control system. Also, this choice will affect not only the control performance but also the economics of the plant. The measurement and manipulated variable selection problem involves selecting the appropriate number, place, and type of actuators and sensors. It is also possible to study the benefits of adding more measurements and manipulated variables.

In this chapter, a review of the available measurements and manipulated variables selection methods is presented. These methods are grouped according to the control system property they address, their effectiveness, applicability, etc. Also, a qualitative assessment and comparison of the reviewed methods is given.

3.2 ***Purpose of Measurement and Manipulated Variable Selection***

In general, there is a large number of measurement and manipulated variables available in a complex process, where the number of measurements usually far exceeds the number of manipulated variables. Each combination of measurement (y) and manipulated variable (u) is called the measurement and manipulated variable (M-MV) set. The number of the candidate M-MV sets grows exponentially with the number of measurements and manipulated variables available. This exponential growth motivates the need for systematic methods to select measurements and manipulated variables. These methods should complement the engineer's experience to quickly and easily assess a large number of candidate measurements and manipulated variable sets. The measurement and manipulated variable selection problem has also been studied separately. In general, the measurement selection problem (sensor location) has been studied more than the manipulated variable selection. The reason is that the number of measurements that can be used to control a specific variable or group of variables is usually much larger than the number of manipulated variables.

In the past, the optimum sensor location (measurement selection) has been studied for different purposes. Originally, the sensor location problem was studied from the control perspective. Later, the sensor location was also studied considering the observability point of view (amount of information required for good monitoring). The design of inferential control schemes was another purpose for studying best sensor location. Also, in the estimation of variables such as states and controlled variables finding the best sensor is the main concern. The sensor location problem has been studied mainly for control and monitoring purposes.

The sensor location problem for control and monitoring purposes was studied by Jorgensen [Jorgensen S. et al. 1984] and Lim K [Lim K. 1992]. In his work, Jorgensen presented a sensor location procedure for chemical processes that distinguishes between the purposes of observability and control. In the observability case, the method requires knowledge of process dynamics and open loop stationary variance. In the control case, additional knowledge of the states required for control is needed. In addition, Lim presented a method for selecting optimum sensor location, based on the combined degree of controllability and observability. Lim used the controllability and observability grammians to weight the projections to reflect the degrees of controllability and observability for different structures.

The sensor location problem also has been studied from an inferential measurement point of view by Romagnoli [Romagnoli J. et al. 1981], Morari M. [Morari M. and O'Dowd M., 1980], Mejdell [Mejdell, 1991] and Kresta [Kresta et al., 1994]. When the controlled variable is not easily measured, it must be inferred from the available measurements. The selection and location of these measurements are very important because the performance of the plant depends on it. Consequently, one can think that the more information that is available about the plant, the better the monitoring and control should be. However, a large number of sensors can increase the cost associated with acquisition, installation, and maintenance of sensors. Furthermore, the implementation of a control strategy that uses a large number of measurements becomes complicated. Romagnoli [Romagnoli et al. 1981] proposed a method that modified the measurements' structure and applied them for optimal control. In addition, Mejdell (1991) and Kresta (1994) presented methods for building inferential models for control purposes, based on Principal Component Regression (PCR) and Partial Least Squares (PLS) methods.

3.3 Review of Techniques for Measurement and Manipulated Variables (M-MV) Selection

This section presents a review of the most relevant methodologies proposed in the literature for the M-MV selection problem. These methodologies are divided into different groups according to the control system property that is addressed, the applications that they solve, and the purpose for this selection. It is important to point out that all the reviewed methods apply to linear, time invariant, and continuous plants. Also, some of the methods assume that the number of measurements is equal to the number of manipulated variables ($n_u = n_y$), leading to square controllers. These characteristics will be mentioned for the specific method considered. It is important to point out that in some cases the measurements (y) are directly related to the control variables (z). Then, the control goals can be formulated in terms of y. This is the case where z can be measured directly ($z = y$) or if an explicit relationship is known between y and z ($z = f(y)$). The key ideas for each of these methodologies are described as follows:

3.3.1. Accessibility

The M-MV selection methods reviewed in this section are based on the use of cause-and-effect graphs. These graphs show the relationship between variables (measurements, manipulated variables, and controlled variables) and can be generated for linear and nonlinear systems. The key idea is that a causal path exists between the manipulated and controlled variables and between the measurements and the controlled variables. In other words, the manipulated variables must have an effect on the controlled variables, and it must be possible to use the measurements to obtain values of the controlled variables [Van der Wal, 2001]. The main problem with this idea is that it is a qualitative technique that might generate a large number of possible candidate M-MV sets. Therefore, additional information should be used to narrow down the number of possible M-MV sets. Govind [Govind and Powers 1982] propose the use of cause-and-effect graphs, along with steady state gains, time constants, and time delays as additional quantitative accessibility measures. Other authors that used the cause-and-effect graphs to solve the M-MV selection problem are Daoutidis [Daoutidis and Kravaris 1992]. They define the relative degree (r_{ij}) of a controlled variable (z_i) with respect to a manipulated variable (u_j) as a measure of the dynamic interaction between manipulated and controlled variables. They assume that $y = z$. Also, r_{ij} is defined as a measure of the sluggishness of the response of the controlled variables to changes in the manipulated variables. Daoutidis used the cause-and-effect graphs to study the paths for the number of variables connecting u_j

with z_i. Details about how to calculate the r_{ij} can be found in Daoutidis (1992). The r_{ij} can be intuitively interpreted as the number of integrations the input has to perform before it affects the output. The heuristic used for the M-MV selection method is as follows: the lower the r_{ij}, the better the accessibility of u_j to z_i. Therefore, they compute

$$r_{zu} = \sum_{i=1}^{n_z} \min(r_{i1}, r_{i2}, \ldots\ldots, r_{in_u}) \tag{3.1}$$

for each manipulated variable set. Then, the preferred M-MV sets are the ones with the smallest r_{zu}.

3.3.2. State Controllability and State Observability.

In this section, methods based on state controllability and observability of the linear model of the plant (state space description) are discussed. The state space description of the plant K is as follows:

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx + Du \end{aligned} \tag{3.2}$$

where x represents the states; u represents the manipulated variables (inputs); y the measurement (outputs); A, B, C, and C are matrices whose elements describe the system dynamics.

State controllability. This system is called state controllable if, for any initial state $x(0)=x_o$, any time $t_f > 0$, and any final state x_f, there exists an input $u(t)$ such that $x(t_f) = x_f$.

State observability. This system is called state observable if, for any time $t_f >$ 0, the initial state $x(0)=x_o$ can be determined from the time history of the input $u(t)$ and the output $y(t)$ in the interval $[0,t_f]$.

The simplest M-MV selection set rule, based on controllability and observability, is to reject candidates for which (A, B) is uncontrollable or (C, A) is unobservable, Zhou et al. (1996). Other criteria for selecting M-MV sets, based on structural state controllability and observability, are presented by Morari [Morari and Stephanopoulos 1980]. They used a structural model to represent the plant. A structural model only requires information about whether a variable is involved in a particular system equation or not, Van de Wals (2001). Then, they check for the necessary and sufficient conditions for structural state controllability and observabillity and select the M-MV sets that satisfy these conditions. An important characteristic of structural models is that they can be used to describe nonlinear systems. Therefore, by linearizing these nonlinear structural models, it is possible to select M-MV sets for nonlinear systems. The main disadvantage with these methods (1. controllability and observability and 2. structural controllability and obserbability) is that they are not selective enough. In other words, a large number of possible M-MV sets might result. Therefore, quantitative methods, based on state controllability and observability were proposed by numerous researchers Muller [Muller and Weber, 1972], TaliMaamar [TaliMaamar and Babary 1994], Dochain [Dochain et al. 1997], among others]. One of the earliest approaches based on optimization was suggested by Muller (1972).

They suggested the use of the determinant of the observability matrix, as a measure of the observability of the system. They defined a function that depends on the observability matrix. Therefore, the sensor location structure that maximizes this function improves the degree of observability; it is also the optimum sensor location from the observability point of view. Different observability measures have been suggested to determine optimum sensor location. For instance**,** TaliMaamar (1994) proposed a method to determine optimum sensor location in a fixed bed bioreactor, by considering the condition number of the observability matrix. They stated that the optimum sensor location is the one in which the condition number is minimized. They tested their method by determining the sensor location that gives the best observability. Damak et al. (1992) used the observability matrix. Georges (1995) selects optimal sensor (measurement) and actuator (manipulated variable) location, based on maximizing the minimum eigenvalue of the controllability ($W_c(t)$) and observability ($W_o(t)$) matrices (for a given t). The key idea is to minimize the input energy to reach a given state and to maximize the output energy generated by a given state Van de Walls (2001). Georges extended his idea to nonlinear systems. Stephanopoulos (1980); Bainum [Bainum and Xing 1997]; TaliMaamar (1997) looked for expressions that consider the degree of controllability and observability. All of these approaches were based on scalar functions of the observability matrix or observability grammian. From the controllability point of view, the best sensor location is the one that minimizes the energy required by the control action to reduce the disturbance. In the case of the observability, the best sensor location is the one that gives maximum signal response for the sensor when disturbances occur. Dochain et al. (1997) proposed a criterion for the degree of observability, based on the use of the condition number of the observability Grammian to select the best observable system. They stated that smaller condition numbers indicate better observable systems. Van den Berg et al. (2000) determined the optimum sensor location in a tubular reactor, using a method based on a robust degree of observability. They proposed two criteria that are scalar measures of the observability Gramian. These criteria are based on the idea of maximizing the signal received by a sensor when the system faces a disturbance. Other controllability-and-observability-based methods can be found in Van der Wall (2001).

3.3.3. Measurement-Manipulated Variables (Input/Output) Controllabillity

A plant is called input/output controllable if acceptable performance can be achieved, in the presence of uncertainties, setpoint changes, disturbances, and sensor noise [Van der Wal, 2001]. Several research studies have been done in this area. In these studies, different groups of controllability measures, based mainly on singular value decomposition analysis (SVD), have been used. Singular Value Decomposition (SVD) is a numerical technique that has been proven to be a very useful tool in modern system theory. Basically, SVD is designed to determine the rank and the condition of a matix and to geometrically map the strengths and weaknesses of a set of equations [Moore, 1987]. During the last two decades, SVD has been extensively used by the process control community for analysis and design of control systems. For instance, Moore (1987) shows how SVD can be used to design a simple but effective multivariable control structure. He proposes a tool, based on the numerical concept of SVD, that provides quantitative information about sensor placement, physical controllability, and controller pairing. SVD analysis decomposes an mxn process gain matrix into three component matrices as follows:

$$K = Y\, \Sigma\, U^{*} \qquad (3.3)$$

where:

K is an nxm matrix.

Y is an nxn orthonormal matrix called the "left singular vectors".

U is an mxm orthonormal matrix called the "right singular vectors".

Σ is an n x m diagonal matrix of scalars, called the "singular values"

Σ=diag$(\sigma_1, \sigma_2, \sigma_3, \ldots \sigma_n) > 0$. σ_i's are the singular values that are organized in descending order such that $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \ldots \sigma_n \geq 0$.

The important aspect of the SVD, in terms of process control, is that when it is applied to a steady state gain matrix (K), the singular vectors and the singular values have a strong physical interpretation [Moore, 1987]. Therefore, important information, such as potential control problems, control structure design, more sensitive measurements, and manipulated variables can be obtained. Moore (1987) gives the following general interpretation of the elements in a singular value analysis:

K= is the steady state gain matrix. This matrix provides information about the sensitivity of each measurement (y, outputs) to changes in each of the manipulated variables (u, inputs) for multivariable systems.

Y= Y_1:Y_2:Y_3.....Y_n form an orthonormal basis for the column (output) space of K. Y_i of Y are called the left (output) singular vectors and they provide the most appropriate coordinate system for viewing the process sensors (outputs). The left singular vectors of this coordinate system point in the direction of the first (Y_1), the second (Y_2), the third (Y_3), etc., most sensitive combination of sensors (outputs).

U= U_1:U_2:U_3.....U_m form an orthonormal basis for the row (input) space of K. U_i of U are called the right (input) singular vectors and they provide the most appropriate coordinate system to for viewing the manipulated variables (inputs). The right singular vectors of this coordinate system point to the combination of manipulated variables (inputs) that have the first (U_1), the second (U_2), the third (U_3), etc., largest effect on the sensor (outputs).

Σ= Σ=diag(σ_1, σ_2, σ_3, . . . σ_n) >0. The singular values represent the "decoupled open loop gains" of the multivariable process. In terms of the process control problem, the magnitude of the singular values is very important for studying control system feasibility. For instance, very small singular values indicate that the system is not sensitive enough for control. When one tries to implement many loops that have small singular values, a problem of valve saturation can occur. This problem can be explained by using the analogy with the process gain. For example, a small process gain requires a large controller gain which, for multivariable control, can lead to a valve saturation problem. On the other hand, a very large singular value indicates a control problem because it requires very small controller outputs which, for multivariable systems, can cause a loss of control performance.

Condition Number (*CN*). The *CN* is an important parameter that can be obtained from the SVD. It is calculated as the ratio of the largest singular value to the smallest non-zero singular value:

$$CN = \frac{\overline{\sigma}_1}{\underline{\sigma}_n} \tag{3.4}$$

The *CN* is an indication of the of the difficulty to control the entire set of control objectives ($n \times n$ multivariable problem). The larger the condition number is the more difficult it is to control all the variables together.

3.3.3.1. Singular Vectors. The M-MV selection methods reviewed in this group are based on the use of the right and left singular vectors from the SVD analysis.

Moore et. al. (1987) proposed three methods for selecting measurements. The key idea in these methods is to find a set of measurements that are sensitive to changes in the manipulated variables on one hand, and that are mutually independent on the other hand. To do so, in the first method, Moore et. al. (1987) calculated the SVD of the process gain matrix and used the left singular vector. They explained that each column in Y (left singular vector) is an orthonormal vector whose coordinate directions are described by each one of the process measurements. Therefore, for each singular vector, they select the measurement (row) with the largest absolute value. Moore et al, stated that the selected measurements are sensitive to the inputs and relatively independent because of the orthogonality of the vectors in Y. Although the first method has been proven to work well, it can show problems of measurement interaction in some cases. For instance, if the row in Y_2 corresponding to the row of the largest absolute value of Y_1 is large and vice versa, then there will be a significant interaction between these two measurements. In order to overcome this interaction problem, Moore et. al. (1987) proposed a second method which is a modified version of the first one. The second method is based on the differences between the absolute-values of the left singular vectors. This method surely reduces the interaction but possibly also reduces sensitivity to manipulated variables. For this method, Moore et. al. stated the following: 1) A large value of the minimum singular value σ_n indicates good sensitivity to manipulated variables, and 2) A small value of CN indicates a good mutual independence of the measurements. Therefore, they calculate the following index:

$$Q(K) = \frac{\sigma_n(K)}{CN(K)} \tag{3.5}$$

Then, they looked for sets of measurements that have large Q values, which means that the measurements exhibit a good compromise between sensitivity to manipulated variables and mutual independence of measurements [Van der

Wal 2001]. Moore et. al. (1987) stated that a similar procedure could be proposed for input selection. Other researchers that use the singular vector information for selecting manipulated variables are Keller and Bonvin (1987). They propose a method for selecting the manipulated variables (*u*) that have the strongest and most orthogonal on the measurements (*y*). To do so, they follow a similar procedure to the one used for Moore et. al., (1987). However, they looked for the largest singular values and the corresponding singular vectors of the matrix *B* (from the state space model), instead of using the gain matrix (*K*). Cao and Biss (1996) also used singular vector information to select the set of manipulated variables that has the largest effect on a fixed number of measurements. They calculate the *SVD* of the *K* matrix for the full manipulated variable set. Then, they calculate the single-input-effectiveness for u_j as follows:

$$v_{u_j}(K) = \sqrt{\sum_{i=1}^{N_y} U_{ji}^{*} U_{ji}} \tag{3.6}$$

The manipulated variables (n_u) that exhibit the largest values of $v_{uj}(K)$ should be selected. More details about this method can be found in Cao and Biss (1996).

Some of the advantages of using Cao's method are: 1) *SVD* can be applied to an existing process or during the design phase, and 2) *SVD* is easy to understand and use.

3.3.3.2. The Minimum Singular Value. The minimum singular value ($\underline{\sigma}_n$) has been also used for selecting M-MV sets [Morari (1983), Luyben (1986), Skogestad and Havre (1996)]. The key idea is to select the M-MV sets that exhibit a large value of $\underline{\sigma}_n$. The main reason for this is that the $\underline{\sigma}_n$ of the plant, evaluated as a function of frequency, is a measure for evaluating the feasibility of achieving acceptable control. For example, the value of $\underline{\sigma}_n$ guarantees that with a manipulated variable (input) of a unit magnitude (measure by the 2-norm), an output magnitude of at least $\underline{\sigma}_n$ can be achieved in any measurement (output) direction [Skogestad and Postlethwaite, 1996]. Therefore, the value of $\underline{\sigma}_n$ in some sense quantifies the effect of the manipulated variables in the measurements. The larger the $\underline{\sigma}_n$, the bigger the effect of the manipulated variables (inputs) on the measurements (outputs). An important issue concerning the magnitude of $\underline{\sigma}_n$ is considered by Morari (1983). Morari explains that for a plant to have good setpoint tracking and disturbance rejection in the case of manipulated variables limitation, $\underline{\sigma}_n$ should be large (to avoid valve saturation). Yu and Luyben (1986) use this idea and call $\underline{\sigma}_n$ the "Morari Resilience Index" (MRI). In their work, they select the manipulated variable set with the largest MRI for the frequency range of interest. Havre et al. (1996) also used this idea. Skogestad and Postlethwaite (1996) give a detailed explanation of the properties of $\underline{\sigma}_n$. They also demonstrate that $\underline{\sigma}_n$ should be large in order to have independent control of all outputs [Van der Wals, 2001].

3.3.3.3. Condition Number. The condition number is another controllability measure that can be used for selecting M-MV sets. The key idea is to select

M-MV sets that exhibit a small condition number. Morari (1983), Skogestad and Postlethwaite (1986) shows that systems with small CN(K) are more robust against uncertainty. Reeves (1991) proposes a method that uses the CN to reduce the number measurements and manipulated variables available, before applying more rigorous methods that are more time consuming and computationally involved. This method starts with the full set of measurements and manipulated variables (N_y x N_u); then a single input or single output is eliminated which produces the reduced sets (N_y x [N_u-1]) or ([N_y-1] x N_u) with smaller CN. The same procedure is performed many times until smaller and more manageable M-MV sets are found. Some variations of the condition number definition are presented by Skogestad and Morari (1987) and Cao and Rossiter (1996). Skogestad and Morari (1987) propose the disturbance condition number (*DCN*) which is a measure of the input magnitude required to reject a disturbance. Therefore, they look for manipulated variable sets with small DCN, which means they are more effective for disturbance rejection**.** Cao and Rossiter (1996) defined the input disturbance alignment (IDA) which uses similar basis as Skogestad and Morari (1987). However, they look for manipulated variable sets with IDA close to 1.

3.3.3.4. Relative Gain Array (RGA). RGA has been extensively used for control configuration selection. (See Chapter 2). In this section, some RGA-based methods for the M-MV selection problem are discussed. The simplest rule for using the RGA to solve this problem is to avoid M-MV sets that exhibit large RGA elements since the corresponding plant would be difficult to control [Chen, Freudenberg, and Nett (1994)]. Reeves (1991) proposed two RGA-based heuristics to reduce the full set of measurements and manipulated variables into a smaller set. These methodologies narrow down the number of M-MV sets available but they do not give an optimal M-MV set. More studies in this area are presented by Cao and Biss (1996) and Chan and Yu (1990).

The main advantage of the M-MV controllability based methods is that all the measures are simple to compute and give insight into how easy it is to control the plant. The main disadvantages are as follows: 1) Some M-MV controllability measures are based on inputs restrictions and uncertainties that are not addressed simultaneously, and 2) Some M-MV controllability measures assume a suitable scaling because the results critically depend on it [Van de Wal, 2001].

3.3.4. Right-half-plane (RHP) zeros

In this section, methods for selecting M-MV sets, based on RHP zero location, are presented. Because different M-MV sets lead to distinct locations of systems zeros, the key idea is to reject M-MV sets which introduce RHP zeros with magnitudes below the desired bandwith. Research studies that use this idea are presented by Hovd and Skogestad (1993) and Bis and Perkins (1993), among others. In the case of unstable plants, M-MV sets with RHP zeros close to the RHP poles should be avoided. The reason is that the exact cancellation of RHP poles and zeros causes the unstable mode to become uncontrollable or unobservable. More details on this can be found in Van de Wall (2001).

3.3.5. Optimization-Based M-MV Selection Methods

Optimization is a common technique that researchers have used to solve the M-MV selection problem. Van de Wal (2001) categorized the use of optimization to solve this problem as follows:

1) In a control system, the objective of the manipulated variables is to take actions to make the system behave as desired. This should be achieved with limited energy. Therefore, optimization can be used to obtain a set of manipulated variables (MV) that minimize an MV-set-dependent-cost function (J_u) in terms of the MV energy. This is called efficiency of manipulation.

2) The objective of the measurements is to maintain the best possible information of the system behavior. Hence, optimization can be used to obtain a set of measurements that minimizes a measurement-depended-cost function (J_y) that involves the estimation error of relevant variables (e.g. states). This is called efficiency of estimation.

3.3.5.1. Efficiency of Manipulation

The manipulated variable set that minimizes this cost function (J_u) given by

$$J_u = \int_0^{t_f} (x(t)^T Qx(t) + u(t)^T Ru(t))dt \tag{3.7}$$

where $Q = Q^T \geq 0$ and $R = R^T > 0$ is the optimal. Al-Sulaiman and Zaman (1994) and Xu, Warnitchai and Igusa (1994) used this idea to solve the M-MV selection problem. Al-Sulaiman and Zaman evaluated J_u after designing a state feedback by pole placement and after running a closed-loop simulation for a disturbance. Therefore, their choice for an MV depends on the choice of the disturbance. Cao, Biss, and Perkins (1996) considered the selection of manipulated variables with magnitude constraints for nonlinear systems. Their cost function is as follows:

$$J_u = \int_0^{t_f} (z(t) - z_r)^T Q(z(t) - z_r)dt \tag{3.8}$$

where z_r is the setpoint for the controlled variables with $Q > 0$, where Q a diagonal weighing matrix. The MV selection problem is solved in the following way: for a given MV set, J_u is minimized as a function of the input signal $u(t)$ and the final time t_f, subject to the constraint $u_t \leq u(\mathrm{t}) \leq u_u$ and subject to the nonlinear system behavior $f(x,x,z,u,t) = 0$ and a given initial and final state. The MV set that yields the smallest J_u is the optimal. The main problem with this method is that it requires a large computational effort [Van de Wals (2001)].

3.3.5.2. Efficiency of Estimation

Estimation is based on the used of secondary measurements to estimate the desired measurements like controlled variables. The key idea in the efficiency of estimation methods is to select secondary measurements that minimize the error in the estimates of relevant variables (controlled variable). Morari and Stephanopoulos (1980) used this idea and looked for a set of measurements that minimizes the cost function (J_u). The error sources considered for the estimation are model uncertainties, process disturbances, and sensor noise.

Morari and Stepanopoulos proposed four measurement selection criteria, based on a static estimator (derived for the steady state model). The objectives of these methods are to minimize the static estimation error (first criteria), to minimize the effect of model uncertainties on the estimates (second criteria), and to minimize the estimation errors if the static estimator is used for the dynamic system (third and fourth criteria). Kumar and Seinfeld (1978) proposed a measurement selection method that minimizes the state-estimation errors, using a dynamic estimator (Kalman filter) instead of a static one. In 1995, Rhodes and Morari proposed a measurement selection method for a nonlinear autonomous plant $\dot{x} = f(x), y = g(x)$. The objective is to determine the smallest number of secondary measurements (y) that allow an accurate recreation of the nonlinear system dynamics. Other methods for measurement selection, based on efficiency of estimation, can be found in Van de Wal (2001).

3.3.5.3. Efficiency of Manipulation and Estimation

The methods presented in this section combine both the efficiency of manipulation and estimation. Norris and Skelton (1989) proposed a M-MV selection method, based on a cost function which is similar to the linear quadratic Gaussian (LQG) control

$$J_{uy} = E\left(\int_0^\infty (z^T(t)Qz(t) + u^T(t)Ru(t))dt\right) \tag{3.9}$$

where $z=Fx$. The simplest approach would be to calculate the J_{uy} for all M-MV sets and to select the set that yields to smallest J_{uy}. However, this requires a high computational effort [Van der Wal (2001)]. In order to overcome this problem, Norris and Skelton (1989) compute J_{uy} only for the full M-MV set. They retain the corresponding estimator and feedback gains. Then, the effectiveness of each manipulated variable and measurement is expressed as the change of J_{uy} if a measurement or a manipulated variable is eliminated [Van der Wal (2001)].

3.3.5.4. Other Measurement Selection Methods Based on Optimization.

Over the last few decades, optimization has been used as a tool to select optimal measurements for different purposes, such as to improve controllability, observability, efficiency of estimation, and economics, among others. One of the earliest approaches based on optimization was presented by Muller and Weber (1972). In their work, they suggested the use of the determinant of the observability matrix as a measure of the observability of the system. They determined the optimum sensor location by maximizing a function, based on the observability matrix.

Optimization was also used to determine the best sensor location for optimal control. Since control of a process is often the main objective behind the sensor installation, it is worth trying to improve control by selecting optimal sensor locations. One of the earliest approaches for control purposes based on optimization was presented by Mellefont and Sargent (1977), who considered the case of linear quadratic (LQ) control. They determined that the optimum sensor location was the one that minimizes an objective function, based on the covariance matrix of the state prediction, error, and cost functions. More detailed explanation of this method can be found in the cited literature. Harris and MacGregor (1980) presented an up to date review of the techniques available for sensor location based on optimization. A later approach also based on optimization was proposed by Maghami and Joshi (1992), who used nonlinear programming to determine sensor location for flexible space structures. Grimble and Johnson (1988) and Miller (1998) determine the best sensor location by using linear quadratic Gaussian (LQG) theory, based on the Levine and Athans (1970) theory.

In general, optimization is associated with the minimization or maximization of an objective function. Nishida et al. (1981) stated that this objective function can be divided into two main categories: control objectives based on pure economic consideration, and control objectives based on control purposes. In the past, researchers used optimization techniques to determine sensor location, only for control purposes without considering the economic point of view. However, Kookos and Perkins (1999) studied the problem of sensor location, based on optimization techniques, considering both aspects. They proposed a mixed-integer linear programming (MILP) problem formulation, based on the assumption that the control objectives can be related to the variability of certain process variables. The selection of an optimum sensor location is based on the minimization of the maximum time domain deviation of these process variables in the presence of disturbances. In other words, the objective is to maintain process variables within the constraints that define the feasible region of operation. These constraints come from safety and operational requirements, quality specifications, and environmental regulation, among others. From this formulation, Kookos and Perkins (1999) claim that the sensor location chosen in this way will be the optimum because process variables are directly related to the economic performance of a plant. A more detailed explanation of this technique can be found in Kookos and Perkins (1999 and 2000).

3.3.6. Combined Robust Stability and Nominal Performance.

The methods discussed in this section use as selection criteria robust stability (RS) and nominal performance (NP). RS guarantees stability in the presence of uncertainties while nominal performance NP guarantees stability and performance in the absence of uncertainties. The key idea for combined RS and NP methods is to reject those M-MV sets for which there is no controller achieving joint RS and NP.

Research studies in this area were presented by Reeves (1991); Banerjee and Arkun (1995); Reeves, Nett, and Arkun (1991); Ross and Swartz (1997); Van de Wal et al. (1997); and Van de Wal (1998). A detailed review of these methods can be found in Van der Wal (2000). The combined RS and NP based M-MV selection methods are useful for initial screening of M-MV sets, but are very time consuming because of the large number of combinations that must be checked.

3.3.7. Robust Performance (RP).

In this section, methods that use robust performance (RP) as a selection criterion are presented. RP guarantees stability and performance in the presence of uncertainty. The key idea for RP methods is to reject those M-MV sets for which there is no controller achieving RP. This method is used for initial screening of M-MV sets. Research studies in this area were presented by Braatz (1993); Trierweiler and Engell (1997); Van de Wal (1998); among others. A detailed review of these methods can be found in Van de Wal (2001).

3.3.8. Search methods

The majority of the M-MV selection methods discussed are evaluated on a per candidate basis which means that all the M-MV sets should be checked for viability. However, it is not always necessary to check all these candidate M-MV sets in order to determine viable ones. Optimization can be used along with other M-MV selection methods to avoid exhaustive testing on a candidate-by-candidate basis. Adding an optimization criterion may lead to a unique solution. In this section, methods that combine optimization and other M-MV selection methods are discussed.

3.3.9. Measurement Selection Method Based on Thermodynamics Information

This method used to determine dominant variables in a process, was presented by Tyreus (1999). In his work, Tyreus stated that economic-related variables, such as flow and production rates, are almost always related to the internal process rates. He identified the dominant variables affecting these internal rates by using a thermodynamic process description that focuses on the power release expression for each process unit. The thermodynamic method consists of using a generalized balance equation to describe all physical processes. Tyreus used the idea, proposed by Schmid (1984), that certain thermodynamic quantities behave as if they were substance-like. Substance-like means any physical quantity that behaves like an actual substance (physical material). Examples of substance-like quantities are as follows: the total mass of material within a process, the amount of chemical components, energy, entropy, and momentum. The generalized equation that is applicable to all substance-like quantities in a system can be written as the continuity equation for the accumulation of the component within the reactor:

$$\frac{dn_i}{dt} = -In_i + \Pi n_i \tag{3.10}$$

The first term of the equation accounts for the accumulation of the substance-like quantity over time. The second term (negative term on the right-hand side) is the net flow of material leaving the system. Finally, the last term models the generation or consumption of the substance-like quantity within the system. To solve the balance equations, quantitative expressions for the flow and production terms are needed. These expressions are called constitutive equations. These equations describe how substance-like quantities affect the state of a particular dynamic system and how the quantities flow in and out of the system, depending on the system state. Examples of constitutive equations are ideal gas law, ideal gas heat capacities, Fourier's law for heat conduction, and Fick's law for material diffusion, among others. Since all physical systems can be modeled through a combination of balance equations and constitutive equations, an important question is which substance-like quantities should be used to describe the dynamics of the system. In the case of chemical systems, they are modeled, using N component balances and one entropy balance as the substance-like quantities. In this approach, energy is seen as the connection between the descriptions of different systems. Energy is also treated as a quantity that is always carried and associated with another substance-like quantity. Since energy cannot be created or destroyed, every system must export as much energy as was carried into the system. In the thermodynamic method, the unit operations are treated as energy exchangers or receivers of energy between different energy carriers. Tyreus (1999) stated that the economic objectives of a process are tied to the rates governed by the constitutive equations of the system. These equations relate the flow and production rate of substance-like quantities with the intensive variables that help establish these rates. Hence, Tyreus used the concept of internal energy exchange (common to all processes) and focused on this rate exchange to determine the variables that tend to dominate the behavior of the system exchange. The main disadvantage of this method is that it requires experience and knowledge of the process to select the M-MV variables (dominant variables).

Other works based on physical insight from thermodynamics for process control were presented by Ydstie et al. (1996, 2000). They linked physics from thermodynamics to key principles of nonlinear system theory in the analysis and control of processes. They describe the process model in terms of its thermodynamic properties which are then used directly to evaluate the stability of the system. They used typical passivity (Lyapunov) and thermodynamics based storage function to determine the stability of the system. Application and extension of this approach can be found Ydstie et al. (2002, 2007).

3.4 <u>Comparison between M-MV selection methods</u>.

In this section, the more relevant current methodologies for the M-MV selection problem are compared, using some evaluation properties presented in Van der Wal (2001). The main contributions of this review are 1) the addition of new M and/or MV selection methodologies to those presented in Van de Wal et al (2001); 2) the addition of three new properties; and 3) the addition of different application of the M-MV selection methods. The properties considered to evaluate these methods are as follows:

1) Well-founded: In this property, the theoretical bases for the M-MV selection methods are considered. Also, the difficulty and transparency of the methods as well as applications used to prove them are considered.

2) Efficient: In this property the capability for the method to quickly evaluate (in polynomial time) a large number of candidate M-MV sets is considered. Algorithms are called efficient if they solve problems in polynomial time in a measure of the problem size.

3) Effective: This property implies that the candidate M-MV sets for which the considered selection criterion cannot be achieved (nonviable M-MV sets) are eliminated while the ones that can be achieved (viable M-MV sets) are kept.

4) Generally Applicable: This property considers the applicability of the methods. For example, if the method can be applied to linear and nonlinear systems, for square and nonsquare systems (N_y>N_u) etc.,

5) Rigorous: This property considers the rigorousness of the selection method used. For example, a M-MV selection method based on robust stability (RS) is more rigorous than a criterion based on nominal performance (NP). The more rigorous the criterion is the smaller the number of viable M-MV sets are.

6) Quantitative: This property evaluates if the methods generate quantitative measures for selecting the best M-MV set.

7) Controller Independent: This property evaluates whether the M-MV selection method is controller independent or not. In general, it is not desirable to impose restrictions on the controller design method, because this can generate biased conclusions on the M-MV sets viability. However, in some cases, restrictions on the

controller design play an important role; therefore, a controller dependent M-MV selection method might be desired. Frequently, M-MV selection methods should not involve complete controller design.

8) Direct: This property evaluates whether the method directly characterizes the viable M-MV sets, instead of performing candidate-by-candidate tests for each particular criterion in other words, if the candidates are evaluated on a one by one basis.

9) Scaling Independent: This property evaluates if the method is scale-independent or not. The reason for checking scaling dependence is because wrong scaling leads to inaccurate results.

10) Plant Model Not Required: This property evaluates whether the methods require a linearized plant model or not.

11) Disturbance and Setpoint Tracking: This property evaluates whether disturbances and setpoint tracking are considered in the M-MV selection.

These properties are the basis for the evaluation and qualitative comparison of the M-MV selection methods reviewed. The grade in which these methods fulfill the properties is expressed by the following symbols:

+: The method exhibits this property to a satisfactory extent

0: The method exhibits this property to a moderate extent

-: The method does not exhibit this property, or only to a minor extent

Table 1 shows the evaluation of these properties for each M-MV selection criterion. This Table presents the essential information about the current M-MV selection methods available and their main advantages and disadvantages. The most important issues considered in Table 1 for each property are discussed below:

1) Most of the M-MV methods lack of a well-known theoretical background. The selection methods that totally satisfy this property are accessibility, state controllability and observability, right-half-plane zeros, and thermodynamic information. The remaining selection methods satisfy this property to a moderate extent.

2) The more efficient methods, regarding computational effort, are accessibility, state controllability and observability, M-MV controllability, and right half-plane zeros. The remaining methods, except for the thermodynamic information method, require more computational effort in their calculations. It is important to point out that a less rigorous M-MV selection method usually requires less details and, therefore, less analytical effort.

Table 3.1 Qualitative Assessment of the Reviewed M-MV Selection Methods

		Desirable Properties for M-MV Selection Methods										
	M-MV Method	1	2	3	4	5	6	7	8	9	10	11
3.1	Accessibility	+	+	+	+	_	_	+	_	+	+	_
3.2	State Controllability and Observability	+	+	+	+	_	0	+	_	_	_	0
3.3	M-MV Controllability	0	+	0	0	0	+	+	0	0	0	+
3.4	Right Half-Plane Zeros	+	+	0	0	_	+	+	_	0	_	0
3.5	Optimization Efficiency of Manipulation and Estimation	0	0	0	+	+	+	_	0	_	_	+
3.6	Robust Stability & Nominal Performance	0	0	0	0	+	+	+	_	0	0	0
3.7	Robust Performance	0	0	_	0	+	+	0	_	0	0	0
3.8	Search Methods & Robust Performance	0	0	+	+	+	+	0	_	_	_	0
3.9	Thermodynamic Information	0	_	+	+	0	0	+	0	+	0	0

3) The more effective methods are accessibility, state controllability and observability, and the search and robust performance method.
4) The methods that fully satisfy this property are accessibility, state controllability and observability, search methods and robust performance, and thermodynamic information. The reason is that these methods have been successfully applied to nonlinear systems. For other M-MV methods, generalizations to nonlinear systems might also be possible.
5) The major disadvantage of the accessibility and state controllability and obserbavility methods is the lack of rigor. The M-MV controllability method is not very rigorous either; however, this can be improved by sequential M-MV selection for distinct M-MV controllability measures [Van der Wall 2001].
6) Almost all M-MV selection methods use some quantitative criterion, except for accessibility, state controllability and observability, and thermodynamic information. The quantitative measure used by accessibility (the relative degree) it is not rigorous enough to indicate whether the intended control can be achieved or not.
7) The majority of M-MV selection methods, are controller independent except for some optimization-based methods, robust performance-based methods, and search methods. For instance, some of the optimization-based methods assume static feedback or output feedback control. In the case of RP methods, some of them assume integral control, LQG control, MPC, etc. Other methods, such as M-MV

controllability, assume perfect control to avoid controller dependence [Van der Wal, 2000]

8) In the majority of the M-MV selection methods discussed in this chapter, all the candidates generated should be evaluated. This implies an exhaustive search for all possible combinations of measurements and manipulated variables, which is inefficient. However, some of the optimization-based methods reviewed can lead to a unique solution, based on the desired control objective. This is also the case for the thermodynamic information-based methods.

9) The M-MV selection methods with the “+” symbol are scaling independent, while the methods with the “-” depend on scaling. The M-MV selection methods that directly depend on scaling are state controllability and observability, optimization-based methods, and search and robust performance methods. It is important to select the appropriate scaling because inappropriate scaling leads to inaccurate results and therefore, wrong conclusions.

10) The M-MV selection methods that fully require a linearized model of the plant are state controllability and observability, optimization-based methods, and search and robust performance-based methods.

11) The M-MV methods that consider setpoint tracking and disturbance rejection are M-MV controllability and optimization-based methods.

As can be seen from this analysis, only a few M-MV selection methods are readily applicable to nonlinear systems. Also, only a few methods give a unique solution for the best set of M-MV variables. There is no single method that satisfies all the properties evaluated. Every method shows different advantages and disadvantages. The development of an M-MV selection method that satisfies all these properties is probably too ambitious. However, these properties can serve as guidelines for the development of new M-MV selection methodologies.

Chapter 4: The Optimal Control Based Measurement Selection Methodology

4.1. Background

The plantwide process control problem involves the design of strategies to control an entire chemical plant, consisting of many interconnected unit operations. This problem is open-ended, which means that there are several possible solutions. In fact, the control structures obtained depend on the economic and control objectives that were considered during the control design stage. Because different objectives lead to different control structures, the most important step in plantwide control design is to define the desired objectives. For example, some of the control objectives that have been used for the Tennessee Eastman process (process simulation) are as follows: to improve the control of key economic variables in the plant, such as production rate and product quality [Ricker, 1996 and Tyreus]; to be able to have rapid changes in the production rate [Luyben, 1996 and Tyreus 1998]; to reduce the variability in the feed streams to the process by not using them (feed streams) for controlling fast loops [McAvoy et. at. 1996]; etc.

In general, the most common economic objective in any chemical process is to maximize profit, while considering the environmental and safety regulations. This objective is closely related to the control performance of key economic variables in the plant (production rate, product quality, and purge losses). Often in complex processes, in order to achieve the desired economic and control objectives (e.g. control some key variables at their setpoints or within a specified range), a few other important variables should be controlled. This means that the setpoints of these key controllers are the manipulators to hold the economic objectives in the desired range. This is called partial control. Works in partial control have been presented by Arbel (1995a, 1995b, 1996, 1997, 1999), and Tyreus (1999), among others. Tyreus (1999a and 1999b) used partial control to improve the control of the production rate. Tyreus used thermodynamic principles to identify the dominant variables that affect the economic variables in the plant (production rate and product quality). Then, he used a partial control scheme to control these dominant variables in order to: 1) increase and hold the production rate by approximately 50% of the steady state value and 2) improve the control performance (transient responses) of the process for disturbance rejection.

The main objective of this Thesis is to determine the set of measurements and manipulated variables (important variables) and to structure them to maximize profit in the plant. A sub-objective that directly affects the main objective is to improve the control performance of production rate and quality. The reason is that by improving the control performance of these variables, the plant can be operated closer to operational constraints. In this Thesis, a methodology based on optimal control theory that uses the idea of partial control is presented to solve this control problem. The optimal control measurement selection methodology uses a linear quadratic regulator (LQR) design method to generate an optimal static output feedback controller (OSOFC). The OSOFC is analogous to a gain matrix in the sense that it can provide dynamic information about the process interaction while the gain matrix contains static information about process interaction. This gain matrix (OSOFC) is used to determine the important measurements and manipulated variables that affect production rate and product quality. Then, control structures (interconnections) for these important variables (manipulated variables and measurements) are determined, using OSOFC. After closing these loops, the setpoints of the important measurements become manipulated variables. Finally, the idea of using partial control for controlling production rate and product quality is implemented as follows. In this methodology, production rate and product quality are controlled by manipulating the setpoint of important manipulated variables. The main difference between the plantwide control design methodology presented in this Thesis and the majority of the current methodologies is as follows. In this methodology, production rate and product quality are controlled by manipulating a set of dominant variables in the plant, while in other methodologies production rate and product quality are controlled using only two manipulated variables (one for each controlled variable). It is important to point out that the original idea of using an LTI process model and optimal control theory for control structure design was presented by Schenelle (1989). More recent research on this subject has been presented by McAvoy and Chen (2002 and 2003). In their work, Chen and McAvoy (2002 and 2003) use the OSOFC for control structure design.

The structure of this chapter is as follows: First, the basic OSOF LQR design Linear Quadratic Regulator (OSOF LQR) is presented. Then, the optimal control-based measurement selection methodology is described. Next, the OSOF LQR design considering economics is addressed. Finally, a discussion and comparison with other schemes is presented.

4.2. The Basic Optimal Static Output Feedback Linear Quadratic Regulator (OSOF LQR) Design

In general, the majority of chemical processes are considered nonlinear. Even though there is an optimal controller design approach for general nonlinear systems [Lewis, 1992], no systematic design approach has been suggested at the present time. In fact, experience is always needed for solving each particular nonlinear problem. By contrast, optimal control theory and LQR are firmly established for linear and time-invariant (LTI) systems. The optimal controller design for linear time invariant (LTI) systems with quadratic performance indices is called the linear quadratic regulator (LQR) problem. In the optimal control theory, LQR is the basic controller design for LTI systems. The general formulation for an optimal LQR, using state feedback, is given in Chapter 1 Section 1.3. However, in practice, only some of the states are available as measured outputs. Therefore, in order to determine the LQR when not all the states are available, two approaches can be used: 1) to estimate the states by using a Kalman filter or 2) to use output feedback instead of state feedback. The second approach is called the optimal static output feedback linear quadratic regulator (OSOF LQR) design problem, and its formulation is presented in Chapter 2 Section

2.4. It is important to understand the OSOF LQR because the methodology proposed in this work (optimal control based measurement and manipulated variables selection methodology) is based on the OSOF LQR.

4.3. ***<u>The Optimal Control Based Measurement and Manipulated Variables Selection Methodology</u>***

The optimal control measurement selection methodology uses a linear quadratic regulator (LQR) design method to generate an optimal static output feedback controller (OSOFC), which is analogous to a process gain matrix. The OSOFC (gain) is used to determine the important measurements and manipulated variables that affect production rate and product quality (those variables for which production rate and product quality are most sensitive). Then, control structures for these important variables (measurements and manipulated variables) are generated, using OSOFC. After closing these loops, the setpoints of the important measurements become manipulated variables. Finally, partial control is used for controlling production rate and product quality by adjusting all the important manipulated variables.

The main problem to be solved in this stage is to find a set of measurements and manipulated variables that affect the production rate and quality, without using these two measurements in the control law. In other words, these two measurements should be used to define the control objective (in the objective function), but they should not be considered as available measurements at this stage. The logic behind this is explained as follows: Production rate and product quality are considered in the objective function in order to define the control objective -- to control production rate and product quality. By not considering them within the available measurements, the idea is to find other dominant variables (measurements and manipulated variables) that can be used to control production rate and product quality. The reasons for using partial control to control production rate and product quality is that, by controlling the dominant variables, there is an improvement in the control performance of production rate and product quality for setpoint changes and disturbance rejection

In order to solve this problem, two methods based on OSOFC are proposed. For both methods, given a LTI state space model (Equation 2.4) an optimal static output feedback controller (OSOFC) is designed to stabilize the system and bring the states from arbitrary initial values to zero, following a trajectory that minimizes a linear quadratic objective function. The output feedback equation is given as:

$$u = -Ky \tag{4.1}$$

where K is a mxp matrix of constant feedback coefficients. The problem to be solved is to find the K that minimizes a quadratic time domain performance index function given by:

$$\min_{K} \quad J = \frac{1}{2}\int_{0}^{\infty}(y^T Q y + u^T R u)dt + \frac{1}{2}\sum_{i}\sum_{j} g_{ij} k_{ij}^{\;2} \tag{4.2}$$

where Q and R are weighting matrices for y and u respectively, while g_{ij} is a weight on element k_{ij} in K. In general, g_{ij}'s are zero. However, when a single input single output (SISO) structure is used, the g_{ij}'s elements are used to force the off-diagonal elements of K to be zero; then the resulting K has only diagonal elements. In order to make the k_{ij} elements small, large values of the corresponding g_{ij} elements should be used.

Two methods are proposed to find the set of measurement and manipulated variables that affect production rate and product quality. Both methods are based on OSOFC. **The first method** to find the set of measurement and manipulated variables that affect production rate and product quality uses the weight matrix Q. By changing the elements of this matrix, the control objectives can be defined. To do so, two sets of measurements are generated: a first set (*Cs*) which includes all the measurements, except the production rate and quality, and a second set (*Cc*) which includes all the measurements including production rate and product quality). Then Equations 2.7, 2.9, and 2.10 are replaced by the following algebraic Riccati Equations:

$$A_C^T P + PA_C + Cs^T K^T RKCs + Cc^T QCc = 0 \tag{4.3}$$

$$RKCsSCs^T - B^T PSCs^T + g * K = 0 \tag{4.4}$$

$$A_C = A - BKCs \qquad X = x(0)x(0)^T \tag{4.5}$$

To achieve the control objective, all the elements in the Q matrix are set equal to zero, except for the elements that correspond to the production rate and product quality in the *Cc* matrix.

The second method to solve this problem uses the g_{ij} elements in Equation 4.4. In this method, only one set of measurements (C) is generated. This set of measurements includes the production rate and product quality. The key idea is to make all the elements in the rows of K matrix corresponding to the production rate and product quality measurements very small. To do so, a large value for the corresponding weighting g_{ij} elements is used. Several simulations were performed using both methods. The results obtained using both methods were the same; however; the computation speed of the second method is much slower. An example that demonstrates that these two methods give the same results is presented in Appendix III. Because both methods give the same results the first method is chosen to be used due to the speed of the calculation. If the first method is used then g_{ij} are equal to 0. On the other hand, R is chosen to be the identity matrix; therefore, all manipulated variables are treated equally. In solving this problem (using method 1)the following conditions are required:

1) R should be positive definite, and Q should be positive semidefinite to ensure $C_C^T Q C_C$ is positive semidefinite.

2) P is positive definite or positive semidefinite as long as A_C is stable $(C_S^T K^T R K C_S + C_C^T Q C_C)$ is positive definite or positive semidefinite.

3) S is positive definite or positive semidefinite as long as A_C is stable and X is positive definite or positive semidefinite.

The OSOFC K solution depends on the initial states x_0 (as explained in Chen's methodology in Chapter 2 Section 2.4), and in most of the cases, x_0 is unknown. This problem can be solved by minimizing the expected value of J [Levine, 1970]:

$$\min_K \quad E\{J\} = E\left\{\frac{1}{2}\int_0^\infty (y^T Q y + u^T R u)dt\right\} + \frac{1}{2}\sum_i \sum_j g_{ij} k_{ij}^{\ 2}$$

Then, Equation 4.5 is replaced by:

$$A_C = A - BKC_C \qquad\qquad X = E\{x(0)x(0)^T\} \tag{4.6}$$

where X is the initial autocorrelation of the states. It is usual to assume that the initial states are uniformly distributed on the unit sphere, therefore $X=I$, the identity matrix. Chen (2002, 2003) used this assumption to solve the OSOFC. Therefore, the control structures obtained using Chen's methodology might not be the most appropriate for specific disturbance rejection and setpoint changes. In contrast, to Chen's methodology, in this methodology, the initial states X are calculated for considering disturbance rejection and setpoint change. Then the initial condition for (4.6) for the proposed methodology is given by

$$X = \left\{ \sum_{i=1}^{n} x_{d_i} x_{d_i}^T + x_{sp_i} x_{sp_i}^T \right\} \tag{4.7}$$

where x_d represents the disturbances states, n represents the total number of disturbances, and x_{sp} is a vector related to setpoint changes in the production rate and quality. The calculation for x_d and x_{sp} is given by

$$x_{d_i} = -A^{-1} * W * d_i \tag{4.8}$$

W is the matrix whose elements describe the dynamics for the disturbances, and d is the vector that considers the disturbances.

$$x_{sp_i} = C * m \tag{4.9}$$

C is the matrix that has information about the measurements and m is the vector that specifies the measurements that are considered for control, in this case production rate and product quality. Therefore, the size of m is the total number of measurements. All the elements of m are zero, except for the elements that correspond to production rate and product quality.

After the OSOFC is obtained, the next question is how to extract information about the best set of measurements and manipulated variables to control production rate and product quality. Since the process model is scaled, the OSOFC is dimensionless. Therefore, the absolute value of the elements in the OSOFC can be compared to one another. In the OSOFC the rows represent manipulated variables while the columns represent measurements, as can be seen form Equation 4.1. Generally, an element with absolute value close to zero indicates a weak relationship between the manipulated variable and the measurement. In this methodology, the L_1-norm of a vector is used as a measure of the degree of importance for the measurements and manipulated variables. The L_1-norm is defined as follows:

$$\|x\|_1 = |x_1| + |x_2| + |x_3| + \ldots\ldots + |x_n| \tag{4.10}$$

In order to determine which measurements and manipulated variables should be used to control production rate and product quality the following rules of thumb are used:

1) The L_1-norm for each row of the OSOFC is calculated as the sum of the absolute value of all the elements in each row. These values are called Σrow_i and represent the total contribution of each manipulated variable. The manipulated variables that have more effect on the production rate and product quality (strongest manipulated variables) are the ones that have the largest values of Σrow (L_1-norm row).

2) The L_1-norm for each column of the OSOFC is calculated as the sum of the absolute value of the elements in each column. These values are called Σcol_i and represent the total contribution of each measurement. The measurements that have more effect on the production rate and product quality (strongest measurements) are the ones that have the largest values of Σcol (L_1-norm col).
3) If a row of the OSOFC contains only small elements the corresponding manipulated variable should not be consider in the control structure for controlling production rate and product quality.
4) If a column of the OSOFC contains only small elements the corresponding measurement should not be consider in the control structure for controlling production rate and product quality.

The Optimal Control-Based Measurement and Manipulated Variable Selection Procedure

In this section, the implementation of the optimal control-based measurement and manipulated variable selection methodology for controlling production rate and product quality is explained. This methodology is one of the most important tasks in the plantwide control design methodology presented in this work. This methodology it is closely related to the plantwide control design methodology presented by Chen and McAvoy (2002, 2003). The reason is that some of their ideas about control structure design and the calculation of the OSOFC are used in this methodology. Therefore, the differences between both methodologies are pointed out in each stage. If the procedure is similar or the same, references are given. The plantwide control design methodology proposed is based on the following ideas: 1) the use of optimal control theory, 2) the use of hierarchical design procedure for process control design, and 3) the use of partial control. The original idea of using optimal control theory for control structure selection was presented by Schenelle (1989) and more recently, by Chen and Mc Avoy (2002 and 2003). In this Thesis, a new idea of using optimal control theory for finding dominant measurement and manipulated variables that affect production rate and product quality is presented**.** The optimal control theory is also used for control structure selection based on Chen and McAvoy (2002, 2003) presented in Chaper 2 Section 2.4. The original idea of using a hierarchical design procedure for plantwide control design was presented by Mc Avoy (1994). The plantwide control design methodology presented in this work uses the idea proposed by McAvoy in the following way: The plantwide control design problem is divided into four sub-problems: 1) controlling variables related to safety issues, 2) controlling the component balances, 3) controlling production rate and product quality variables, and 4) controlling the unit operations with the available degrees of freedom. The reason for dividing the problem into sub-problems is that, from the plantwide design point of view, it is easier to solve an optimization problem, when not all the objectives are being considered at the same time. In fact, a hierarchical design procedure can provide a systematic and practical way to locate satisfactory solutions in a small search space. Finally, partial control was used by Tyreus (1999) for controlling economic operating objectives in a plant. Tyreus uses a thermodynamic-based method for the identification of the dominant variables. Then the partial control structure is implemented by feedback control of all the dominant variables and by manipulating the setpoint of the dominant variables manually. In the methodology presented in this work, optimal control theory is used to identify the dominant variables (measurement and manipulated variables). Then optimal control is also used to generate control structures to pair these measurements with the manipulated variables. Finally, a model predictive control (MPC) is built on top of the resulting control structure to manipulate the set point of these loops, in order to change the production rate and product quality.

Data Requirements

In order to use this methodology, the following data should be available:

1) A linearized model (a state space linear time invariant process model). The linear model can be obtained from the first principle nonlinear model by numerically calculating the first order Taylor expansions coefficients of the nonlinear model around the operating point. Also, the linear model can be obtained from model identification using process data.

2) Steady state process data for state variables, manipulated variables, and measurements.

3) Operating ranges of the measurements and manipulated variables.

4) Defined control objectives, i.e. the control of key economic variables (production rate and quality)

5) Process constraints used to define the safety variables.

6) Information about possible disturbances and/or setpoint changes.

The optimal control-based measurement and manipulated variable selection procedure for plantwide control design consists of 6 stages. Even though the methodology presented in this work, has many similarities with Mc Avoy and Chen's plantwide control design methodology (2002) the main differences between them are listed at the end of this section.This methodology is tested in two-process simulations: 1) the Tennessee Eastman Process, presented in Chapter 5, and the Vinyl Acetate process, presented in Chapter 6.

1) Stage 1: Preparation.

The first stage, the preparation, is divided into three substages:

1.1) Scaling the model: The main purpose of this scaling is to obtain an optimal gain matrix (K) that has no units; therefore, every element of this matrix can be compared directly with each other. Because K depends on the scaling of the models, a proper scaling is required. The scaling can be made using the following:

- State Variables: They can be scaled by their steady state values or by the ranges of their desired movements.
- Measurements: They can be scaled by the range of the transmitter or by the range of desired movements (operational ranges). The operational ranges are decided by engineering judgment.
- Manipulated Variables (MVs): They are either valve opening percentages or setpoints of inner cascade controllers. The MVs can be scaled by the physical valve range or by the range of desired movements (operational ranges).

In this work, the operation range values are used for scaling, and their values are decided by engineering judgment.

To scale the model given by Equation 2.1, x, u and y are scaled using

$x = N_x x_s, \; y = N_y y_s, u = N_u u_s$.

N_y = diagonal scaling matrix for the measurements

N_u = diagonal scaling matrix for the manipulated variables

N_x = diagonal scaling matrix for the state variables.

Therefore, the scaled model is

$$\begin{cases} \dot{x}_s = A_s x_s + B_s u_s \\ y_s = C_s x_s \\ x_s(0) = (N_x)^{-1} x_0 \end{cases} \tag{4.11}$$

where $A_s = (N_x)^{-1} * A * N_x \quad B_s = (N_x)^{-1} * B * N_u \quad C_s = (N_y)^{-1} * C * N_x$

$Q_s = (N_x)^{-1} * Q * N_x \quad R_s = (N_u)^{-1} * R * N_u$

The scaling values used in this work are given in Chapters 5 and 6 for the Tennessee Eastman process and Vinyl acetate process, respectively.

The $K_s = N_u^{-1} K N_y$ that minimizes $J = \frac{1}{2}\left[\int_0^\infty (y_s^T Q_s y_s + u_s^T R_s u_s) dt\right]$ depends on the values of the scaling factors in the matrices N_x, N_y or N_u

1.2) Closing the inner cascade loops (secondary loops): In this step, flow loops and temperature loops are closed. The manipulated variables then become the setpoints of the flow and temperature loops. The main advantage of closing the inner cascade loops is that the upset (disturbances) can be caught more quickly. For example, if the secondary (inner) loop has a response that is five times faster (or more) than the master (outer) loop, then upsets entering the inner loop can be caught and corrected before they affect the primary loop. Therefore, better control of the primary variables is achieved because they are less affected by disturbances. The main difference between the performance of cascade loops and direct loops can be seen in the presence of disturbances.

1.3) Steady state correlation analysis: In this step a correlation analysis is carried out on the steady state gain matrix to identify variables (measurements) that are highly correlated. This is an important issue for overall plantwide control because when there are two or more variables that are highly correlated, trying to control all of them at the same time results in severe interactions. In addition, several simulations showed that when highly correlated variables (measurements) are considered simultaneously, the algorithm used to calculate the OSOFC did not converge, or the calculation was very slow. The reason for this is that the condition number of the C matrix increases significantly whenever two or more highly correlated variables are considered simultaneously. Because the algorithm used to calculate the OSOFC involves the inversion of the C_*S_*C' matrix (equation 4.4), it is recommended not to work with ill-conditioned systems to avoid convergence problems. In order to overcome this problem, a condition number analysis is used to determine how the condition number of the C matrix is affected when highly correlated measurements are considered simultaneously. To do so, the condition number (CN) of the C matix is calculated, eliminating one variable at a time from each correlated group until there is not significant change in the CN.

In this stage, the differences between this methodology and Chen's methodology are as follows:

In this methodology, a correlation analysis and condition number analysis are performed, while Chen does not consider these analyses. The reason for this is that the problem solved with this methodology is much larger than the problem solved by Chen's methodology. For instance, the problem of finding the dominant variables that affect production rate and product quality through calculating an OSOFC is a large optimization problem because all the available measurements in the plant are considered simultaneously. These analyses are used for identifying highly correlated variables that make the system ill-conditioned, causing slow calculation and convergence problems. Chen does not require these analyses because he solves smaller optimization problems in each stage. In these problems, he chooses the controlled variables, based on experience, and he calculates the OSOFC to find the best manipulated variables to control them.

In this stage, inner cascade loops, such as flows and temperatures, are closed while Chen does not consider inner cascade loops.

2) Stage 2: Generate decentralized control structure candidates.

In this stage the safety variables identified in Chen's first stage are used. Then, decentralized control structures are generated for these safety variables. The procedure used here is similar to the one proposed by Chen (2002). Details on this procedure can be found in Chapter 2 Section 2.4 or Chen (2002, 2003). However, the main difference is that in this procedure the initial states are calculated for specific disturbances and setpoint changes (Equations 4.7, 4.8, and 4.9) while Chen's assumed that the initial states are uniformly distributed on the unit sphere. The control structures for the safety variables are determined using Chen's guidelines. Then, these loops are closed, using proportional-only controllers. The tuning of the controllers is carried out by generating a diagonal optimal static output feedback controller (OSOFC) for each control candidate. This tuning method was proposed by Chen (2002), and it can be used to automatically tune proportional-only controllers. More details can be found in Chaper 2 Section 2.4. In this methodology the calculation of the diagonal OSOFC is also done for specific disturbance rejection and setpoint changes while Chen uses generic forcing ($X=I$).

3) Stage 3: Control Structure for Inventory Variables (Inventory Control).

The goal of this stage is to maintain component balances. The plant chemical components are characterized by Luyben (1999) as reactants, products, and inerts. In chemical processes it is very important to satisfy the overall component balance of all chemical species at steady state. In fact, this is particularly important in processes with recycle streams because any imbalance of any component will cause an accumulation of the component that is in excess [Luyben, 1999]. In this methodology, the component balance control design is done before the production rate and product quality control design, while in Chen's methodology, the sequence of these two stages is inverted. The reason for doing the component balance control design early (in the plantwide control design process), is to avoid the use of the feed streams (manipulated variables used to control component) to satisfy other control objectives, instead of keeping the component balances. Although Chen does the production rate and product quality control design (Stage 3 in Chen's methodology) before the component balance control design (Stage 4 in Chen's methodology), he does not close the product loops until he closes the component balances. For instance, in Chen (2003), he said, "Before product loops are tuned (Stage 3), the component balances should be examined in Stage 4 because these balances might reduce the number of manipulated variables that can be used in Stage 3." Therefore, it is not clear why he first considers the production rate and product quality control design.

In 1992, Downs pointed out the importance of verifying whether the control structure in the plant satisfies the component balance. To do so, it is necessary to check the specific mechanism or control loop that guarantees that there will be no accumulation of that chemical component (Downs drill). There are three ways to ensure this: 1) to limit the feed flow of reactants, 2) to control their reaction, or 3) to adjust the product or the purge in the plant. In order to verify the component balances, Luyben (1999) recommended the use of a Downs drill analysis. This is shown in a Table that lists each chemical component, its input, its generation or consumption, and its output. In this methodology, Downs drill Tables are generated for each candidate obtained in Stage 2. However, a difference from Chen's methodology is that, in this methodology only the reactants, inerts, and byproducts are considered for this analysis since the products will be controlled in the next stage. The Downs drill Tables generated have the following information: list of the components of the plant (reactant, inerts, and byproducts) and their categories, whether the components are regulated or not, why they are self-regulating, and all possible measurements and manipulated variables for controlling each component. After the number of control loops for the uncontrolled chemical components are identified, the same number of manipulated variables should be used. In general, the manipulated variables used to control the inventory of a component are their feed flows. In the case of the inerts the purge is used. The measurements used in this stage are not available for future stages. Then, the new manipulated variables are the setpoints of the component inventories. These loops are tuned by generating a diagonal optimal static output feedback controller (OSOFC) for each control candidate.

4) Stage 4 : Control Structure for Production Rate and Product Quality

The objective in this stage is to determine the set of measurements and manipulated variables that have more effect on the key economic variables in the plant (production rate and product quality). The measurements used in this stage are all the remaining measurements (measurements not used to close loops) from the previous stages. It should be pointed out that production rate and product quality are not included in the set of available measurements. They are only considered to define the control objective. On the other hand, the setpoints of the loops, closed in Stages 1, 2, and 3, become manipulated variables for this stage. Then, an OSOFC is calculated to determine the set of variables that have the strongest effect on production rate and product quality. The OSOFC can be a non-square system. The initial states used can be: 1) not known then, the initial states are assumed uniformly distributed on the unit sphere, X=I; and 2) calculated based on disturbance rejection and setpoint change.

The parameters used for the calculation of the OSOFC are as follows:

Parameter	**Value**
R	Identity matrix, which gives the same importance to all the manipulated variables
g_{ij}	0, which means there is no control structure specified
Cs	All remaining measurements from stages 1, 2, and 3 except for the production rate and product quality
Cc	All remaining measurements from stages 1,2, 1and 3, and the production rate and product quality
Q	Q is the weight matrix that can be used to define the desire control objective. All the elements of this matrix should be zero except for those that correspond to the variables associated with production rate and product quality in *Cc*.
X	The initial states are calculated for setpoint change and disturbance rejection using Equations 4.7, 4.8, and 4.9.

The OSOFC obtained from this procedure is similar to a gain matrix in which the elements of each row and column can be compared to one another because the OSOFC is dimensionless. In the OSOFC matrix, the rows represent the manipulated variables while the columns represent the measurements. To obtain the information about the important measurements and manipulated variables from the OSOFC, the following rules of thumb are used:

1) The sum of the absolute value of the elements of each column is called Σ*col*. The Σ*col* is calculated for each column.

$$\sum col_j = \sum_{i=1}^{n} \left| K_{i,j} \right| \qquad j = 1,\ldots\ldots,m \tag{4.12}$$

The best measurements (strongest measurements) are the ones that have the largest values of Σcol.

2) The sum of the absolute value of all the elements in a row is called Σrow . The Σrow is calculated for each row.

$$\sum row_i = \sum_{j=1}^{m} \left| K_{i,j} \right| \qquad i = 1,.......n \qquad (4.13)$$

The best manipulated variables (strongest manipulated variables) are the ones that have the largest values of Σrow.

3) An element with absolute value close to zero indicates a weak relationship between the manipulated variable and the measurement.

These rules of thumb provide information about the strongest measurements and manipulated variables; however, there is no rule to decide how many of these variables should be used in the final control structure. Since only the manipulated variables will be used to build the MPC, control structures for the important measurements should be determined, using the available manipulated variables. To do so, the following procedure is carried out:

- **Control Structures for Important Measurements.** In this section, decentralized control structures are identified to control the strongest measurements. An OSOFC is calculated where the control objective is to control the strongest measurement. All the strongest measurements and all the manipulated variables are used. The reason for using all the manipulated variables, instead of using only the strongest ones, is because now the objective is to control the strongest measurements. Therefore, different manipulated variables, rather than the strongest ones, might be needed for this new objective. The following parameters are used for the calculation of the OSOFC:

Parameter	**Value**
R	Identity matrix, which gives the same importance to all the manipulated variables
g_{ij}	0, which means there is no control structure specified
Cs	All the strongest measurements
Cc	All the strongest measurements
Q	Q is the identity matrix that gives the same importance to all the measurements
X	The initial states are calculated for setpoint change and disturbance rejection using Equations 4.7, 4.8, and 4.9.

From the OSOFC, the best manipulated variables to control strongest measurements are the ones with the largest values in the column. These loops are tuned by generating a diagonal OSOFC. The tuning method used is the same as the one used in stages 2 and 3. The proportional gains for these loops are given in Appendix IV. After closing these loops, the setpoints of these variables become manipulated variables.

- **Determination of Control Structures for Controlling Production Rate and Product Quality.**

After the loops that correspond to the strongest measurements are closed, the setpoints of these control systems become new manipulated variables. Then, two possible alternatives are considered to build the MPC: 1) to use the manipulated variables generated by closing the important measurement loops first, and then to add the strongest manipulated variables, one at a time, and 2) to recalculate an OSOFC to check for any changes in the strongest manipulated variables, once the important measurements loops are closed. The second alternative is used in this work. The reason is that it takes into consideration any changes in the order of importance of the manipulated variables due to the addition of the important measurements loops that were closed.

As mentioned above, an MPC is used to control production rate and product quality by adjusting the strongest manipulated variables. This MPC will have two outputs or controlled variables (production rate and product quality) and many inputs or manipulated variables. The questions become how many manipulated variables and which ones should be used. To answer these questions, the manipulated variables are added, one at a time, in descending order of Σrow, until there is no significant improvement in the control performance for disturbance rejection and setpoint changes. In order to identify the cut-off for the manipulated variables, a multivariable OSOFC is used as a quick screening tool, to have an initial idea about the numbers of important manipulated variables that should be used (check length. The reason for using a multivariable OSOFC before the MPC is that the multivariable OSOFC will give insight about the effects of the addition of a manipulated variable in control performance; it is easier to implement, and therefore, it is less time consuming than generating a new MPC every time a new manipulated variable is added. When a new manipulated variable is added, a new control structure or candidate is generated. The resulting control structures are evaluated for disturbance rejection and setpoint changes. The control performance of the resulting candidates is compare using transients' response characteristics, such as settling time and offset value for critical variables in the plant, as well as the integral of the absolute value for the error (IAE). The critical variables in the plant are selected depending on the control objectives. The offset of the critical variables is calculated as the difference between the setpoint of a critical variable and the final steady state value, reached after a disturbance or setpoint change. Then, the summation of the absolute value of the offset for the critical variables is calculated for disturbances and setpoint changes, for each candidate using the following Equation:

$$Offset\,Value_k = \sum_{j=1}^{m}\sum_{i=1}^{n} \alpha_* abs(critical\ variables\ offset(j,i)) \qquad (4.14)$$

α: weights for the critical variables (selected depending on importance of control objectives)

i: critical variables offsets. *i*= 1 to *n*, where *n* is the total number of critical variables *j:* Disturbances and setpoint change. *j*= 1 to *m*, where *m*, where *m*, is the summation of the disturbances and setpoint changes

k: total offset value for each candidate *k*=1 to max number of candidates.

Equation 4.14, shows that the offset values per candidate are the summation of the offset for the all the critical variables for disturbances and the setpoint changes.

The IAE is calculated, using Equation as follows:

$$IAE\ \ for\ critical\ variables_k = \int_0^\infty \left[SP(t) - CV(t)\right]dt \qquad (4.15)$$

The IAE for each candidate is calculated as follows

$$I\mathrm{AE} = \sum_{j=1}^{\mathrm{m}} \sum_{i=1}^{\mathrm{n}} I\mathrm{AE\ for\ critical\ variables(j,i)} \qquad (4.16)$$

i: IAE for critical variables: selected depending on control objectives. *i*= 1 to *n*, where *n* is the total number of critical variables

j: Disturbances and setpoint change. *j*= 1 to *m*, where *m*, where *m*, is the summation of the disturbances and setpoint changes

k: total IAE for the critical variables for each candidate. *k*=1 to max number of candidates

Every time a new manipulated variable is added, a new candidate is generated, and the values for the summation of the offset and IAE for this candidate are compared with the previous candidate. The goal is to evaluate whether there is significant improvement or not when a new manipulated variable is added. It can be said that there is significant improvement under the following conditions:

a) The percentage of change in the IAE with the addition of a new manipulated variable is greater than 5%. The percentage of change is calculated as the change between two consecutive candidates. If it is less than 5%, there might be no significant improvement. Therefore, the addition of a new manipulated variable will not give significant control benefits. However, since this is just an initial screening tool if the % change is between 1 to 5%, it might be checked with the nonlinear simulation, just to corroborate that the variable does not significantly improve the control performance.
b) The total summation of the offset value decreases more than 5% between two consecutives candidates.

The most important difference between this methodology and Chen's methodology is in this stage. The difference is the way in which both methodologies handle the production rate and product quality control design. For instance, Chen solves the problem of finding the best set (two) of manipulated variables to control production rate and product quality (one manipulated variables for each measurement). In Chen's methodology, based on experience, he chooses the controlled variables (in this case production rate and product quality are the controlled variables); then he uses optimal control theory, process insight, and experience to find the best manipulated variable for each controlled variable. Therefore, production rate and the product quality are controlled by adjusting only two manipulated variables, one for each controlled variable. On the other hand, in the methodology proposed in this work, production rate and product quality are controlled using the partial control idea by manipulating several dominant variables. The main benefit for using the partial control idea for controlling production rate and product quality is that there is an improvement in the control performance of production rate and product quality for setpoint changes and disturbance rejection. In addition, the product quality can be kept under specifications, even though the product quality analyzer has problems.

5) Stage 5: Control Structure for Individual Unit Operations

The number of valves available in a plant is equal to the number of degrees of freedom. In general these valves are used to: 1) set production rate, 2) control gas and liquid inventories, 3) control product quality, and 4) avoid safety and environmental constraints [Luyben, 1999]. In this stage, the degrees of freedom that are still available are determined. Then, control loops for individual unit operations are determined, using the remaining degrees of freedom. If there is more than one loop that needs to be closed, an OSOFC is used to determine the control structure. If, at the end of this stage, there are still degrees of freedom available, they can be used for process optimization, which is not considered in this work.

6) Stage 6: Control Production Rate and Product Quality Using MPC

The objective in this stage is to improve the control of the production rate and product quality by adjusting the setpoints of the important variables in the plant (strongest manipulated variables determined in stage 4). One important question to consider in this stage is whether to use a multivariable controller (OSOFC which is a proportional controller used in stage 4) or a model predictive control (MPC) for implementing the production rate and product quality control. In this work, multivariable controller (OSOFC) is used as a screening tool to determine how many strongest manipulated variables should be used. The reason is that multivariable controller uses the linear model of the plant (which is available) and it is easier to implement than the MPC applied to the nonlinear model. Once the system is defined an MPC is used for implementing the resulting control structure because of the following reasons:

1) The MPC is a more general model based control methodology, in which the dynamic optimization problem is solved on-line at each control execution while the OSOFC is solved offline. The MPC drives the outputs to their steady-state optimal values (dynamic output optimization) and the inputs to their steady-state optimal values, using the remaining degrees of freedom (dynamic input optimization)
2) The MPC formulation can handle process constraints (inputs and outputs) while the OSOFC cannot. This is very important because, in general, the most efficient operation is achieved by operating the process at an optimum set of constraints that represent the physical limitations of the equipment in the plant or quality specifications of the products. In the MPC, process input and output

constraints can be included directly in the process formulation; therefore, future constraint violations are anticipated and prevented. Then by using MPC, the process can be operated closer to the true process equipment and product quality constraint achieving more economic benefits.

3) The MPC allows moving the system from different steady states. The inputs may receive the steady state operating point from a plantwide steady state optimizer.

4) The MPC prevents excessive movement of the manipulated variables because it has weights for the manipulated variables movement that can be adjusted.

In this particular case, the outputs of the MPC are production rate and product quality, while the inputs are the important manipulated variables.

Another difference from this methodology and Chen's methodology is the way in which control performance is evaluated. In this methodology, the performance of the final control structure candidates is evaluated, using nonlinear process simulation, while in Chen's methodology, only linear process simulations are considered. If the process is kept close to the operating point, there should not be a big difference between using linear and nonlinear simulations. However, if the process is moved far form the operating point (for example big changes in production rate, changes between different operating modes in the plant, etc.), then it is necessary to evaluate the control performance of the candidate by using nonlinear simulations.

Important Considerations:

Chen (2002 and 2003) presented three groups of numerical algorithms to solve for the OSOFC (see Chapter 2, Section 2.4). In this methodology the Moerder and Caliese's algorithm is chosen to calculate the OSOFC because of its simplicity and efficiency. Also, Chen (2003) presented three methods (Moerder and Calise's, Toivonen, Toivonen and Malika's algorithms) for calculating an initial guess for K that makes an unstable open-loop process model asymptotically stable. The method chosen in this methodology is the first method (Moerder and Calise's algorithm) because of its simplicity and efficiency. In this method random numbers, ranging between $\pm\alpha$, are generated for the elements of K until $A\text{-}BKC$ is asymptotically stable. α is a design parameter, and its value is given by users, with a default value of 1.0 [Chen 2003]. More details about whether the system can be stabilized or not, what the sufficient conditions are for global convergence, what the convergence properties are, and how the calculation of an initial stabilizing SOF controller K is done are presented in Chen (2003).

Tuning

In each stage a diagonal OSOFC is generated for each candidate. There are two possible ways to obtain the diagonal OSOFC [Chen, 2002]:

1) to force all the off-diagonal elements in the OSOFC to be 0 by using large g_{ij}'s that correspond with the off diagonal elements. The computation speed is much slower than using zero g_{ij}'s.

2) to generate a diagonal initial OSOFC and keep it diagonal while it is updated by solving the design equations. More details in this method and the algorithm can be found in Chen (2002).

In this methodology the second method is selected because it runs much faster and give the same results as the first method.

4.4. __Summary and Discussion__

In this section important aspects of the optimal control based approach for measurement and MVs for controlling key economic variables are discussed.

4.4.1.- Comparison between Optimal Control Approach with other Approaches

Comparing this method with the methods presented in the previous Chapters:

1) The optimal control based measurement selection approach extracts information from a linear time invariant (LTI) state space model. Therefore, there is more insight of the process in the sense of information about the dynamic of the process than the approaches that use steady state information [Moore (1992) and Tyreus (1999)].

2) This method is a plantwide measurement selection based approach instead of a unit operation based approach. This is an important fact because the plantwide approach finds the measurements and manipulated variables that have more effect in certain control objectives taking into account the interaction between unit operations. For instance, in general, when the units

are controlled alone they show good control performance but when all the unit operations are combined the interaction between variables causes an overall bad control performance.

3) The use of this method does not require an experienced control engineer because the amount of engineering judgment involved is limited, making this methodology very attractive.

4) This method represents a systematic way to determine measurements and manipulated variables that affect key economic variables in the plant.

5) The main difference between this methodology and other proposed ones [Chen et. al. (2002, 2003), McAvoy et. al. (1994), among others, is that, in this methodology, the key economic variables (production rate and product quality) are controlled by manipulating the important MVs in the plant, instead of using just one manipulated variable for each controlled variable. There are three main advantage of this approach: 1) It uses dynamic process information to select measurement for global plants which means that the interaction between units is considered; 2) It finds the best set of measurements and manipulated variables for specific control objectives and 3) Decentralized control structures can be generated to pair these variables. Then a MPC controller is built on top of them to control the production rate and product quality in the plant by adjusting their setpoints. In Chapter 5 and 6 this methodology is applied to the Tennessee Eastman Process and to the Vinyl Acetate process respectively.

4.4.2.- Effects on Scaling

Scaling is very important in many process control applications because it makes the controller design (weight selection) and the analysis of the results much simpler. There are few practical cases in which scaling does not affect the analysis of the results (for example, RGA analysis). However, whenever the results depend on scaling (for example: OSOFC results, SVD, etc.), it is very important to use the appropriate scaling. Mainly in the literature authors have used the maximum physical limits imposed by the process design for scaling measurements and manipulated variables. Another option is to use the operational range. The operational range for measurements is the allowed deviation value for each measurement while for the manipulated variables is the allowed magnitude of each input signal. In this research work, the scaling on the measurements is done according to their relative importance with respect to the control objective desired while the manipulated variables are scaled according to the physical limits obtained from the process design.

Chapter 5: Case Study: Tennessee Eastman Process

5.1. <u>Introduction</u>

For many years, researchers in plantwide control design have been using realistic process simulation to test new technologies and algorithms. This chapter presents the application of the optimal control-based approach for measurement selection to a well-known process, the Tennessee Eastman (TE) Challenge, in order to demonstrate the effectiveness of this method. This process consists of five operating units that involve the production of 2 products, G and H, from four reactants, A, D, E, and C. In addition, there is an inert B that enters with one of the feed streams, and two side reactions that occur. The exothermic irreversible reactions are:

$$A(g) + C(g) + D(g) \quad G(l) \qquad \text{Product 1} \tag{5.1}$$

$$A(g) + C(g) + E(g) \quad H(l) \qquad \text{Product 2} \tag{5.2}$$

$$A(g) + E(g) \quad F(l) \qquad \text{Byproduct} \tag{5.3}$$

$$3D(g) \quad 2F(l) \qquad \text{Byproduct} \tag{5.4}$$

The model of the process has 50 states, 12 manipulated variables, and 41 measurements. A schematic diagram of the plant is shown in Figure 5.1.

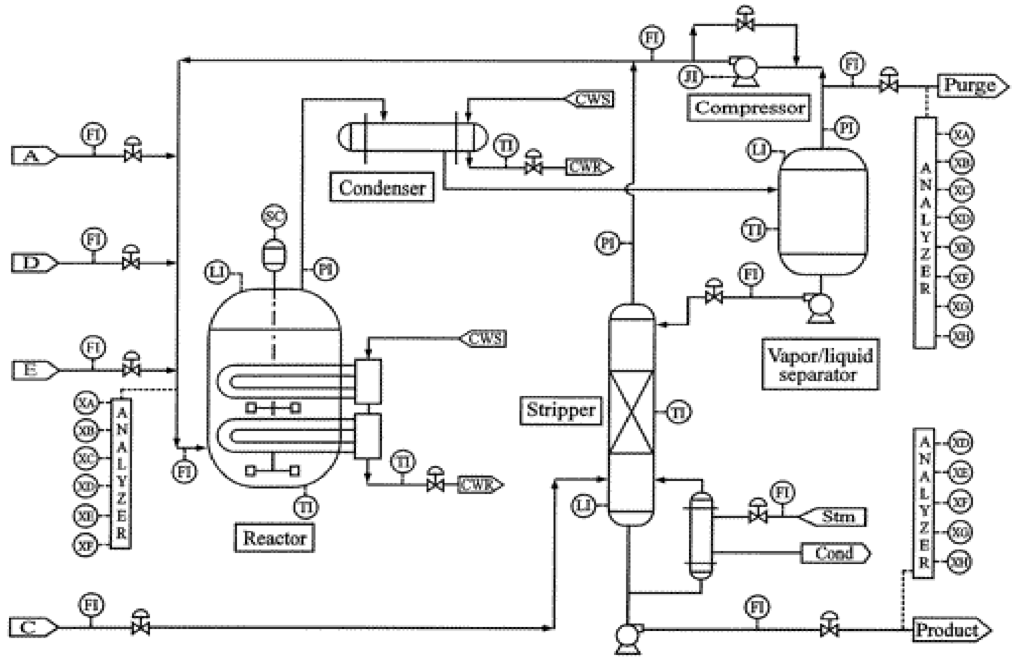


Figure 5.1 Tennessee Eastman Plant

Downs and Vogel (1993) provided 6 operating modes at three different G/H (Product 1/Product 2) mass ratios that are listed in Table 5.1

Table 5.1 Operational Modes for TE Process

Mode	G/H mass ratio	Production rate
1	50/50	7038 kg h-1 G and 7038 kg h-1 H
2	10/90	1408 kg h-1 G and 12669 kg h-1 H
3	90/10	10000 kg h-1 G and 1111 kg h-1 H
4	50/50	maximum production rate
5	10/90	maximum production rate
6	90/10	maximum production rate

In 1994, Ricker calculated the optimal steady states process values for each of the 6 operating modes. Ricker's results showed that the base case provided by Downs is far from optimal. A detailed description of the TE process, model formulations, physical property data, and steady state process values for each operating mode can be found in Downs and Vogel (1993), Ricker (1994), and Ricker and Lee (1995).

Different decentralized control structures for the TE process have been published during last decade. In 2002, Chen categorized these control structures and proposed a plantwide design methodology, based on optimal control that was tested on the TE process. The majority of the authors evaluated their control structures by their capability to reject the disturbances listed in Downs (1993), using nonlinear simulations. Other authors such as Tyreus (1999), Luyben (1996), and Ricker (1996) also evaluated the ability of their structures to move the process over wide areas of steady state operation. To do so, Tyreus (1999) and Luyben (1996) demonstrated that their control structures could achieve the maximum production rate for optimal mode 1. Ricker (1996) not only achieved the maximum production rate for mode 1 but also for operation modes 2 and 3. Tyreus (1999), Luyben (1996), and Ricker (1996) used process-oriented approaches, which are based on engineering experience and process insight to generate their control structures. Tyreus (1999) used thermodynamic analysis to identify the dominant variables that affect production rate and product quality in the plant. Then, he used these dominant variables to apply partial control to the Tennessee Eastman Process. On the other hand, Luyben (1996) used the general plantwide control procedure developed by Luyben et al. (1996) to generate a simple regulatory control structure for the TE process. More details on this procedure can be found in Luyben (1996). Ricker (1996) developed a plantwide control design procedure which relies on heuristics and insight into the process dynamics to assign the available degrees of freedom for control. Details on this design procedure are given in Ricker (1996). He generated a decentralized control structure for the TE Process. Results for Ricker's structure showed good performance for disturbance rejection, and the production rate could be maximized for any of the three operation modes.

In this chapter, the optimal control-based approach for measurement selection is applied to the TE process to generate plantwide control structures that are feasible for all the three optimal operation modes. These control structures should be able to reject disturbances and change the production rate to its maximum value for each operation mode as shown in Ricker (1994). The methodology used is based on optimal control theory and uses a linear dynamic model of the process in designing the planwide control structures. Because the nonlinear model (first-principle dynamic model) of the process is available, the linear models for each mode are obtained by numerically calculating the first order Taylor expansion coefficients of the nonlinear model. More details can be found in Chen (2002).

The optimal control-based approach for measurement selection consists of 6 stages. In Stage 1, the process model is scaled, the inner cascade loops are closed, and a correlation and a condition number analysis are carried out. In Stage 2, the variables related to safe process operation (safety variables) are identified, and control structures for these variables are generated. Chen (2002) used engineering judgment to identify the safety variables for the Tennessee Eastman Process. Then he used optimal control theory to identify control structures for these safety variables. The safety variables identified by Chen are used in Stage 2 of this work. In Stage 3, control structures for inventory variables (components) are designed. In Stage 4, important measurements and manipulated variables that affect production rate and product quality are identified. Then, control structures are designed to control the important measurements with the available manipulated variables. In Stage 5, control structures are designed for other variables related to individual unit operations using the available degrees of freedom. In Stage 6, a Model Predictive Controller (MPC) is designed in the top on the resulting control structure to manipulate the set point of these loops, in order to change the production rate and product quality.

The structure of this chapter is as follows: First, control structures are designed for the three operational modes. Then, an alternative method with economic considerations is applied and compared with the previous results. Next, the control structure design to improve purge control is presented. Finally, a discussion and comparison with other schemes is presented.

5.2. <u>Control Structure Design for the Three Operation Modes</u>

In some cases, a process should operate in different steady states (operation modes). This is the case for the TE process which has three operation modes. Some control structures may be feasible for one or more operation modes, but not for all of them. If the process needs to alternate (to be moved) frequently between the different operation modes, it is desirable to find a control structure that works in all the operation modes.

The objective in this section is to find control structures that are feasible for the three operation modes of the TE process. These control structures should be able to reject disturbances 1 and 2 (Downs, 1992) and to change the production rate to its maximum value for each mode (Ricker, 1994). The current methodology uses the linear dynamic model of the process to determine the control structure. Since the TE plant has three different linear models that describe the three operation modes, three control structures can be obtained. In order to find a single control structure that is feasible for all the operation modes, the following procedure is applied:

1) Find the control structure for each operation mode individually. This step not only gives the structure but also the tuning parameters for the controller.
2) If the control structure obtained for the each mode is the same, then trial and error is used to find a set of tuning parameters that works for the three operation modes.
3) If the control structure obtained is different for any operating mode, then the Multiple Steady State Operation Design Procedure, proposed by Chen et. al. (2003), is applied. The only limitation of this method is that if specific forcing is desired, then the forcing must have the same effect on each state for each operating mode.

In all the optimal operation modes in Ricker (1994), the agitator rate is fixed at its maximum speed, the gas recycle flow is fixed at its maximum value, and the steam flow is fixed at its minimum value. Therefore, there are nine manipulated variables available for control. However, Downs (1992) stated that the A,C, and D feed streams have frequency constraints. For these reason, it is not desirable to use these manipulated variables to control loops that require fast responses.

The main goal in this section is to generate control structures that improve the control performance of key economic variables in the plant, such as product rate and quality. The optimal control-based approach for measurement selection is used to generate the control structures. This methodology divides the design problem into 4 sub-problems, based on the control objectives: 1) controlling variables related to the safety operation of the process; 2) controlling the component balances; 3) controlling variables related to production rate and product quality; and 4) controlling unit operations with available degrees of freedom. The steps in this design procedure are as follows:

5.2.1. Preparation

This stage consists of three parts. First, the model is scaled. Then the inner cascade loops are closed. Finally, a steady state correlation analysis and a condition number analysis on the C matrix of the state space model are carried out.

a) Scaling the state space model is done, as explained in Chapter 4, using the following scaling factors:

-The measurements are scaled using the following scaling factors: 200 KPa for pressures; 30C for temperatures; 50% for levels; and steady state values for mass flow rates, volumetric flow rates, molar compositions and compressor work.

-The manipulated variables are scaled, using the measurement scaling factors because the inner loops are closed, and, therefore, the manipulated variables are the set points of the inner loops.

b) Closing the inner cascade loops eliminates 10 measurements, and the setpoints of the inner cascade loops become manipulated variables. Table 5.2 presents the measurements and manipulated variables available after closing the cascade loops. Ten proportional-only controllers were used for the inner cascade loops. The proportional gains used are given in Appendix IV.

Table 5.2 Measurements and Manipulated Variables after Closing Cascades Loops

# Measur.	Measurements	Manipulated Variables
1	Recycle Flow	D Feed Set Point
2	Reactor Feed	E Feed Set Point
3	Reactor Pressure	A Feed Set Point
4	Reactor Level	C Feed Set Point
5	Reactor Temperature	Purge Set Point
6	Separator Temp	Separator Exit Flow Set Point
7	Separator Level	Stipper Exit Flow Set Point
8	Separator Pressure	Product Flow Set Point
9	Stripper Level	Reactor Cooling Water Temp SP
10	Stripper Pressure	Condenser Cooling Water Temp SP
11	Stripper temperature	
12	Compressor work	
13-18	Reactor Feed Composition	
19-26	Purge Compositions	
27-31	Product Composition	

c) Steady state correlation and condition number analysis of C matrix:

Several simulations were conducted, and results show that the algorithm used to calculate the optimal static output feedback controller (OSOFC) did not converge or the calculation was very slow, whenever highly correlated variables were considered simultaneously. For this reason, a steady state correlation analysis is carried out to identify the variables that are highly correlated. The equations used for this analysis can be found in Appendix I. Results show that the following group of variables are highly correlated:

Group # 1: Reactor pressure, separator pressure, and stripper pressure

Group # 2: Composition of G and H in the purge

Group # 3: Reactor feed and recycle flow

Then, the condition number of the C matrix is calculated. The objective is to determine how the condition number of the C matrix is affected when highly correlated measurements are considered together. The measurements considered for this analysis are presented in Table 5.2. These measurements are divided into two groups:

1) Highly correlated measurements: reactor pressure, separator pressure, stripper pressure, composition of G in the purge, composition of H in the purge, reactor feed, and recycle flow.

2) Basic measurements (BM) all the measurements in Table 5.2 except for the highly correlated measurements. Table 5.3 shows the values of the condition number of the C matrix.

The results from Table 5.3 demonstrate that the condition number of the C matrix has a significant increase when two or more highly correlated variables are considered simultaneously.

Table 5.3 Condition Number of C Matrix

Measurements included	**CN of the C matrix**
BM + Reactor pressure	982.0030
BM + Reactor and separator pressure	1.6637e+004
BM + Reactor and stripper pressure	1.3718e+004
BM + Reactor, separator and stripper pressure	2.3442e+012
BM + Composition of G in the purge	9.0452e+004
BM + Composition of H in the purge	5.9808e+004
BM + Compositions of G and H in the purge	7.5591e+016
BM + Reactor feed	1.2037e+004
BM + Reactor feed and recycle flow	2.5037e+007

Because the algorithm to calculate the OSOF gain involves the inversion of the $C*S*C'$ matrix (discussed in Chapter 4 in section 4.3 Stage 1), it is recommended not to work with ill-conditioned systems to avoid convergence problems. Therefore, only one variable in each group of highly correlated variables is considered. Table 5.4 shows the available measurements and manipulated variables after eliminating the correlated measurements.

Table 5.4 Meas. and Manipulated Variables after eliminating the correlated Variables

# Measur	Measurements	Manipulated Variables
1	Reactor Feed Rate	D Feed Set Point
2	Reactor Pressure	E Feed Set Point
3	Reactor Level	A Feed Set Point
4	Reactor Temperature	C Feed Set Point
5	Separator Temp	Purge Set Point
6	Separator Level	Separator Exit Flow Set Point
7	Stripper Temperature	Separator Exit Flow Set Point
8	Stripper Level	Product Flow Set Point
9	Compressor work	Reactor Cooling Water Temp SP
10	Comp of A in Feed	Condenser Cooling Water Temp SP
11	Comp of B in Feed	
12	Comp of C in Feed	
13	Comp of D in Feed	
14	Comp of E in Feed	
15	Comp of F in Feed	
16	Comp of A in Purge	
17	Comp of B in Purge	
18	Comp of C in Purge	
19	Comp of D in Purge	
20	Comp of E in Purge	
21	Comp of F in Purge	
22	Comp of G in Purge	

5.2.2. Control Structure for Safety Variables

In this stage, the safety variables are identified and decentralized control structures candidates are generated. The safety variables are the variables related to safe process operation. These variables are those that have limits of operation and can cause the shutdown of the plant if they exceed some shutdown limit. Chen, (2002) used eigenvalue analysis, the process gain matrix, and engineering judgment to determine the safety variables in the plant. Moreover, Chen (2002) used an optimal control-based plantwide control design methodology to generate control structure candidates for the safety variables. Details on the identification of the safety variables and the generation of control structures candidates can be found in Chen (2002).

In this stage, the control structure candidates for controlling the safety variables proposed by Chen (2002) for the operational modes of the Tennessee Eastman process are used. Table 5.5 shows the control structures recommended by Chen (2002)

Table 5.5 Control Structures for Controlling the Safety Variables

Candidate	Reactor P	Reactor L	Reactor T	Separator L	Stripper L
1	Purge	E	RCT CW	Sep.Bottom	Str.Bottom
2	Purge	CON CW	RCT CW	Sep.Bottom	Str.Bottom
3	CON CW	E	RCT CW	Sep.Bottom	Str.Bottom
4	Purge	E	RCT CWT	Sep.Bottom	Str.Bottom
5	Purge	CON CW	RCT CWT	Sep.Bottom	Str.Bottom
6	CON CW	E	RCT CWT	Sep.Bottom	Str.Bottom
7	Purge	E		Sep.Bottom	Str.Bottom
8	Purge	CON CW		Sep.Bottom	Str.Bottom
9	CON CW	E		Sep.Bottom	Str.Bottom

In this work, only candidates 4, 5, 6, 7, 8, and 9 are considered for the following reason: Candidates 1, 2 and 3 are almost the same as candidates 4, 5 and 6 respectively. The difference between them is that in candidates 1, 2, and 3, the reactor temperature is controlled using the reactor cooling water valve, while in candidates 4, 5, and 6, a cascade configuration is used. In this configuration, the reactor temperature is controlled by manipulating the setpoint of the reactor cooling water temperature setpoint. In this work, candidates 1, 2, and 3 are not evaluated for the following reasons: 1) there is not a significant difference between candidates 1, 2, 3, and 4, 5, and 6 and 2) the reactor cooling water valve (RCT CW) is already used to control the reactor cooling water temperature (RCT CWT); therefore the RCT CW is not longer available.

In this section, candidate 4 is considered first. The same procedure is applied to the remaining candidates. Five proportional-only controllers are automatically tuned for candidate 4 using the tuning method proposed by Chen (2002). The tuning is obtained by calculating an optimal static output feedback (OSOF) controller that contains only diagonal terms. The only difference is that, in this work, the tuning is calculated for a different type of process forcing (disturbance rejection and setpoint change) while in Chen's, it is calculated for the generic forcing (initial states around unitary sphere, X=I). Averaging level control is used for the two integrating levels (separator and stripper levels). The gains for the averaging level controls are +1 or –1 (%/%), depending on the sign of the process gain. The proportional gains for these loops are given in Appendix IV. After the safety loops are closed, the measurements corresponding to these variables are no longer available as measurements. Instead, the setpoints of these loops become the new manipulated variables. This procedure drops the number of available measurements from 22 to 17.

5.2.3. Control Structure for Inventory Variables (Components)

It is well known that to satisfy the material balance in a plant, all the reactants fed into the system must be consumed in the reaction or leave the system as impurities in the product or purge streams. In the case of the inerts, they should also be removed from the process through the purge or product streams (Luyben,1992). In chemical plants, any imbalance in the number of moles of any reactant will cause an accumulation of the reactant that is in excess. For this reason, it is very important to control the inventory of components so that exactly the right amount of the reactants is fed in. There are three ways to avoid component accumulation: 1) limit the feed flow of reactants, 2) control their reaction or 3) adjust the product in the plant.

Downs (1992) has pointed out the importance of verifying if the control structure in use satisfies component balances. To do so, it is necessary to check, for each component, the specific mechanism or control loop that guarantees that there will be no accumulation of that chemical component. This procedure is called Downs Drill Analysis. Luyben (1992), recommended the use of this analysis for checking component balances in a control scheme. Chen (2002) used Downs Drill Analysis to identify the components that need to be controlled for his proposed control schemes. He explained that the inventory of components should be controlled unless they are self-regulating or made self-regulating by closing other loops. Chen analyzed reactants, inerts, and products. In this case, only the reactants, inerts, and byproducts are considered for the Downs Drill Analysis since products will be controlled in the next stage. The Downs Drill Analysis for reactants and purge components for candidate 4 is given in Table 5.6. The Downs Drill Analysis for the other candidates and operating modes can be seen in Appendix IV.

Table 5.6 Downs Drill Analysis

Candidate	**Component**	**Self-Reg**	**Why Self-Reg**	**Manipulated Var**	**Measurement**
Candidate 4	A (reactant)	No		A Feed	%A RCT Feed, %A Purge
	B (inert)	Yes	Purge-RCT P		
	C (reactant)	No		C Feed	%C RCT Feed,%C Purge
	D (reactant)	No		D Feed	%D RCT Feed,%D Purge
	E (reactant)	Yes	E Feed-RCT L		
	F (byproduct)	Yes	RCT CW-RCT T		

The second column of Table 5.6 tells if the component is self-regulating or not. If it is self-regulating, the third column shows which loop makes it self-regulating. For example, the component B is self-regulated because the purge is used to control the reactor pressure (RCT P). The fourth and fifth columns indicate the measurement and manipulated variables that can be used to control the inventory variables. From the Downs Drill Analysis for this control structure, components A, C, and D are left uncontrolled after stage 2 and they need to be controlled. The manipulated variables used for controlling the inventories of A, C, and D are their respective feeds (See Chen, 2002). There are two analyzers in the gas loop that can be used for measuring the inventories of A, C, and D. One is in the reactor feed, and the other is in the purge stream. In this case, the analyzer in the reactor feed is used because it is located closer to the manipulated variables. It should be pointed out that, even though A, C, and D feeds have frequency constraints, these feeds can be used to control the compositions of A, C, and D in the reactor feed without affecting upstream processes. In other words, there will be no aggressive changes in the A, C, and D feeds because of the following: 1) in general, loops that involve analyzers are slow because of delays in the measurements, and 2) no aggressive tuning parameters are being used. So far, candidate 4 contains 8 loops (5 safety variables, compositions of A, C, and D). Three proportional-only controllers are automatically tuned to control the inventory loops (%A in the reactor feed - A feed, %C in the reactor feed - C feed, and %D in the reactor feed - D feed). These loops are included into the model for use in later stages. The tuning method used is the same as the one used in stage 2. The proportional gains for these loops are given in Appendix IV.

5.2.4. Control Structure for Production Rate and Product Quality

In this stage, the optimal static output feedback controller (OSOFC) is calculated to determine the best set of measurements and manipulated variables that affect production rate and product quality. The idea is to control these variables to improve the control of the production rate and quality variables. At this point, the available measurements and manipulated variables are shown in Table 5.7.

Table 5.7 Measurements and Manp Variables after Closing the Safety and Inventory Variables

# Measur.	Measurements	Manipulated Variables
1	Reactor Feed	%A in Feed Set Point
2	Separator Temp	Reactor Pressure Set Point
3	Stripper temperature	%C in Feed Set Point
4	Compressor work	%D in Feed Set Point
5	Comp of B in Feed	Reactor Temperature Set Point
6	Comp of E in Feed	Cond Cooling Water Temp SP
7	Comp of F in Feed	Reactor Level Setpoint
8	Comp of B in Purge	Separator Level Set Point
9	Comp of E in Purge	Stripper Level Set Point
10	Comp of F in Purge	
11	Comp of G in Purge	

Then, an OSOFC is calculated, as discussed in Chapter 4, Section 4.2. The OSOFC is analogous to a process gain matrix and represents the dynamic information about process interaction. The control objective is to control the production rate and product quality. The following parameters are used for the calculation of the OSOFC:

1) $R = I$, this gives the same importance to all the manipulated variables.

2) $g_{ij}=0$. In setting g_{ij} equal 0 we do not solve for a specific SISO control structure.

3) Q is the weight matrix that can be used to define the desire control objective. All the elements of this matrix should be zero except for those that correspond with the variables associated with production rate and product quality.

To extract information about the important measurements and manipulated variables to control production rate and quality (control objective) from the OSOFC matrix, the absolute value of each element is considered. Since the process model has been scaled, the OSOFC matrix is dimensionless, and therefore it's elements can be compared to one another. Generally, an element with absolute value close to zero indicates a weak relationship between the manipulated variable and the measurement. The following rules of thumb are used:

5) The sum of the absolute value of the elements of each manipulated variables (element in each row) is calculated for each measurement (columns). This is called Σcol. The best measurements (strongest measurements) are the ones that have the largest values of Σcol.

6) The sum of the absolute value of the elements of each measurement (element in each column) is calculated for each manipulated variable (rows). This is called Σrow. The best manipulated variables (strongest manipulated variables) are the ones that have the largest values of Σrow.

Table 5.8 shows the OSOFC matrix. The numbers that are in bold case in Table 5.8, correspond to the strongest measurements and manipulated variables to control product rate and product quality. From Table 5.8, the strongest manipulated variables are reactor temperature, composition of D in the reactor feed, condenser cooling water temperature SP, composition of A in the reactor feed, reactor level, and composition of C in the reactor feed.

Table 5.8 OSOFC Matrix

Control Objective: to Control Product Rate and Quality

SP	RF	**SpT**	**StT**	CpW	BF	E F	F F	BP	EP	FP	**GP**	Σ*row*
%A	0.036	0.676	-0.185	0.043	-0.029	-0.022	-0.013	-0.019	0.006	-0.013	-0.211	**1.252**
RP	0.054	-0.514	0.028	0.021	0.023	0.011	0.012	-0.002	0.013	0.001	0.190	0.871
%C	0.026	0.571	-0.368	-0.011	-0.001	0.014	-0.000	-0.013	-0.017	-0.014	-0.176	**1.212**
%D	0.225	-2.839	0.236	0.211	0.045	-0.145	0.025	0.006	0.048	0.033	1.065	**4.876**
R T	-0.120	4.923	-0.822	0.087	-0.190	-0.147	-0.073	-0.057	0.034	-0.065	-1.579	**8.097**
CCW	-0.238	2.102	-0.353	-0.264	0.054	-0.049	0.047	-0.186	0.075	-0.096	-0.599	**4.065**
R L	-0.093	1.327	-0.197	-0.126	0.005	0.241	0.008	-0.002	0.002	-0.025	-0.503	**2.530**
S L	-0.101	0.237	0.070	-0.098	0.027	-0.030	-0.005	-0.047	0.043	-0.010	-0.183	0.851
St L	-0.011	-0.388	0.236	-0.002	0.016	-0.024	-0.002	-0.014	0.025	0.008	0.119	0.845
Σ*col*	0.905	**13.58**	**2.496**	0.863	0.390	0.681	0.185	0.346	0.263	0.265	**4.626**	

This result seems to be very reasonable, considering that throughput changes can be achieved only by altering, either directly or indirectly, conditions in the reactor. In addition, to obtain the composition of D as a dominant variable is reasonable, because it affects the rate of formation of component G, which is one of the control objectives.

The strongest measurements are separator temperature, composition of G in the purge, and stripper temperature. In this case only the separator temperature is considered as the important measurement for three reasons: 1) It has the largest value in Σcol which is more than twice the value of closest important measurement; 2) There is no need to control product G in the purge because it is going to be controlled in the product stream by adjusting the important manipulated variables; and 3) The manipulated variable that is most often used to control the stripper temperature, the steam flow, is fixed at its minimum value for all the optimal operating modes. The other manipulated variables are located too far to the stripper temperature or do not seem to have big effect in the stripper temperature.

Once these important variables are identified, the final objective is to build an MPC that will have two outputs (production rate and product quality) and several inputs (important manipulated variables in the plant). As can be seen in Table 5.8, this methodology, not only gives information about the important manipulated variables but also about the important measurements. Since only the manipulated variables will be used to build the MPC, control structures for the important measurements are determined, using the available manipulated variables. In this example, the separator temperature is a measurement and, therefore, cannot be manipulated. For this reason, decentralized control structures are generated for the separator temperature. Once the important measurements are closed, these loops become new manipulated variables, available for the MPC.

Control Structure for Important Measurement

In this stage, the control objective is to control the separator temperature. An OSOFC is calculated, using the separator temperature and all the manipulated variables. The following parameters are used for the calculation of the OSOFC:

1) $R = I$, this gives the same importance to all the manipulated variables.

2) $g_{ij} = 0$. In setting g_{ij} equal 0 we do not solve for a specific SISO control structure.

3) Q is the weight matrix that can be used to define the desired control objective. All the elements of this matrix should be zero, except the ones that correspond to the control objective (in this case, the separator temperature).

The OSOFC is given in Table 5.9

Table 5.9 Optimal Static Output Feedback Controller (OSOFC)

Man Var	**S T**
%A	-0.022
RP	-0.001
%C	-0.009
%D	0.007
RCT T SP	0.129
CCW SP	**0.512**
RCT L SP	0.009
Sep L SP	-0.004
Stp L SP	0.000

From Table 5.9, the best manipulated variable to control the separator temperature is the condenser cooling water setpoint (largest value in the column), followed by the reactor temperature setpoint. Controlling the separator temperature by manipulating the setpoint of the reactor temperature was proposed by Luyben (1999). Luyben explains that changes in the separator temperature affect the stripper. A low separator temperature drops too many light components into the stripper and, therefore, the product quality is affected. The tuning method used is the same as the one used in Stage 2. The proportional gain for this loop (separator temperature) is given in Appendix IV along with the proportional gains for the safety and inventory variables controllers. The separator temperature loop is included in the model for use in later stages.

After closing the important measurements, two possible alternatives are considered to build the MPC: 1) to use the manipulated variables generated by closing the important measurement loops first, and then to add the strongest manipulated variables, one at a time, and 2) to recalculate an OSOFC to check for any changes in the strongest manipulated variables, once the important measurements loops (in this case the separator temperature-condenser cooling water temperature) are closed. The second alternative is evaluated below. The OSOFC is calculated in the same way; the only difference is that, this time, the separator temperature set point is a manipulated variable and it replaces the condenser cooling water temperature set point (See underlined variables in Table 5.10). In addition, the separator temperature is removed from the set of measurements being evaluated. Table 5.10 shows the OSOFC results for this case.

Table 5.10 OSOFC Matrix

Control Objective: to Control Product Rate and Quality

SP	RF	**StT**	CpW	BF	E F	F F	BP	EP	FP	**GP**	Σ*row*
%A	0.071	-0.080	0.072	-0.050	0.014	-0.010	0.028	0.022	0.001	-0.070	**0.418**
RP	0.018	-0.065	0.008	0.024	0.007	0.014	-0.021	0.010	-0.011	0.053	0.231
%C	0.048	-0.263	0.044	-0.047	-0.004	-0.008	0.044	0.007	0.003	-0.084	**0.552**
%D	0.016	-0.301	0.047	0.083	-0.202	0.022	-0.136	-0.028	-0.032	0.375	**1.243**
R T	0.193	-0.017	0.321	-0.302	0.025	-0.089	0.255	0.051	0.066	-0.389	**1.709**
SepT	-0.171	-0.110	0.093	-0.054	-0.092	-0.003	0.006	0.066	-0.018	-0.297	**0.909**
R L	0.025	0.077	-0.018	-0.021	0.281	0.014	0.083	0.066	0.003	-0.197	**0.784**
S L	-0.092	0.127	-0.079	0.016	-0.040	-0.009	-0.037	0.058	-0.003	-0.135	**0.597**
St L	-0.038	0.205	-0.024	0.024	-0.031	-0.001	-0.029	0.015	0.001	0.020	0.388
Σ*col*	0.671	**1.246**	0.707	0.622	0.695	0.171	0.638	0.324	0.137	**1.620**	

As can be seen from comparing Tables 5.8 and 5.10, the order of importance for the manipulated variables and the measurements remains almost the same. However, the main differences are that now the separator level is in the fifth place of importance, and that %A and %C switched their order of importance. In this case, the separator level and stripper level are not considered for the following reasons: 1) These levels use averaging level control, and 2) These levels are affected by the separator temperature. Since the order of importance for measurements and manipulated variables is practically the same, the results from Table 5.10 regarding key manipulated variables and their order of importance are used in the next step.

Determination of Control Structure for controlling Production Rate and Product Quality

In this section, the objective is to identify how many and which manipulated variables should be used to control production rate and product quality. Because there is no rule to decide how many and which of these important manipulated variables should be used as inputs to the MPC, the strongest manipulated variables will be added, one at a time, in descending order of importance according to the Σrow value in Table 5.10. Every time a new manipulated variable is added, a new control system is generated, and each new control system is called a Candidate (See Table 5.11). Each candidate starts with the number of the base candidate (candidate for safety variables in Table 5.5) being evaluated, in this case, Candidate 4. Each candidate has two control variables or outputs (production rate and product quality) and a different number of manipulated variables or inputs. According to Table 5.10, the order in importance of the manipulated variables (from the strongest to the weakest) is as follows: separator temperature, composition of D in the reactor feed, separator temperature setpoint, reactor level, and composition of C and A in the reactor feed. Table 5.11 shows all the generated candidates.

Because building an MPC for each one of the generated candidates can be a very time consuming task, a multivariable OSOFC is used instead, as a quick screening tool, to have an initial idea about the numbers of important variables that should be used, and to eliminate candidates (manipulated variables) with poor performance. These linear simulations are used to obtain an initial insight about the resulting control structure. The resulting control structures are evaluated, using nonlinear process simulations and model predictive controller (MPC). The MPC and the multivariable OSOFC will have two outputs (production rate and product quality) and different inputs, depending on the candidate being evaluated. All the generated candidates are tested for a setpoint change of a 50% increase in the production rate, and to reject the first two process disturbances IDV(1) and IDV(2), in Downs (1993). These process disturbances are step upsets.

To compare the control performance of these candidates the following control objectives presented by Downs and Vogel (1992) are considered: 1) maintain the process variables at the desired values, 2) recover quickly and smoothly from disturbances, and 3) minimize the variability of production rate and product quality during disturbances. The Product variability (product flow and quality) should be less than ±5%. Transients' response characteristics, such as settling time and offset value for critical variables in the plant, as well as the integral of the absolute value for the error (IAE), are used as a measure of the candidates' performance. These critical variables in the plant are: some of the safety variables (reactor pressure, temperature, and level) and the economic variables in the plant (production rate and product quality) Production rate and product quality are considered critical variables because they are directly specified as control objectives by Downs and Vogel (1992). The safety variables are considered critical variables because they are directly related to safety and operational constraints. The separator level and the stripper level are not considered among the critical variables because they are averaging level control. Indirectly, the purge flow (another economic variable) is already taken into consideration because the purge flow is used to control the reactor pressure.

The offset value is calculated as the difference between the setpoint of a critical variable and the final steady state value reached by that particular variable after a disturbance or setpoint change. Then, the summation of the absolute value of the offset for the critical variables is calculated for disturbances IDV(1), IDV(2), and for setpoint changes, for each candidate. Because the offsets of different critical variables will be added together, these offset values are scaled by dividing them by the steady state values. In order to calculate the summation of the offset, the following weights are given to the critical variables: production rate: 0.25, product quality: 0.25, reactor temperature: 0.20, and reactor level: 0.20, reactor pressure: 0.1. These weights are chosen based on the control objectives of the plant and the operating cost function given by Downs and Vogel (1992). The summation of the offset values for each candidate is calculated as follows:

$$Offset\ Value_k = \sum_{j=1}^{3} \sum_{i=1}^{5} \alpha_* abs(critical\ variables\ offset(j,i)) \tag{5.5}$$

α: weights for the critical variables (0.25, 0.25, 0.20, 0.20, 0.10)

i: critical variables offsets: production rate, product quality, reactor temperature, reactor level and reactor pressure

j: Disturbances and setpoint change. *J*=1 IDV(1), *J*=2 IDV(2), and *J*=3 set point change

k: total offset value for each candidate *k*=1 to7.

As can be seen in Equation 5.5, the offset values per candidate are the summation of the offset for the all the critical variables for disturbances IDV(1), IDV(2) and the setpoint change.

The IAE is calculated, using Equation 5.6.

$$IAE \ for \ critical \ variables_k = \int_0^{\infty} \left[SP(t) - CV(t) \right] dt \tag{5.6}$$

The IAE for each candidate is calculated as follows

$$IAE = \sum_{j=1}^{3} \sum_{i=1}^{5} IAE \ for \ critical \ variables(j,i) \tag{5.7}$$

i: IAE for critical variables: production rate, product quality, reactor temperature, level, and pressure

j: Disturbances and setpoint change. *J*=1 IDV(1), *J*=2 IDV(2), and *J*=3 set point change.

k: total IAE for the critical variables for each candidate *k*=1 to7.

There are three conditions that a candidate has to pass in order to be considered: 1) to reject disturbances IDV(1), and IDV(2), 2) to increase production rate by 50% in less than five hours, and 3) to have less than ±5% product rate and product quality variability for disturbance rejections. As mentioned above, every time a new manipulated variable is added, its values for the summation of the offset and IAE are compared with the previous candidate to evaluate whether there is significant improvement or not. It can be said that there is significant improvement when:

- The percentage of change in the IAE with the addition of a new manipulated variable is greater than 5%. The percentage of change is calculated as the change between two consecutive candidates. If it is less than 5%, there might be no significant improvement. Therefore, the addition of a new manipulated variable will not give significant control benefits. However, since this just an initial screening tool if the % change is between 1 to 5% it might be checked with the nonlinear simulation, just to corroborate that the variable does not improve significantly the control performance.
- The total summation of the offset value decreases more than 5% between two consecutives candidates.

Transients of 6 measurements (production rate; product quality; purge flow; reactor pressure, level, and temperature) are calculated for each disturbance (IDV(1) and IDV(2)) and production rate set point change for 60 hours. Table 5.11 shows all the candidates generated, the controlled and manipulated variables for each candidate, the ability of each candidate to reject disturbances IDV(1) and IDV(2) and to achieve maximum production rate change in less than five hours. In addition, it shows the summation of the offset (see Eq 5.6), and the IAE values (see Eq 5.7) for the critical variables in the plant for each candidate. It also shows the percentage of change for the summation of the offset values and the IAE between consecutives candidates.

Table 5.11 Candidates for Alternative 1

Candidate number	**Controlled Variables**	**Manipulated Variables**	**Can maximize production rate and reject disturbances?**	**Summation offset values / % change btw candidates**	**IAE / % change btw candidates**
Candidate 4-1	Production rate Product Quality	**Reactor Temperature SP**	SP change No IDV(1) Yes IDV(2) Yes	0.0092	330.67
Candidate 4-2	Production rate Product Quality	Reactor Temperature SP **%D in Reactor Feed SP**	SP change No IDV(1) Yes IDV(2) Yes	0.0094 2.12	321.89 2.8
Candidate 4-3	Production rate Product Quality	Reactor Temperature SP %D in Reactor Feed SP **Sep Temp SP-CCWT**	SP change Yes IDV(1) Yes IDV(2) Yes	**0.0083** **13.25**	**291.29** 10.51
Candidate **4-4**	Production rate Product Quality	Reactor Temperature SP %D in Reactor Feed SP Sep Temp SP-CCWT **Reactor Level SP**	SP change Yes IDV(1) Yes IDV(2) Yes	**0.0072** **15.27**	**231.70** 25.71
Candidate 4-5	Production rate Product Quality	Reactor Temperature SP %D in Reactor Feed SP Sep Temp SP-CCWT Reactor Level SP **%C in Reactor Feed SP**	SP change Yes IDV(1) Yes IDV(2) Yes	0.0072 0	230.70 0.43
Candidate 4-6	Production rate Product Quality	Reactor Temperature SP %D in Reactor Feed SP Sep Temp SP-CCWT Reactor Level SP %C in Reactor Feed SP **%A in Reactor Feed SP**	SP change Yes IDV(1) Yes IDV(2) Yes	0.0071 1.40	229.17 0.67
Candidate 4-7	Production rate Product Quality	Reactor Temperature SP %D in Reactor Feed SP Sep Temp SP-CCWT Reactor Level SP %C in Reactor Feed SP %A in Reactor Feed SP **Reactor Pressure SP**	SP change Yes IDV(1) Yes IDV(2) Yes	0.0071 0	229.16 0.002

After running the linear simulations, using a multivariable OSOFC and evaluating the values for the summation of the offset, IAE for each candidate and their respective percentage of change, and the transient responses, the following statements can be made: 1) For disturbance IDV(1) and IDV(2): all the candidates are able to reject both disturbances. 2) Candidates 4.1 and 4.2, are not able to achieve maximum production rate. 3) For maximizing production rate: At least the setpoint of three loops need to be considered (reactor temperature, composition of D in the reactor feed, and separator temperature). 4) Candidates 4.3 to 4.7 are able to achieve maximum production rate in less than 5 hours. 5) It can be said that there is no significant improvement in the control performance after candidate 4.4, when the reactor level setpoint is added. Therefore, the addition of extra manipulated variables, after candidate 4.4, will not give control benefits. According to Table 5.10 the most important manipulated variables are reactor temperature SP, % D in feed, separator temperature SP, and reactor level. However, by evaluating the summation of the offset and the IAE and their respective %of change between candidates (see Table 5.11) it appears to be that reactor level is more important than separator temperature. These linear simulations are used to obtain an initial insight about the resulting control structure. Then, the resulting control structures are evaluated, using nonlinear process simulations and model predictive controller (MPC).

5.2.5. Control structure for individual unit operations using the available degrees of freedom.

So far, the only degrees of freedom that have not been used are the agitator speed, the recycle valve, and the stripper steam flow. The stripper steam can be used for unit operation control (control of the stripper temperature). However, as was mentioned at the beginning of this section, in all the optimal operation modes (Ricker, 1994) the agitator speed and the recycle valve are fixed at their maximum values, and the steam flow is fixed at its minimum value. Moreover, Ricker (1994) and Tyreus (1999) clearly state that the stripper temperature and the heat to the reboiler are not dominant variables and serve no purpose in a feedback control.

5.2.6. Control production rate and product quality, using MPC.

In this stage, a Model Predictive Controller (MPC) is built on the top of the resulting control structure. The main objective is to improve the control of the production rate and product quality by adjusting the setpoint of the important loops (i.e. the ones with the strongest manipulated variables) in the plant. The control structure implemented is the best control structure obtained in step 5.2.4, Candidate 4-4 from Table 5.11. The resulting control structure is implemented and its performance is studied using nonlinear process simulations. The controller tuning parameters used for these simulations were obtained from linear calculations. The first two process disturbances, IDV(1) and IDV(2), in Downs (1993), which are step upsets, and a 50% setpoint change in the production rate (maximize production rate for operating mode 1) are considered. Transients of 16 measurements (production rate; product quality; purge flow; reactor pressure, level, and temperature; separator level; stripper level; composition of A, B, C and D in the reactor feed; A feed; D feed; E feed; and C feed) are calculated for each disturbance (IDV(1) and IDV(2)) and production rate set point change for 60 hours. Since proportional gains are available from the design phase, nonlinear simulations using proportional-only controllers, are used to show the control performance of the resulting structure. However, for the final control structure, the one that is feasible for all the three operation modes, proportional-integral controllers will be used. As mentioned above, at least the setpoint of three loops (reactor temperature, composition of D in the reactor feed, and separator temperature) should be adjusted by the MPC in order to achieve the maximum production rate, while avoiding valve saturation and plant shutdown. There is improvement in the transients for production rate and product quality variables until candidate 4.4 (when the reactor level SP is added is added to the MPC inputs). The model predictive controller is build using the function scmpcnl in Matlab. This function designs an MPC controller for constrained problems and simulates closed loop systems with hard constraints. This MPC is tested using the nonlinear model simulations. In other words, the input values calculated by the MPC are fed continuously into the nonlinear simulation for the Tennessee Eastman Plant. The scmpcnl function uses the plant model in Simulink format.

The tuning parameters for the MPC are the following:

1) The control horizon (M). This is the number of control moves
2) Length of prediction horizon (P)
3) Penalty weighting for changes in manipulated variables (uwt)
4) Penalty weighting for setpoint tracking (ywt)

The MPC is tuned by trial and error using the following guidelines:

The control action becomes more aggressive when: P decreases, M increases, and uwt decreases. Even thought, this is a general trend, for some controllers the adjustment of P and M does not have significant effect in the control performance. In these cases, uwt is used as the main tuning parameter. In this work, the same weight (ywt) is given to both controlled variables (production rate and product quality). P and M are used to give an initial tuning while uwt is used to obtain a fine tuning. Different values of uwt are given to the manipulated variables depending on how fast these variables can be manipulated, and the desired control performance.

Figures 5.2, 5.3, show the nonlinear simulations for a 50% setpoint change in the production rate (maximum production rate for Candidate 4-4). Figure 5.2 shows transients of the 8 variables (product flow, product quality, purge flow, reactor pressure, reactor level, reactor temperature, separator level and stripper level. Figure 5.3 shows transients for 8 variables %A feed, %B feed, %C feed, %D feed, A feed, Dfeed, E feed and C feed. Figure 5.2 shows how the large and fast changes in the production rate are handled. It is worth noting that the production rate changes more than 50% in less than two hours. Although this is a big change, the proposed control structure can handle it without valve saturation and/or plant shutdown. An important consideration from the economic point of view is the amount of purge used. In this case, the purge flow is less than what Tyreus (1999) reported for his control scheme. Figure 5.2 shows the purge flow.

Figure 5.2 Maximum Production Rate for Operation Mode 1 (Candidate 4-4)

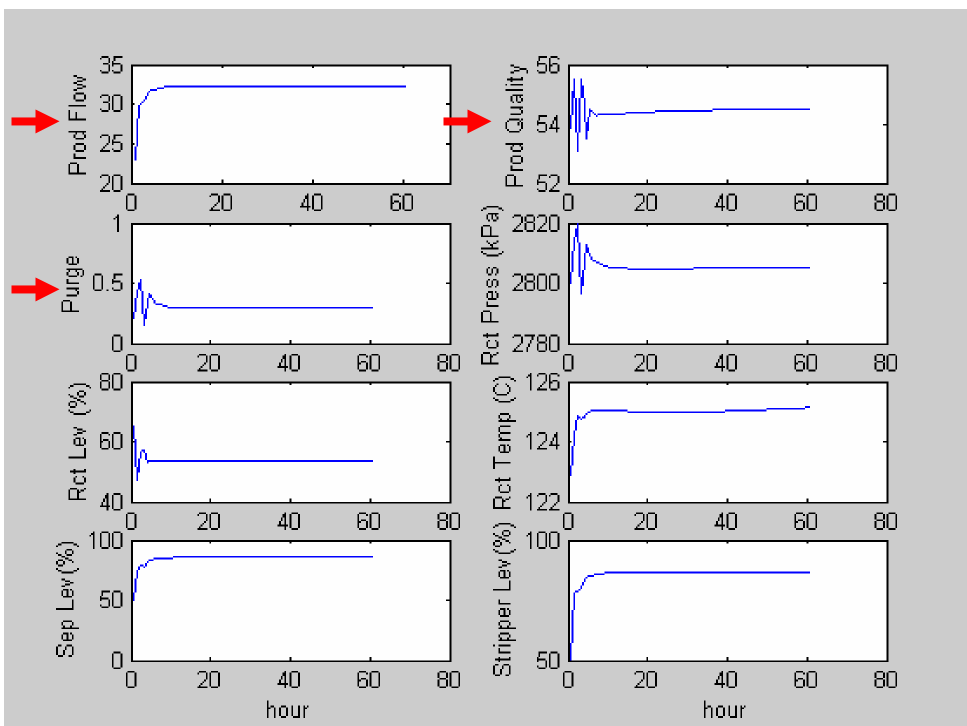


Figure 5.3 Maximum Production Rate (Candidate 4-4)

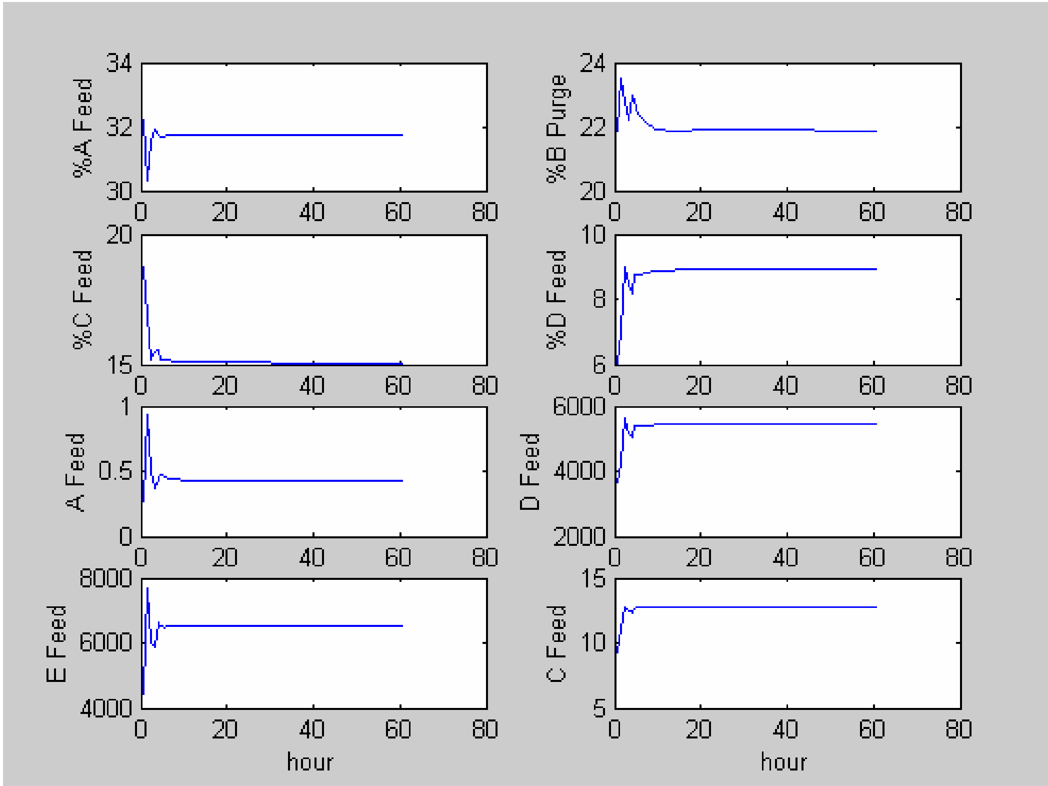


Figure 5.4 and 5.5 show the response of the proposed control scheme for IDV(1) a change in the composition of A, and C in the C feed stream. This figure shows that the control scheme can easily reject IDV(1). When the amount of A in the system decreases the A feed increases to counteract this fact.

Figure 5.4 IDV(1) for Operation Mode 1 (Candidate 4-4)

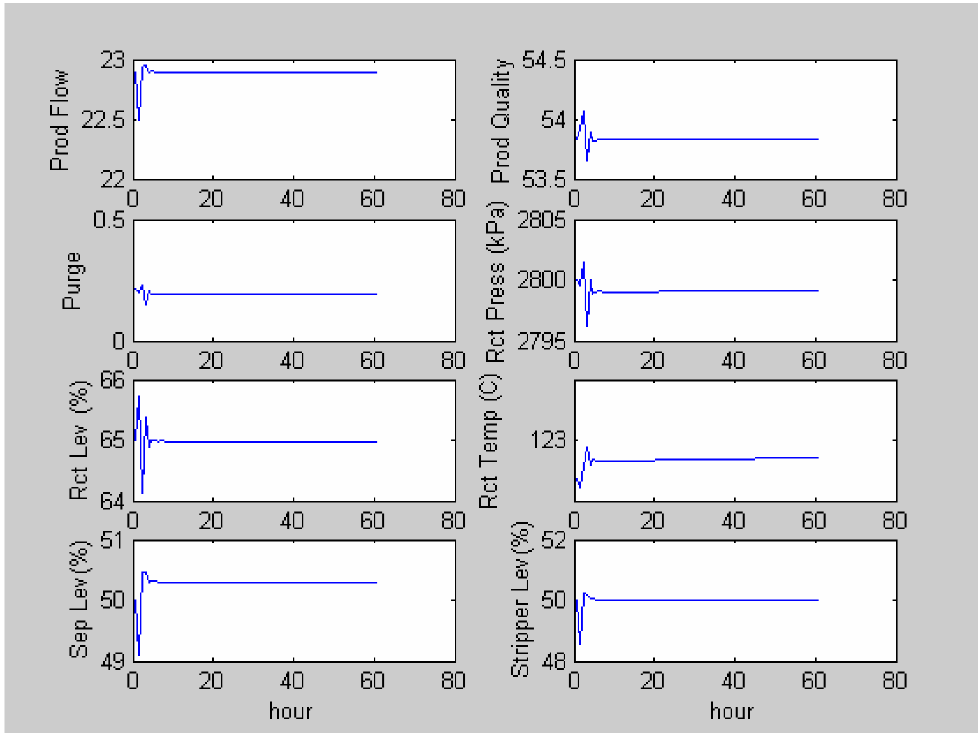


Figure 5.5 IDV(1) for Operation Mode 1 (Candidate 4-4)

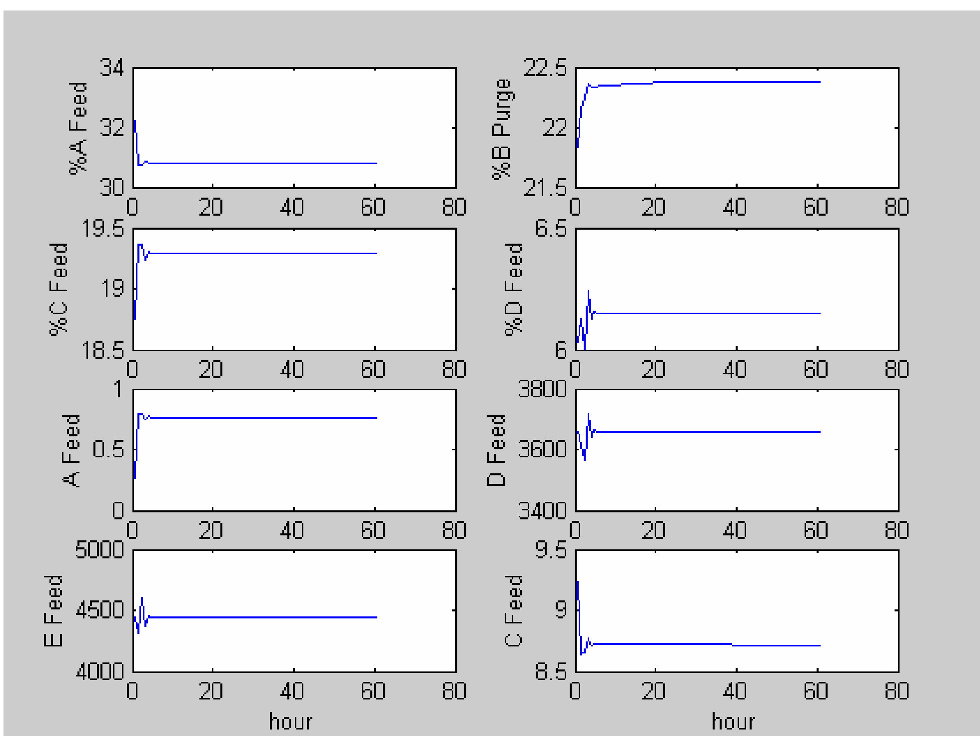


Figure 5.6 and 5.7 show the response of the proposed control scheme for IDV(2) a change in the composition of B in the C feed stream. This figure shows how the system opens the purge to control the amount of B (inert).

Figure 5.6 IDV(2) for Operation Mode 1 (Candidate 4-4)

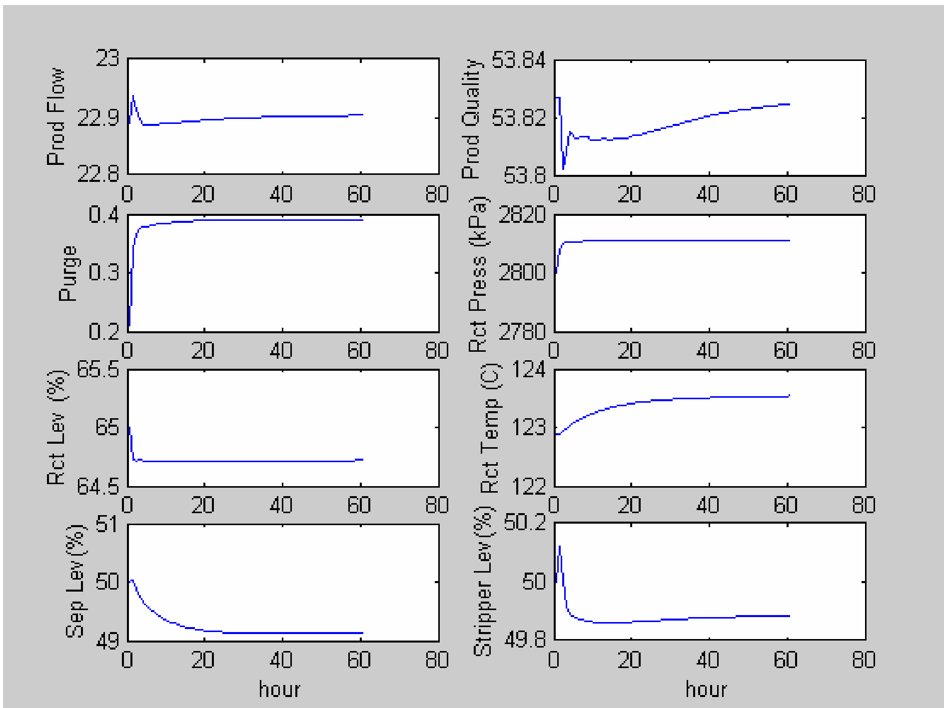
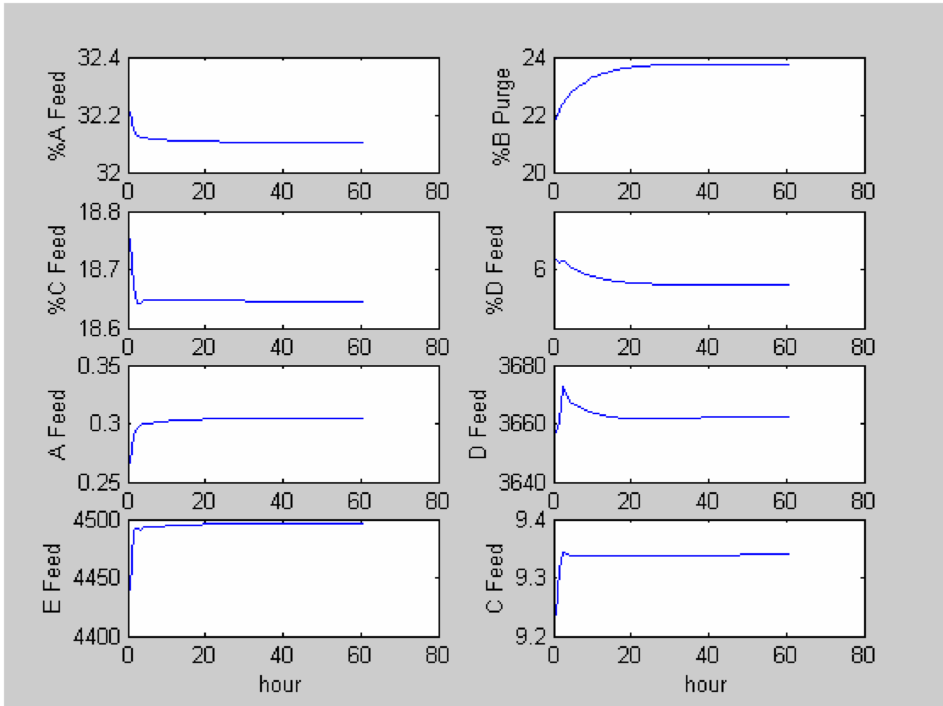


Figure 5.7 IDV(2) for Operation Mode 1 (Candidate 4-4)



Control Structure for Candidate 4 for Operation Modes 2 and 3

Since the TE process needs to operate in 3 different operation modes, it is desirable to determine a control structure that is feasible for each mode. So far, only candidate 4 (from Table 5.5) for operating mode 1 has been evaluated. To determine the control structure for the same candidate for operation modes 2 and 3, the same procedure is applied. Stages 1 (preparation), 2 (control structure for safety variables), and 3 (control structure for inventory variables) from the procedure are the same for each operation mode. Stage 4 (control structure for production rate and quality) is the key stage in determining the control structure because this stage is the one that gives information about the strongest measurements and manipulated variables to control production rate and product quality. If stage 4 gives the same strongest measurements and manipulated variables for operation modes 2 and 3 as the ones given in mode 1, then the same MPC design is used for these modes. Since there are three different set of tuning parameters (one for each mode), trial and error is used to find a single set of tuning parameters that works for the three operation modes.

In the case that a different set of strongest measurements and manipulated variables are obtained for any mode then, 1) the scaling factor should be evaluated since the OSOF solutions depends on how measurements, manipulated variables and states are scaled; and 2) the multiple steady state operation design procedure, proposed by Chen et. al. (2003), is applied.

Results for Candidate 4 for Operating modes 2 and 3 as well as the rest of the rest of the candidates in Table 5.5 with their respective operating modes (1, 2 and 3) are shown in Appendix IV

5.3. __Discussion and Comparison with Other Control Schemes__

During the last decade, several control structures were proposed for the TE process. The main differences among these control schemes are the ways in which the production rate (throughput), the reactor pressure, and the liquid levels are controlled. The majority of authors have focused on controlling production rate with one or more flow rates. For example, McAvoy and Ye (1994) use the flowrate of C feed as a throughput manipulator; Lyman and Georgakis (1995) recommended using the coolant rate for the condenser; Ricker (1996) uses all material streams in ratio to the product flow; Chen (2002) also uses C feed; and Luyben (1996) uses the product flow as the throughput manipulator. A different idea to control production rate, using the partial control idea was introduced by Tyreus (1999). He controls the production rate by manipulating the set point of reactor pressure, reactor temperature, and separator temperature. In the proposed control structure, the production rate is controlled by manipulating the setpoint of the reactor temperature, the separator temperature, the reactor level, and the compositions of D, C, and E in the reactor feed.

The plantwide design control problem is open-ended, which means there is no unique correct solution. A control structure is considered acceptable if it is able to achieve the desired control objectives. Because different control objectives lead to different control strategies, one of the most important steps in plantwide control design is to define the control objectives. For the TE process, Downs (1992) listed the following control objectives:

1) Maintain process variables at desired values.
2) Keep process operating conditions within equipments constraints.
3) Minimize variability of product rate and product quality during disturbances.
4) Minimize movement of valves which affect other processes (frequency constraints).
5) Recover quickly and smoothly from disturbances, production rate changes or product mix changes.

Several authors have proposed different control structures for the TE process. It seems that they had interpreted these control objectives in different ways and, therefore, they obtained different control structures. For example, McAvoy et. al.

(1994) consider all control objectives. However, it seems that their control structure attempts to reduce the variability of feed flows (objective 4). On the other hand, Luyben (1996) and Tyreus (1999) control objective is to achieve rapid changes in the production rate. These authors also considered all the control objectives presented in Downs (1992), except for objective 4 (Minimize movement of valves that affect other processes). Luyben (1996) and Tyreus (1999) ignore the frequency constraint on the C feed and used this valve to control reactor pressure, which is a fast loop. Ricker (1996) proposed a control structure that not only satisfies the control objectives (Downs, 1992), but also attempts to satisfy economic objectives. He also demonstrated through nonlinear simulations that his control structure could achieve the maximum production rate and could work for all operation modes. Although the change in production rate is not as fast as Luyben's, Tyreus, or the proposed control structure, Ricker ramped the SP, which is more like what actually happens in real processes. The majority of the investigators have not demonstrated how to maximize production rate with their control schemes.

One of the most important factors that should be considered when comparing control structures is the economic benefit obtained by using any given control structure. In this section, some of control structures proposed in the literature for the TE problem are compared to the proposed control structure in this work, from the economic point of view. To do so, the objective function given by Downs and Vogel (1992) and based on operating cost, is used. The operating costs for the TE process are mainly determined by the loss of raw materials through the purge stream and the product stream, and by means of the two side reactions. Costs of the compressor work and stripper steam costs are also included. The objective function is as follows:

Total operating cost at base case:

Total Costs = (Purge Cost)(Purge Rate) + (Product Stream Cost)(Product Rate) + (Compressor Costs) (Compressor Work) + (Steam Costs)(Steam Rate)

Where:

Purge Costs = 7.5973 $/Kgmol

Product Stream Costs = 0.1434 $/Kgmol

Compressor Costs = 0.0536 $/kWh

Steam Costs = 0.0318 $/Kg

The larger cost for the base operating mode [Downs and Vogel, 1992] is caused by purge losses, followed by the product stream losses. The purge losses cost represents 67% of the total cost, while the product losses cost represents 17%. It is obvious that a control strategy that reduces the purge losses is translated into economic benefits. Therefore, in order to evaluate the economic benefits for using any given control structure for the TE plant, their respective purge losses costs are calculated and compared. These purge losses are calculated by using steady date information of the purge rate and compositions for the control schemes where the data is available.

Comparison with Tyreus's Control

The proposed control structure in this research and Tyreus's control structure are able to achieve the desired change in production rate. However, from the economic point of view, the control scheme proposed in this work has better performance than Tyreus' scheme. The control scheme proposed allows working with a larger amount of component B in the purge (21%) than Tyreus' scheme (15%). Therefore, the amount of purge (0.3 kscmh) in the proposed scheme is less than the amount of purge (0.5 kscmh) in Tyreus' control scheme. By using the proposed control scheme the purge losses cost is reduce by 68 $/h, which is about more than half a million dollars a year. Some limitations with Tyreus' control structure for the Tennessee Eastman plant are the following:

1) His control structure is difficult to apply in a real process since the final product flow controller requires changing 4 setpoints (3 dominant variables and %B purge) simultaneously. Also, the values of these setpoints should be calculated continuously in order to change the product rate.
2) Tyreus' control structure ignores the frequency constraints on the C, D, and A feeds.
3) Negative RGA pairing results from his structure.
4) Tyreus did not demonstrate that his control structure is able to work for all operating modes for the TE process.

Comparison with Luyben's Control Structure

Luyben used common heuristics to determine a decentralized control structure for the TE plant. He demonstrated through nonlinear simulations that his control structure is able to do the following: 1) to decrease the production rate of the plant in 50% almost immediately, and 2) to reject disturbance 1 (change in the C Feed composition). A direct comparison between the proposed control structure (optimal control-based control structure) and Luyben's control structure cannot be made because Luyben applied his control structure to the base case (Downs 1992), while the proposed control structure is applied to the optimal operating modes (Rickers 1994). However, it should be pointed out that the main limitation with Luyben's control structure is that he ignored frequency constraints by using C Feed to control reactor pressure. Therefore, he did not consider one of the control objectives stated in Downs (1992): "Minimize the movement of valves which affect other processes." Also, Luyben did not demonstrate that his control structure is able to work for all operating modes for the TE process.

Comparison with Chen's Control Structure

Even thought the methodology presented in this work has a lot of similarities with Chen's proposed methodology, it can be said that this methodology gives better control results that Chen's methodology. The reason is that, this methodology, is not only is able to reject disturbances as Chen's, but also to increase the production rate by 50% in less than 5 hours while decreasing the purge flow. Chen's methodology is not able to have such a large change in the production rate. In addition, this methodology is tested using the nonlinear model for the Tennessee Eastman Plant, while Chen's only uses the linear model of the plant.

Comparison with Ricker's Control

Ricker proposed one of the best control structures for the TE process, considering that his structure satisfies all the control objectives presented in Downs (1992). In his design methodology, Ricker, explained very clearly how to: determine the degrees of freedom in the process, select variables that must be controlled, set production rate, and decide what to do with the remaining degrees of freedom. When comparing Ricker's control structure with the proposed one, it should be pointed out that both structures are able to reject disturbances and maximize production rate for all operating modes in the plant with similar results in control performance.

From the results of the linear and nonlinear simulations it can be said that the most important variables in the plant to control production rate and product quality are: reactor temperature, composition of D in the reactor feed, separator temperature setpoint, and reactor level setpoint. The proposed methodology has proven to be a reliable method to determine the key manipulated variables and measurements in the plant. In addition, it can be said that the resulting control strategy gives better control results than Chen's and Tyreus' and similar results to Ricker's control structure.

Chapter 6: Case Study: Vinyl Acetate Process

6.1. <u>Introduction</u>

For many years, academic researchers in process design, control, and related areas have been interested in industrial examples of realistic processes that can be used in developing and testing new technologies. These processes should have a realistically large process flowsheet containing standard chemical unit operations, and typical industrial characteristics of recycle streams and energy integration [Luyben et. al., 1998]. One process with these characteristics is the Tennessee Eastman Process [Downs et. al., 1993]. This process (presented in Chapter 5) has been highly used by researchers in the process control field to test their ideas and technical developments. In fact, many publications have appeared about the Tennessee Eastman Process. Because of the continuous interest among researchers to have additional industrial examples of realistic processes, Luyben et al. (1998) presented design details of an industrial process for the production of vinyl acetate monomer (the Vinyl Acetate process). This process has a flowsheet with the typical unit operations in chemical plants. In contrast with the Tennessee Eastman Process, the Vinyl Acetate Process has real components and two recycle streams (gas and liquid) that make the problem more realistic. On the other hand, unlike Downs et al. (1993), Luyben et. al. (1998) does not make available any code to simulate the Vinyl Acetate (VA) Process. A nonlinear dynamic model for the VA Process was developed by Luyben and Tyreus in TMODS, which is a Dupont in-house process simulation software system. Because

TMODS is not accessible for the public use, a first principle model has been developed by Chen et al. (2001). The code for this model can be downloaded from the Internet [Chen et. al., 2003].

This chapter presents the application of the optimal control-based approach for measurement and manipulated variables selection to the Vinyl Acetate (VA) Process. This process consists of 10 basic unit operations: a vaporizer, a catalytic plug-flow reactor, a feed-effluent heat exchanger (FEHE), a separator, a gas compressor, an absorber, a carbon dioxide (CO_2) removal system, a gas removal system, a tank for the liquid recycle stream, and an azeotropic distillation column with a decanter. The flowsheet for the Vinyl Acetate (VA) process is shown in Figure 6.1.

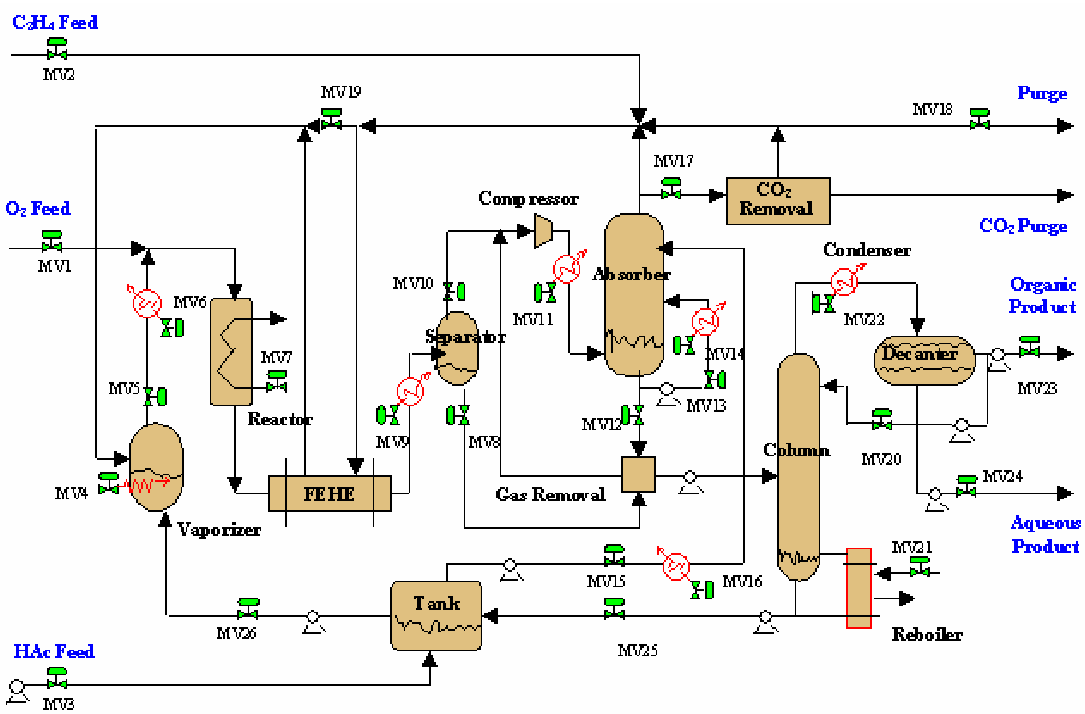


Figure 6.1 The Vinyl Acetate Process

There are seven chemical components in this process. Three reactants, Ethylene (C_2H_4), oxygen (O_2), and acetic acid (HAc), react to produce vinyl acetate product (VAc), and two byproducts (water (H_2O) and carbon dioxide (CO_2)). There is an inert component, ethane (C_2H_6) that enters with the fresh ethylene feed. The reactions that take place in the reactor are:

$$C_2H_4 + CH_3COOH + 1/2O_2 \rightarrow CH_2 = CHOCOCH_3 \tag{6.1}$$

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \tag{6.2}$$

More details for this process can be found in Chen et. al., (2003) and Luyben et. al., (1998). The model of this process has 246 states, 26 manipulated variables and 43 measurements.

At present, there are four decentralized control structures available for the VA Process. Luyben (1998) proposed the first control structure based on engineering experience and process insight. In 2003, Chen et al., proposed four control structures, by using their plantwide control design methodology that is based on optimal control. One of the control structures proposed by Chen is exactly the same control structure proposed by Luyben et al. (1998). These authors evaluated their control structures by their capability to reject process disturbances and to change setpoints. Luyben et al., tested his proposed control structure for: 1) 8^{o}C decrease in the reactor temperature, 2) 6^{o}C increase in the reactor temperature, 3) 10^{o}C decrease in the reactor temperature, 4) 5 minutes shutoff of column feed, 5) 20% increase in acetic acid recycle flow, and 6) increase in the column base water composition from 9 to 18%, while Chen et al. [Chen et al. 2003], tested for the 1^{o}C reactor outlet temperature setpoint change. In addition, the control system must be able to change the production rate (as measure by steady organic flow from the decanter) by at least 20% (up or down) in a period of six hours [Luyben and Tyreus, 1998]. This is because of limits on tank storage. It is important to mention that neither Chen et al. (2003) nor Luyben et al. (1998) have demonstrated that their control schemes are able to make this change in the production rate.

In this work, two additional process disturbances are considered: 1) step change in the composition of ethane in the fresh ethylene feed stream from 0.001 to 0.003 mol fraction, and 2) 0.0003 mol fraction of water (impurity) in the fresh acetic acid feed stream. The last disturbance is generated for this work in order to have another possible disturbance scenario for testing the methodology proposed for specific disturbance rejection and setpoint changes. There are two key safety constraints that must be considered: 1) the oxygen composition must not exceed 8 mol % anywhere in the gas recycle loop to remain outside the explosivity envelope of ethylene, and 2) the pressure in the gas recycle loop and distillation column cannot exceed 140 psia. There are other operational constraints that should be considered, such as:

1) the peak reactor temperature along the length of the tube must remain bellow 200^{o}C, otherwise mechanical damage occurs to the catalyst requiring shutdown.

2) liquid levels in the vaporizer, separator, absorber base, distillation column base, and decanter must operate within the limits of 10-90%.

3) reactor inlet temperature must exceed 130^{o}C to prevent condensation of liquid in the reactor.

4) the hot side exit temperature from the feed-effluent heat exchanger (FEHE) must remain above 130^{o}C to avoid condensation in the exchanger, which has been design to handle only vapor-phase flow.

5) the acetic acid in the decanter organic phase in the distillation column must not exceed 600 mol/million to prevent product contamination.

6) the vinyl acetate composition in the in the bottoms stream must remain bellow 100 mol/million to minimize polymerization and fouling in the column reboiler and vaporizer.

In this Chapter, the optimal control-based approach for measurement and manipulated variable selection is applied to the VA Process in order to generate control structures that are able to reject process disturbances and to make rapid and large changes in the production rate. As presented in Chapter 4, this methodology is based on optimal control theory and requires a linear dynamic model of the process. Because only the nonlinear model of the process is available, the linear model is obtained by numerically calculating the first order Taylor expansion coefficients of the nonlinear model [Chen, 2002]. This methodology divides the design problem into 4 sub-problems, based on the control objectives: 1) controlling variables related to the safety operation of the process; 2) controlling the component balances; 3) controlling variables related to production rate and product quality; and 4) controlling unit operations with available degrees of freedom. The structure of this chapter is as follows: the control structures are designed for the VA process and a discussion and comparison with other schemes proposed for the VA process are presented.

6.2. Control Structure Design for Vinyl Acetate Process

The main goal in this section is to generate control structures that improve the control performance of key economic variables in the plant. The optimal control-based approach for measurement and manipulated variable selection method is used to generate the control structures. This methodology consists of 6 stages. In Stage 1, the process model is scaled, the inner cascade loops are closed, and a correlation and a condition number analysis are carried out. In Stage 2, the variables related to safe process operation (safety variables) are identified, and control structures for these variables are generated. Chen (2003) used optimal control theory to identify the safety variables for the Vinyl Acetate Plant(VAP) and to generate control structures for controlling these variables. These results are used in this stage. In Stage 3, control structures for inventory variables (components) are designed. In Stage 4, important measurements and manipulated variables that affect production rate and product quality are identified. Then, control structures are designed to pair the important measurements with the available manipulated variables. In Stage 5, control structures are designed for other variables related to individual unit operations using the available degrees of freedom. In Stage 6, a Model Predictive Controller (MPC) is designed in the top of the resulting control structure to manipulate the set point of these loops, in order to change the production rate and product quality.

6.2.1. Preparation

a) Scaling the state space model is done using the following scaling factors:

- The measurements are scaled using the following scaling factor:

Pressures: 10 psia

Temperatures: minimum value between 40 C and the steady state value of the variable being scaled

Levels: 50%

Molar Flows: steady state values

Molar fraction: 20% of the steady state value if the molar fraction is greater than 0.04 otherwise, the steady state value composition is used

- The manipulated variables are scaled using their full range given in Chen (2003) and Luyben (1996). In the case of the cascade loops, these variables are scaled using the measurement scaling factors because the inner loops are closed and, therefore, the manipulated variables become the setpoints of the inner cascade loops.

b) Closing the inner cascade loops eliminated three measurements. Then the setpoints of these loops become manipulated variables for later stages. Three proportional-only controllers were used for the inner cascade loops. The proportional gains for these loops are given in Appendix V. Table 6.1 shows the inner cascade loops.

Table 6.1 Cascade Loops

Measurements	Manipulated Variables
Compressor Exit Temperature	Compressor Heater Duty
Circulation Cooler Exit Temperature	Circulation Cooler Duty
Scrub Cooler Exit Temperature	Scrubber Cooler Duty

c) Steady state correlation and condition number analysis of the C matrix are performed to identify the variables that are correlated. The reason for doing this analysis is because, after conducting several simulations, results show that the algorithm used to calculate the optimal static output feedback controller (OSOFC) did not converge, or the calculation was very slow when highly correlated variables were considered simultaneously. This happens because the algorithm used to calculate the OSOF gain involves the inversion of the $C*S*C'$ matrix (discussed in Chapter 4 in section 4.3). Therefore, in order to avoid convergence problems, it is not recommended to use ill-conditioned systems. One way to avoid having ill-conditioned systems is by eliminating variables that are highly correlated. Therefore, a correlating analysis is performed on the gain matrix to identify variables that are correlated. The equations used for the correlation analysis can be found in Appendix I. The measurements considered for this analysis are listed in Table 6.2. These measurements include all the available measurements except for the measurements used to close the cascade loops (Table 6.1).

Table 6.2 Available Measurements and Manipulated Variables

1	Vaporizer Pressure	(1)	Fresh O_2 Feed
2	Vaporizer Level	(2)	Fresh C_2H_4 Feed
3	Vaporizer Temperature	(3)	Fresh HAc Feed
4	Heater Exit Temperature	(4)	Vaporizer Steam Duty
5	Reactor Exit Temperature	(5)	Vaporizer Vapor Exit
6	Reactor Exit Flowrate	(6)	Vaporizer Heater Duty
7	FEHE Cold Exit Temperature	(7)	Reactor Shell Temperature
8	FEHE Hot Exit Temperature	(8)	Separator Liquid Exit
9	Separator Level	(9)	Separator Preheater Temperature
10	Separator Temperature	(10)	Separator Vapor Exit
11	Absorber Pressure	(12)	Compressor Exit Temp Set Point
12	Absorber Level	(13)	Absorber Liquid Exit
13	Gas Recycle Flowrate	(16)	Absorber Circulation Flow
14	Organic Product Flowrate	(17)	Circulation Cooler Exit Temp Set Point
15	Decanter Level (Organic)	(18)	Absorber Scrub Flow
16	Decanter Level (Aqueous)	(19)	Scrub Cooler Exit Temp Set Point
17	Decanter Temperature	(20)	CO_2 Removal Inlet
18	Column Bottom Level	(21)	Purge
19	Tray 5 Temperature	(22)	FEHE Bypass Ratio
20	HAc Tank Level	(23)	Column Reflux
21	VAc Organic Product Comp	(24)	Column Reboiler Duty
22	H_2O Organic Product Comp	(25)	Column Condenser Duty
23	HAc Organic Product Comp	(26)	Column Organic Exit
24	VAc Column Bottom Comp	(27)	Column Aqueous Exit
25	H_2O Column Bottom Comp	(28)	Column Bottom Exit
26	HAc Column Bottom Comp	(29)	Vaporizer Liquid Exit
27	O_2 Gas Recycle Comp	(30)	
28	CO_2 Gas Recycle Comp	(31)	
29	C_2H_4 Gas Recycle Comp	(32)	
30	C_2H_6 Gas Recycle Comp	(33)	
31	VAc Gas Recycle Comp	(34)	
32	H_2O Gas Recycle Comp	(35)	
33	HAc Gas Recycle Comp	(36)	
34	O_2 Reactor Feed Comp	(37)	
35	CO_2 Reactor Feed Comp	(38)	
36	C_2H_4 Reactor Feed Comp	(39)	
37	C_2H_6 Reactor Feed Comp	(40)	
38	VAc Reactor Feed Comp	(41)	
39	H_2O Reactor Feed Comp	(42)	
40	HAc Reactor Feed Comp	(43)	

The correlation analysis shows that the following groups of variables are correlated:

Group 1: Vaporizer Pressure and Absorber Pressure

Tray 5 Temperature, VAc, H2O, and HAc Column Bottom Composition, H2O Gas Recycle, VAc Gas Recycle, H2O Reactor Feed, HAc Reactor Feed,

Group 2: O_2 Gas Recycle Composition and O_2 Reactor Feed Composition

C_2H_6 Gas Recycle Composition and C_2H_6 Reactor Feed Composition

VAc Gas Recycle Composition and VAc Reactor Feed Composition

C_2H_4 Gas Recycle Composition and C_2H_4 Reactor Feed Composition

CO_2 Gas Recycle Composition and CO_2 Reactor Feed Composition

Group 3: VAc Gas Recycle Composition, HAc Gas Recycle Composition, VAc Reactor Feed

Group 4: Reactor Exit Flow, Organic Product Flowrate

Results from the correlation analysis show that there are several variables that are correlated. One alternative would be to consider only one variable from each group and to eliminate the rest of them. However, at this point, it is not obvious which variables from each group should be eliminated. The reason is that some of these variables might be required in later stages. In addition, it is important to point out that the correlation analysis is performed using steady state information (the gain matrix), which means it does not consider the process dynamics. Therefore, even though two variables seem correlated if there is a significant delay between them, they can be controlled simultaneously. A condition number analysis on the C matrix (CN-C) is performed to determine which of the correlated measurements have the greatest effect on the condition number. The measurements considered for this analysis are presented in Table 6.2. The condition number of the C matrix that includes all the measurements in Table 6.2 is calculated and is called CN-AM (condition number of all measurements). Then, correlated variables from each group are eliminated, one at a time, to determine their effect on the condition number.

Table 6.3 shows the values of the condition number of the C matrix.

Table 6.3 Condition Number of C Matrix

Measurements included	CN of the C matrix
CN-AM	1.3033e+018
CN-AM - HAc Column Bottom Composition HAc Gas Recycle Composition H2O Reactor Feed Composition HAc Reactor Feed Composition Organic Product Flowrate	2.0554e+004

The results from Table 6.3 show that the condition number of the C matrix has a significant decrease when the highly correlated variables (HAc column bottom composition, HAc gas recycle composition, H2O reactor feed composition, and HAc reactor feed composition, and organic product flowrate) are considered simultaneously. The rest of the correlated variables did not produce a large change in the condition number when they were eliminated. Therefore, they remain in the group of available measurements because they can be used in later stages

6.2.2. Control Structure for Safety Variables

The objective in this stage is to identify the safety variables and to generate decentralized control structures to control them. The safety variables are the variables that have hard constraints. This means that they have limits of operation that can cause the shutdown of the plant if they exceed these limits. Also, the integrating variables and the variables that can cause instability are identified in this stage. Chen (2002) identified the safety, integrating variables and the variables that cause instability for the VA Plant by using the process gain matrix, eigenvalue analysis, and engineering judgment. In addition, he used an optimal control-based plantwide control design methodology that involves the calculation of an OSOF and a sensitivity matrix to generate control structures for these variables. More details for these procedures can be found in Chen (2002). Results from Chen's analysis show that the VA plant does not have process instabilities (the overall model does not have positive eigenvalues). The integrating variables for this process are the seven levels, the tray 5 temperature, and the bottom composition of VAc. In his work, Chen found that controlling the tray 5 temperature results in both of these variables being controlled (tray 5 temperature and bottom composition of VAc). The correlation analysis results show that these two variables are correlated. Finally, the safety variables identified by Chen (2002) according to Luyben et al. process constraints are: % O_2 in the reactor inlet stream, vaporizer pressure, absorber pressure, heater exit temperature, reactor exit temperature, and FEHE exit temperature. Then, the OSOFC and the sensitivity matrix are calculated in order to determine control structures for the safety variables. In this stage, the OSOFC is calculated for a specific type of process forcing (disturbance rejection and setpoint change) while in Chen's, it is calculated for the generic forcing (initial states around unitary sphere, X=I). A more detailed explanation can be found in Chapter 4. The control structure candidates obtained using this method are similar to the ones obtained by Chen (2002). Table 6.4 shows the control structures for the safety variables for the Vinyl Acetate Process.

Table 6.4 Control Structures for Controlling the Safety and Integrating Variables

	Candidates			
Variables	**1**	**3**	**7**	**9**
Vaporizer level	Vap steam duty	Vap steam duty	Vap liquid inlet	Vap liquid inlet
Separator level	Sep liquid exit	Sep liquid exit	Sep liquid exit	Sep liquid exit
Absorber level	Abs liquid exit	Abs liquid exit	Abs liquid exit	Abs liquid exit
Organic level	Col organic exit	Col organic exit	Col organic exit	Col organic exit
Aqueous level	Col aqueous exit	Col aqueous exit	Col aqueous exit	Col aqueous exit
Column base level	Col bottom exit	Col bottom exit	Col bottom exit	Col bottom exit
HAc tank level	Fresh HAc feed	Fresh HAc feed	Fresh HAc feed	Fresh HAc feed
Tray 5 temperature	Col reboiler duty	Col reboiler duty	Col reboiler duty	Col reboiler duty
% O_2 reactor feed	Fresh O_2 feed	Fresh O_2 feed	Fresh O_2 feed	Fresh O_2 feed
Vaporizer pressure	Vap vapor exit	Vap vapor exit	Vap vapor exit	Vap vapor exit
Absorber pressure	Fresh C_2H_4 feed	Sep vapor exit	Fresh C_2H_4 feed	Sep vapor exit
Reactor input temp	Vap heater duty	Vap heater duty	Vap heater duty	Vap heater duty
Reactor exit temp	Reactor shell temp	Reactor shell temp	Reactor shell temp	Reactor shell temp
FEHE exit temp	FEHE bypass ratio	FEHE bypass ratio	FEHE bypass ratio	FEHE bypass ratio

In this section, Candidate 1 is considered first. The same procedure is applied to the remaining candidates. Fourteen proportional-only controllers are automatically tuned for Candidate 1. The tuning is obtained by calculating an optimal static output feedback (OSOF) controller that contains only diagonal terms. The only difference is that, in this work, the tuning is calculated for a specific type of process forcing (disturbance rejection and setpoint change) while in Chen's, it is calculated for the generic forcing (initial states around unitary sphere, X=I). More details in the tuning method can be found in Appendix II. The seven integrating levels are controlled, using averaging level control. The reasons for this are: 1) there is not a requirement for tight level control and 2) the liquid capacities can filter out flow disturbances. The gains for the averaging level controls are +1 or –1 (%/%), depending on the sign of the process gain. The proportional gains for these loops are given in Appendix V. After the safety loops are closed, the measurements corresponding to these variables are no longer available as measurements. Instead, the setpoints of these loops become the new manipulated variables that are used later in the process.

6.2.3. Control Structure for Inventory Variables (Components)

In this stage, the Downs Drill Analysis (recommended by Luyben (1992) and used in Chen (2002, 2003) and in Chapter 5 of this work) is used to check component balances in a control scheme, in order to identify the components that need to be controlled. This analysis helps to determine whether a component (reactant, product, and inert) leave or are consumed in the process. Chen (2003) used Downs Drill Analysis to identify the components that need to be controlled for his proposed control schemes for the VA process. He explained that the inventory of components should be controlled, unless they are self-regulating or are made self-regulating by closing other loops. Chen analyzed reactants, inerts, and products. In this work, only the reactants, inerts, and byproducts are considered for the Downs Drill Analysis since products will be controlled in the next stage. Table 6.5 shows the Downs Drill Analysis for Candidate 1 for the VA process. Appendix V shows the Downs Drill Analysis for the remaining Candidates in Table 6.4.

Table 6.5 Downs Drill Analysis for Candidate 1

Candidate	Component	Self-Reg	Why Self-Reg	Manipulated Var	Measurement
Candidate 1	O_2 (react)	Yes	O_2 Feed - %O_2		
	C_2H_4 (react)	Yes	C_2H_4 feed -Abs pressure		
	HAc (react)	Yes	HAc feed-HAc level		
	C_2H_6 (inert)	No		Purge	% C_2H_6 **in gas recycle –** reactor feed
	H_2O (byprod)	No		Organic reflux	%H_2O **Column bottom -** organic product composition
	CO_2 (byprod)	No		CO_2 removal inlet	%CO_2 **in gas recycle –** reactor feed

The third column of Table 6.5 shows whether the components are self-regulating or not. If they are self-regulating, the fourth column shows which closed loops make them self-regulating. Then, the fifth and sixth columns indicate the measurement and manipulated variables available that can be used for controlling these components. From the Downs Drill Analysis for Candidate 1 the following information is obtained: 1) All the reactants are being controlled. 2) The inert and byproducts (H_2O and CO_2) are left uncontrolled after Stage 2. The manipulated variables used for controlling the inert (C_2H_6) and the byproduct CO_2 are the purge and the CO_2 removal inlet, respectively. These two components (C_2H_6 and CO_2) are essentially in the gas phase. There are two analyzers in the gas phase that measure the compositions of the inert (C_2H_6) and the CO_2. One is located in the gas recycle stream and the other, in the reactor feed. The analyzer located in the gas recycle stream is chosen for controlling the inert (C_2H_6) and CO_2 compositions because it is located closer to the manipulated variables (purge and CO_2 removal inlet). Moreover, to measure the other component (H_2O), which is essentially in the liquid phase, there are two analyzers that can be used. One is located in the column bottom, and the other, in the organic product. From engineering judgment, the analyzer located in the column bottom is selected.

The manipulated variables (degrees of freedom) available for controlling the inventory of H_2O are: MV9, MV10, MV13, MV15, MV20, MV22, and MV26. None of these manipulated variables is able to control the inventory of

H_2O except for the organic reflux stream flowrate (MV20) or the condenser duty (MV22). Even though the condenser duty changes the reflux temperature and, therefore, the effective reflux ratio, the organic reflux stream flowrate (MV20) is selected for controlling the inventory of H2O because is a more direct way to control. It is important to point out that Luyben et. al. (1998) used the organic reflux stream to control the inventory of component H_2O. At this point, Candidate 1 contains 17 loops (14 safety variables and compositions of C_2H_6, CO_2, and H_2O). Three proportional-only controllers are automatically tuned to control the inventory loops: 1) composition of C_2H_6 in the recycle stream - purge, 2) composition of CO_2 in the recycle stream – CO2 removal inlet, and 3) composition of H_2O in column bottom –organic reflux). These loops are included into the model for use in later stages. The tuning method used is the same as the one used in Stage 2. The proportional gains for these loops are given in Appendix V. Table 6.6 shows the measurements and manipulated variables available after closing the safety variables and the inventory variables. Therefore, the measurements corresponding to these loops are no longer available as measurements. Instead, the setpoints of these loops become the new manipulated variables.

Table 6.6 Available Measurements and Manipulated Variables after Closing Safety loops and Inventory Control Loops

1	Vaporizer Temperature (3)	$\%O_2$ Reactor Feed Set Point
2	FEHE Cold Exit Temperature (7)	Absorber Pressure Set Point
3	Separator Temperature (10)	HAc Tank Level
4	Gas Recycle Flowrate (16)	Vaporizer Level Set Point
5	Organic Product Flowrate (17)	Vaporizer Pressure Set Point
6	Decanter Temperature (20)	Heater Exit Temperature Set Point
7	VAc Column Bottom Comp (27)	Reactor Exit Temperature Set Point
8	HAc Column Bottom Comp (29)	Separator Level Set Point
9	C2H4 Gas Recycle Comp (32)	Separator Preheater Temperature
10	VAc Gas Recycle Comp (34)	Separator Vapor Exit
11	H_2O Gas Recycle Comp (35)	Compressor Exit Temperature Set Point
12	HAc Gas Recycle Comp (36)	Absorber Level Set Point
13	C_2H_4 Reactor Feed Comp (39)	Absorber Circulation Flow
14	VAc Reactor Feed Comp (34)	Circulation Cooler Exit Temperature Set Point
15	H_2O Reactor Feed Comp (42)	Absorber Scrub Flow
16	HAc Reactor Feed Comp (43)	Scrub Cooler Exit Temperature Set Point
17		CO_2 Gas Recycle Comp Set Point
18		C_2H_6 Gas Recycle Comp Set Point
19		FEHE Exit Temperature Set Point
20		H_2O Column bottom comp Set Point (reflux)
21		Tray 5 Temperature Set Point
22		Column Condenser Duty
23		Organic Phase Level Set Point
24		Aqueous Phase Level Set Point
25		Column Base Level Set Point
26		Vaporizer Liquid Inlet

6.2.4. Control Structure for Production Rate and Product Quality

In this stage, the optimal static output feedback (OSOF) is calculated to determine the best set of measurements and manipulated variables (dominant variables) that affect production rate and product quality. For this stage the available measurements and manipulated variables are shown in Table 6.6.

Product rate and composition measurements are not included within the available measurements because the objective is to determine what other measurements and manipulated variables can be used for controlling production rate and product quality. The production rate measurement is the organic flowrate from the decanter (17). However, this measurement does not show any relationship to any other variable in the linearized model. Therefore, the reactor exit flowrate is chosen as the production rate measurement. Then, an OSOFC is calculated, as discussed in Chapter 4, section 4.2. The OSOF is analogous to a process gain matrix and represents the dynamic information about process interaction. The control objective is to control the production rate and product quality. The following parameters are used for the calculation of the OSOFC:

1) $R = I$ This gives the same importance to all the manipulated variables.

2) $g_{ij} = 0$ In setting gij equal 0 (not solving for a specific SISO control structure).

3) Q is the weight matrix that can be used to define the desired control objective. All the elements of this matrix should be zero, except for those that correspond with the variables associated with production rate and product quality.

To extract information about the important measurements and manipulated variables to control production rate and quality from the OSOF matrix, the absolute value of each element is considered. Since the process model has been scaled, the OSOF matrix is dimensionless, and therefore, its elements can be compared to one another. Generally, an element with an absolute value close to zero indicates a weak relationship between the manipulated variable and the measurement. The following rules of thumb are used:

1) The sum of the absolute value of the elements of each manipulated variable (element in each row) is calculated for each measurement (columns). This is called Σcol. The best measurements (strongest measurements) are the ones that have the largest values of Σcol.

2) The sum of the absolute value of the elements of each measurement (element in each column) is calculated for each manipulated variable (rows). This is called Σrow. The best manipulated variables (strongest manipulated variables) are the ones that have the largest values of Σrow.

Table 6.7 shows the OSOFC matrix.

Table 6.7 OSOF Matrix

Control Objective: to Control Product Rate and Quality

SP		VapT 1	FEHET 2	SpT 3	GRF 4	DecT 5	O_2GR 6	C_2H_4GR 7	VAcGR 8	H_2OGR 9	HAcGR 10	CO_2 11	C_2H_4RF 12	C_2H_6RF 13	VAcRF 14	Σrow
1	**%O_2**	0.017	−0.000	0.000	−0.031	0.001	0.004	−0.001	−0.010	0.002	0.009	−0.000	0.017	0.008	0.001	0.101
2	**AbP**	0.003	−0.001	0.001	−0.043	0.002	0.019	0.008	−0.016	0.002	0.016	−0.007	0.012	0.011	0.002	**0.143**
3	**HAcL**	0.001	0.000	0.000	−0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.003
4	**VapL**	−0.038	−0.003	−0.001	−0.122	−0.002	0.013	0.008	0.009	0.000	0.002	−0.009	0.006	0.001	0.004	**0.218**
5	**VapP**	−0.100	−0.003	0.001	0.317	−0.000	−0.025	−0.008	0.004	−0.003	0.003	0.002	−0.126	−0.047	0.001	**0.640**
6	**HET**	−0.004	−0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	−0.002	−0.001	0.000	0.007
7	**RET**	−0.009	−0.000	0.000	0.013	0.000	−0.001	0.000	0.002	0.000	−0.001	0.002	−0.009	−0.004	−0.001	0.042
8	**SepL**	−0.013	−0.001	−0.000	−0.003	−0.000	0.003	0.002	0.002	0.000	0.000	−0.002	−0.007	−0.003	0.001	0.037
9	**SepT**	0.049	−0.001	−0.001	−0.097	−0.001	0.026	0.012	−0.003	0.003	0.003	−0.020	0.066	0.025	0.007	**0.314**
10	**SepV**	0.034	0.004	−0.001	0.426	−0.000	−0.046	−0.022	0.008	−0.003	−0.018	0.017	−0.052	−0.028	−0.005	**0.664**
11	**CET**	0.015	0.001	−0.000	−0.001	−0.000	−0.002	−0.001	0.001	0.000	−0.003	0.001	0.011	0.003	0.000	0.039
12	**AbL**	−0.026	−0.002	−0.001	−0.008	−0.001	0.007	0.004	0.004	0.000	0.000	−0.007	−0.013	−0.005	0.003	0.081
13	**AbCF**	−0.056	−0.003	0.001	0.003	0.000	0.010	0.006	−0.003	0.000	0.010	−0.005	−0.040	−0.010	0.001	**0.148**
14	**CCET**	0.022	0.001	−0.000	−0.001	−0.000	−0.004	−0.002	0.002	0.000	−0.005	0.002	0.016	0.004	0.000	0.059
15	**AbSF**	0.042	0.007	0.004	0.109	0.001	−0.030	−0.023	−0.028	0.004	0.025	0.007	0.007	0.010	0.000	**0.297**
16	**SCET**	0.003	0.000	0.000	0.001	0.000	−0.001	−0.001	0.000	0.000	−0.001	−0.001	0.002	0.000	0.000	0.010
17	**%CO2 GR**	0.003	0.000	0.000	0.002	0.000	−0.001	−0.001	0.003	−0.000	−0.003	0.001	0.002	−0.000	−0.001	0.017
18	**%C2H6 GR**	−0.000	0.000	0.000	0.000	0.000	0.000	0.000	−0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
19	**FEHE ET**	0.002	0.000	0.000	0.003	0.000	−0.002	−0.001	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.009
20	**%H2O Col**	−0.005	−0.000	0.000	−0.017	0.000	0.005	0.002	0.001	0.000	0.001	−0.003	−0.001	0.001	0.000	0.036
21	**T5T**	−0.018	−0.001	0.001	−0.044	0.001	0.014	0.006	−0.007	0.001	0.009	−0.008	−0.008	0.003	−0.003	**0.124**
22	**CondD**	−0.191	−0.018	−0.015	−0.177	−0.023	0.067	0.053	0.123	−0.003	−0.069	−0.075	−0.036	−0.050	0.047	**0.947**
23	**OrgL**	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
24	**AqL**	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
25	**ColL**	−0.005	0.000	0.000	−0.013	0.000	0.004	0.002	−0.002	0.000	0.002	−0.003	−0.002	0.001	−0.001	0.035
26	**VapI**	0.165	0.015	0.001	0.295	0.001	−0.116	−0.062	−0.005	−0.001	−0.018	0.058	0.039	0.001	−0.011	**0.788**
	Σ col	**0.821**	0.061	0.028	**1.727**	0.033	0.400	0.225	0.233	0.022	0.198	0.230	**0.476**	0.216	0.089	

The numbers that are in bold case, underlined in Table 6.7, correspond to the strongest measurements and manipulated variables to control product rate and product quality. From Table 6.7, the most important manipulated variables are vaporizer pressure setpoint-vaporizer vapor exit, separator vapor exit, column condenser duty, vaporizer liquid inlet. Other manipulated variables that seem to be important are separator preheater temperature, vaporizer level setpoint - vaporizer steam duty, absorber scrub flow, absorber circulation flow, absorber pressure - fresh C_2H_4 feed, tray 5 temperature - column reboiler duty, composition of O_2 in the recycle gas setpoint - fresh O_2 feed. From the group of important manipulated variables, the condenser duty and the tray 5 temperature setpoint directly affect the product composition while the others affect the production rate. This result seems to be very reasonable, considering that throughput changes can be achieved only by altering (either directly or indirectly) conditions in the reactor. However, some of the important manipulated variables are not considered for controlling production rate and product quality, and the reasons are explained as follows: The absorber scrub flow and the absorber circulation flow are not considered because their flowrates are comparatively small. Also, the composition of O_2 setpoint in the recycle gas is not considered because this is a safety variable that has a hard constraint (The O_2 composition must not exceed 8 mol % anywhere in the gas loop). On the other hand, from Table 6.7, the strongest measurements are the gas recycle flowrate, the vaporizer temperature, and the composition of C_2H_4 in the reactor feed. In this case, only the gas recycle gas flowrate and the vaporizer temperature are considered as important measurements (IM) because their value of Σcol is more than twice the value of closest important measurement. Also, the inventory of C_2H_4 has already been regulated in the plant by the absorber pressure – fresh C_2H_4 feed loop. The strongest manipulated variables can be used to achieve the desired control objective. However, the recycle gas flowrate and the vaporizer temperature are measurements and cannot be manipulated by the MPC. For this reason, decentralized control structures are generated for the strongest measurements using all the available manipulated variables. Once the important measurements are closed, these loops become new manipulated variables, available for the MPC.

Control Structure for Important Measurements

In this stage, the control objective is to control the gas recycle flowrate and the vaporizer temperature. An OSOFC is calculated, using the gas recycle flowrate, the vaporizer temperature and all the manipulated variables. The following parameters are used for the calculation of the OSOFC:

1) $R = I$ This gives the same importance to all the manipulated variables.

2) $g_{ij} = 0$ In setting g_{ij} equal 0 (not solving for a specific SISO control structure).

3) Q is the weight matrix that can be used to define the desired control objective. All the elements of this matrix should be zero, except the ones that correspond to the control objective (in this case, the vaporizer temperature).

The OSOFC is given in Table 6.8

Table 6.8 Optimal Static Output Feedback Controller (OSOFC)

Man Var	VapT	GRF
1 $\%O_2$	0.0048	-0.0754
2 AbP	-0.0606	**-0.2154**
3 HAcL	-0.0020	-0.0009
4 VapL	**-1.6866**	**-1.0319**
5 VapP	0.0641	0.0955
6 HET	0.0000	-0.0034
7 RET	0.0110	-0.0044
8 SepL	0.0043	-0.0163
9 SepT	-0.0091	0.2915
10 SepV	**-1.0898**	**-1.4209**
11 CET	0.0000	0.0151
12 AbL	0.0043	-0.0212
13 AbCF	-0.0016	-0.0588
14 CCET	0.0010	0.0247
15 AbSF	0.0244	-0.2043
16 SCET	0.0040	0.0085
17 %CO2 GR	0.0035	-0.0025
18 %C2H6 GR	-0.0210	0.0889
19 FEHE ET	-0.0196	-0.0073
20 %H2O Col	0.0003	-0.0011
21 T5T	0.0019	0.0035
22 CondD	-0.0266	0.1151
23 OrgL	0.0000	0.0000
24 AqL	0.0000	0.0000
25 ColL	-0.0009	0.0019
26 VapI	**1.1462**	**1.7788**

Table 6.8 shows that there are four manipulated variables that can be used to control gas recycle flowrate and three to control the vaporizer temperature. In order to identify the best manipulated variable for each measurement a sensitivity matrix is calculated. (Details on the sensitivity matrix are given in Chapter 2, Section 2.4). In this methodology, the OSOFC is analogous to a gain matrix, while the sensitivity matrix is analogous to a relative gain array. The sensitivity matrix considers the interaction between variables. Therefore, the sensitivity matrix is calculated whenever there is more than one important measurement that is being considered. Details on how to calculate the sensitivity matrix are given in Chapter 2. The sensitivity matrix is presented in Table 6.9.

Table 6.9 Sensitivity Matrix

Man Var	VapT	GRF
1 $\%O_2$	-0.1668	-0.0940
2 AbP	-1.0315	**1.1399**
3 HAcL	0.2085	-0.0087
4 VapL	**1.7161**	-1.7362
5 VapP	0.4249	-0.0623
6 HET	0.0090	-1.5685
7 RET	0.2321	0.0068
8 SepL	1.2170	-0.5262
9 SepT	0.0691	-0.0724
10 SepV	**0.8883**	-0.1819
11 CET	-0.0256	-0.6564
12 AbL	2.2914	-0.5815
13 AbCF	-0.3848	-0.3147
14 CCET	-0.2273	-0.6358
15 AbSF	0.9090	-0.6022
16 SCET	1.0058	-0.0991
17 %CO2 GR	0.1609	0.0130
18 %C2H6 GR	0.9323	8.5377
19 FEHE ET	0.3612	0.0270
20 %H2O Col	1.8822	1.4605
21 T5T	4.1147	-0.6486
22 CondD	1.3595	1.9686
23 OrgL	-1.2152	-0.1586
24 AqL	0.0854	-1.7638
25 ColL	0.2903	0.0436
26 VapI	**0.9047**	-0.1231

Then, decentralized control structures for the important measurements are generated, using OSOFC, the sensitivity matrix, and engineering judgment. Chen (2002) proposed the following heuristics: 1) Only pairings with elements having an absolute value greater than 0.2 in the OSOFC are considered. 2) Only pairings with values between 0.2 and 5 in the sensitivity matrix are considered. 3) The pairings accepted by 1 and 2 are checked, using engineering judgment.

From these heuristics and by looking at the bold and underlined elements in Table 6.9 there are three possible manipulated variables that can be used to control vaporizer temperature and one to control gas recycle flowrate. The vaporizer liquid inlet is chosen for controlling the vaporizer temperature. The separator vapor flowrate and the vaporizer level are ruled out by using engineering judgment. The first one is ruled out because it is located far away from the controlled variable, and the second one is ruled out because the vaporizer level is controlled, using average level control; therefore, precise control of the vaporizer temperature is not possible. Then, the recycle gas flowrate is controlled, using the absorber pressure, and the vaporizer temperature is controlled, using the vaporizer liquid inlet. The tuning method used is the same as the one used in Stage 2. The proportional gains for these loops are given in Appendix V. These loops are included in the model for use in later stages. Next, an OSOFC is calculated, after closing the important measurements, to check for any changes in the strongest manipulated variables. The OSOFC is calculated in the same way as in Table 6.7; the only difference is that now the vaporizer temperature and the gas recycle flow are removed from the set of measurements, and their setpoints become new manipulated variables. Table 6.10 shows the OSOFC after closing the important measurements loops.

Table 6.10 OSOF Matrix

Control Objective: to Control Product Rate and Quality

SP	FEHET 1	SpT 2	DecT 3	O_2GR 4	C_2H_4GR 5	VAcGR 6	H_2OGR 7	HAcGR 8	CO_2 9	C_2H_4RF 10	C_2H_6RF 11	VAcRF 12	Σrow
1 %O_2	0.0033	0.0007	0.0006	0.0023	0.0018	-0.0066	0.0004	0.0052	-0.0081	0.0055	0.0040	0.0039	0.0424
2 RGF-AbP	-0.0093	-0.0004	-0.0002	0.0072	0.0101	-0.0013	0.0002	-0.0013	-0.0331	0.0073	0.0068	0.0020	0.0791
3 HAcL	0.0000	0.0005	0.0010	-0.0012	-0.0018	-0.0015	-0.0017	0.0022	0.0048	-0.0024	-0.0005	-0.0010	0.0184
4 VapL	-0.0003	0.0004	-0.0027	-0.0105	-0.0013	0.0284	-0.0128	-0.0231	-0.0570	0.0362	0.0113	0.0189	**0.2029**
5 VapP	-0.0249	-0.0028	-0.0002	-0.0084	-0.0189	0.0428	0.0015	-0.0094	0.1635	-0.0726	-0.0429	-0.0457	**0.4336**
6 HET	0.0004	0.0001	-0.0001	-0.0002	-0.0002	0.0003	0.0003	0.0003	0.0010	-0.0003	-0.0001	-0.0000	0.0033
7 RET	0.0181	0.0031	0.0001	-0.0018	-0.0102	-0.0023	0.0068	0.0167	0.0637	-0.0144	-0.0045	-0.0041	**0.1457**
8 SepL	-0.0016	-0.0006	-0.0014	-0.0006	0.0012	0.0091	-0.0009	-0.0077	-0.0036	0.0013	-0.0009	0.0005	0.0293
9 SepT	-0.0014	-0.0021	-0.0025	0.0173	0.0156	-0.0001	-0.0009	-0.0098	-0.0785	0.0340	0.0135	0.0149	**0.1906**
10 SepV	-0.0335	-0.0052	0.0004	0.0030	0.0117	0.0728	-0.0106	-0.0409	0.1602	-0.0977	-0.0462	-0.0615	**0.5438**
11 CET	0.0013	-0.0001	-0.0001	-0.0002	-0.0001	0.0021	-0.0009	-0.0029	-0.0019	0.0004	-0.0003	0.0001	0.0105
12 AbL	-0.0037	-0.0012	-0.0028	-0.0006	0.0026	0.0172	-0.0016	-0.0128	-0.0088	0.0037	-0.0011	0.0017	0.0578
13 AbCF	-0.0045	0.0004	0.0002	0.0009	0.0015	-0.0057	0.0031	0.0096	0.0086	-0.0016	0.0008	-0.0003	0.0372
14 CCET	0.0007	-0.0001	-0.0001	-0.0001	0.0001	0.0012	-0.0006	-0.0017	-0.0012	0.0003	-0.0001	0.0001	0.0061
15 AbSF	0.0041	-0.0007	-0.0012	0.0232	0.0190	-0.0340	0.0130	0.0244	-0.0490	0.0326	0.0169	0.0184	**0.2365**
16 SCET	0.0125	-0.0023	-0.0021	0.0419	0.0336	-0.0684	0.0261	0.0468	-0.0845	0.0599	0.0283	0.0342	**0.4405**
17 %CO2 GR	-0.0039	-0.0001	-0.0020	0.0015	0.0469	0.0021	0.0013	0.0001	-0.0420	-0.0057	0.0173	0.0056	0.1285
18 %C2H6 GR	-0.0003	0.0000	0.0000	-0.0000	-0.0002	0.0001	-0.0000	0.0002	-0.0000	-0.0002	0.0001	-0.0002	0.0014
19 FEHE ET	0.0009	0.0002	0.0001	-0.0008	-0.0011	0.0003	-0.0001	0.0004	0.0026	-0.0007	-0.0003	-0.0003	0.0077
20 %H2O Col	0.0004	0.0001	-0.0001	0.0017	0.0015	-0.0020	0.0006	0.0013	-0.0083	0.0032	0.0020	0.0016	0.0228
21 T5T	0.0001	0.0007	0.0003	0.0052	0.0039	-0.0103	0.0031	0.0068	-0.0221	0.0064	0.0061	0.0024	0.0674
22 CondD	-0.0004	-0.0166	-0.0263	0.0119	0.0353	0.1116	-0.0094	-0.0759	-0.1062	0.0867	-0.0003	0.0598	**0.5406**
23 OrgL	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	-0.0000	0.0000	0.0000	0.0000	0.0000
24 AqL	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	-0.0000	0.0000
25 ColL	-0.0014	0.0007	0.0006	-0.0006	-0.0007	0.0027	-0.0029	-0.0010	-0.0041	-0.0009	0.0011	-0.0007	0.0175
26 Vap T	-0.0136	0.0028	0.0025	-0.0498	-0.0408	0.0802	-0.0301	-0.0541	0.1050	-0.0726	-0.0344	-0.0413	**0.5272**
Σ col	0.1406	0.0421	0.0477	0.1912	0.2603	0.5030	0.1286	0.3546	1.0175	0.5464	0.2396	0.3194	

Comparing Tables 6.7 and 6.10, it can be said that the majority of important manipulated variables remains the same. However, there are three manipulated variables that become important which are reactor exit temperature setpoint (7), separator temperature setpoint (9), and vaporizer level (4). It appears that the order of importance of the remaining manipulated variables is almost the same in both tables (6.7 and 6.10). Therefore, results from Table 6.10 regarding the order of the importance of the key variables, are used in the next step.

Determination of Control Structure for controlling Production Rate and Product Quality

The objective in this section is to identify how many and which of the important manipulated variables should be used to control production rate and product quality. Because there is no rule to decide how many and which of these important manipulated variables should be used as inputs to the MPC, the strongest manipulated variables will be added, one at a time, in descending order of importance according to the Σrow value in Table 6.10. Each time a new manipulated variable is added, a new control system is generated, and each these control systems is called Candidates (See Table 6.11). Each candidate starts with the number of the base candidate (candidate for safety variables in Table 6.4) being evaluated (in this case - Candidate 1). Each of the generated candidates has two control variables or outputs (production rate and product quality) and a different number of manipulated variables or inputs.

In this stage, a multivariable OSOFC is used as a quick screening tool, to determine the number and which manipulated variables should be used to control the economic variables with the MPC. These linear simulations give an initial insight about the manipulated variables that have better control performances for production rate and quality control. Candidates with poor control performance will be eliminated and that particular manipulated variable will not be considered as an inputt to the MPC. The resulting control structures are evaluated, using nonlinear process simulations and model predictive controller (MPC). The final control structure will have two outputs (production rate and product quality) and a different number of inputs, depending on the candidate being evaluated. All generated candidates are tested for the following disturbances and setpoint changes:

1) 20% increase in the production rate (measured as organic product flowrate)
2) DTB(1): Step change in the composition of ethane in the fresh ethylene feed stream, from 0.001 to 0.003 mol fraction
4) DTB(2): 6^{o}C increase in the reactor temperature

The control performance of the generated candidates, are evaluated and compared using transients' response characteristics such, as offset value for critical variables in the plant and the integral of the absolute value for the error (IAE). To do so, the transients and the final steady state values for disturbance rejection and setpoint changes, of the critical variables are compared for the generated the Candidates. The critical variables in the plant are: the following safety variables: %O_2 reactor feed, absorber pressure, heater exit temperature, reactor exit temperature, FEHE hot exit temperature, tray 5 temperature, and the following economic variables in the plant: reactor exit flowrate and VAc organic product composition. The safety variables are considered critical variables because they are directly related to safety and operational constraints, while the economic variables are related to the economic objectives.

The offset value is calculated as the difference between the setpoint of a critical variable and the final steady state value reached by that particular variable after a disturbance or setpoint change. Then, the summation of the absolute value of the offset for the critical variables is calculated for all the disturbances and for setpoint changes, for each candidate. Because the offsets of different critical variables will be added together, these offset values are scaled by dividing them by the steady state values. In order to calculate the summation of the offset, the following weights are given to the critical variables: production rate: 0.2, product quality: 0.2, %O_2 reactor feed: 0.1, absorber pressure: 0.1, heater exit temperature: 0.1, reactor exit temperature: 0.1, FEHE hot exit temperature: 0.1, and tray 5 temperature: 0.1. These weights are chosen based on the control objectives of the plant. The summation of the offset values for each candidate is calculated as follows:

$$Offset\ Value_k = \sum_{j=1}^{3}\sum_{i=1}^{8} \alpha_* abs(critical\ variables\ offset(j,i)) \qquad (6.3)$$

α: weights for the critical variables (0.2, 0.2, 0.1, 0.1, 0.1,0.1,0.1,0.1)

i: critical variables offsets: $\%O_2$ reactor feed, absorber pressure, heater exit temperature, reactor exit temperature, FEHE hot exit temperature, tray 5 temperature, reactor exit flowrate, and VAc organic product composition

j: Disturbances and setpoint change. *j*=1 DTB(1), *j*=2 DTB(2), and *j*=3 set point change

k: total offset value for each.

As can be seen in Equation 6.3, the offset values per candidate are the summation of the offset for the all the critical variables for disturbances DTB(1), DTB(2), and the setpoint changes.

The IAE is calculated, using Equation 6.4.

$$IAE\ for\ critical\ variables_k = \int_0^{\infty} [SP(t) - CV(t)]dt \qquad (6.4)$$

The IAE for each candidate is calculated as follows

$$IAE = \sum_{j=1}^{3}\sum_{i=1}^{8} IAE\ for\ critical\ variables(j,i) \qquad (6.5)$$

i: IAE for critical variables: $\%O_2$ reactor feed, absorber pressure, heater exit temperature, reactor exit temperature, FEHE hot exit temperature, tray 5 temperature, reactor exit flowrate, and VAc organic product composition *j:* Disturbances and setpoint change. *j*=1 DTB(1), *j*=2 DTB(2), and *j*=3 set point change

k: total IAE for the critical variables for each

There are four conditions that a candidate has to pass in order to be considered: to reject disturbances DTB(1), DTB(2), and to increase production rate by 20% in 6 hours. As mentioned above, every time a new manipulated variable is added, its values for the summation of the offset and IAE are compared with the previous candidate to evaluate whether there is significant improvement or not. It can be said that there is significant improvement when:

- The percentage of change in the IAE with the addition of a new manipulated variable is greater than 5%. The percentage of change is calculated as the change between two consecutive candidates. If it is less than 5%, there might be no significant improvement. Therefore, the addition of a new manipulated variable will not give significant control benefits. However, since this just an initial screening tool if the % change is between 1 to 5% it might be checked with the nonlinear simulation, just to corroborate that the variable does not improve significantly the control performance.
- The total summation of the offset value decreases more than 5% between two consecutives candidates.

Since DTB(2) is setpoint changes in the reactor temperature proportional integral (PI) controllers are used for the final control structure. The tuning parameters for the controllers can be found in Appendix V. These PI controllers are included in the state space model formulation. The derivation to incorporate PI controllers into state space model in presented in Appendix VI. Transients of 8 measurements (Production rate, Product quality, $\%O_2$ reactor feed, absorber pressure, reactor exit temperature, separator temperature, vaporizer pressure, temperature, tray 5 temperature are calculated for each disturbance and setpoint change. Table 6.11 shows all the candidates generated, the controlled and manipulated variables for each candidate, the ability of each candidate to reject disturbances DBT(1), DBT(2), and to achieve 20% increase in the production rate. In addition, it shows the summation of the offset (see Eq 6.3), and the IAE values (see Eq 6.5) for the critical variables in the plant for each candidate. It also shows the percentage of change for the summation of the offset values and the IAE between consecutives candidates. Only candidates that are able to reject both disturbances and achieve maximum production rate will be considered for this analysis.

Table 6.11 Candidates for Alternative 1

Candidate number	**Controlled Variables**	**Manipulated Variables**	**Can maximize production rate and reject disturbances?**	**Summation offset values / % change btw candidates**	**IAE / % change btw candidates**
Candidate 1-1	Production Rate Product Quality	GRP SP- Ab Pressure (IM)	SP change No DTB(1) Yes DTB(2) Yes	Not considered, do not satisfy all conditions for SP and disturbance	Not considered, do not satisfy all conditions for SP and disturbance
Candidate 1-2	Production Rate Product Quality	GRP SP- Ab Pressure (IM) **Vaporizer Temp SP (IM)**	SP change No DTB(1) Yes DTB(2) Yes	Not considered, do not satisfy all conditions for SP and disturbance	Not considered, do not satisfy all conditions for SP and disturbance
Candidate 1-3	Production Rate Product Quality	GRP SP- Ab Pressure (IM) Separator Vapor Exit	SP change No DTB(1) Yes DTB(2) Yes	Not considered, do not satisfy all conditions for SP and disturbance	Not considered, do not satisfy all conditions for SP and disturbance
Candidate 1-4	Production Rate Product quality	GRP SP- Ab Pressure (IM) Separator Vapor Exit Decanter Temp SP	SP change Yes DTB(1) Yes DTB(2) Yes	0.9989	2.7205e+004
Candidate 1-5	Production Rate Product Quality	GRP SP- Ab Pressure (IM) Separator Vapor Exit Decanter Temp SP **Vaporizer Pressure SP**	SP change Yes DTB(1) Yes DTB(2) Yes	0.9979 < 5%	2.7203e+004 < 5%
Candidate 1-6	Production Rate Product Quality	GRP SP- Ab Pressure (IM) Separator Vapor Exit Decanter Temp SP **Scrub Cooler Exit Temp SP**	SP change Yes DTB(1) Yes DTB(2) Yes	0.9989 < 5%	2.7205e+004 < 5%
Candidate 1-7	Production Rate Product Quality	GRP SP- Ab Pressure (IM) Separator Vapor Exit Decanter Temp SP **Separator Temperature SP**	SP change No DTB(1) Yes DTB(2) Yes	0.9979 < 5%	2.7202e+004 < 5%
Candidate 1-8	Production Rate Product Quality	GRP SP- Ab Pressure (IM) Separator Vapor Exit Decanter Temp SP **Vaporizer Level SP** Reactor Exit Temp SP	SP change Yes DTB(1) Yes DTB(2) Yes	0.9970 < 5%	2.7197e+004 < 5%

After running the linear simulations and evaluating the transients for disturbances DTB(1), DTB(2), and for increasing production rate by 20%, the following statements can be made: 1) For disturbance rejection: All the cases are able to reject disturbances DTB(1) and DTB(2). 2) for setpoint changes only the following candidates: 1.4, 1.5, 1.6, 1.7 and 1.8 are able to increase the production rate. When a new manipulated variable is added, if this variable does not have significant effect in the IAE or in the summation of the offset values, the variables will not be considered for the next candidate and it will be eliminated from the list of manipulated variables. In table 6.11 all the variables that are in bold does not have significant effect and therefore are not considered for the final control structure.

From table 6.11 it can be seen that the best candidate is 1.8. This candidate has two outputs production rate and product quality and four manipulated variables that are gas recycle –Absorber pressure SP, Separator vapor exit flow, Decanter temperature setpoint.

These linear simulations are used to obtain an initial insight about the resulting control structure. The resulting control structures are evaluated, using nonlinear process simulations and model predictive controller (MPC).

6.2.5. Control Structure for Individual Unit Operations Using the Available Degrees of Freedom.

So far, the only degrees of freedom that have not been used are separator preheater temperature (MV9), column condenser duty (MV22), absorber circulation flow (MV13), and absorber scrub flow (MV15). The separator preheater temperature (9) can be used to control the separator temperature (10), and the column condenser duty (22) can be used to control the decanter temperature (20). The absorber circulation flow and the absorber scrub flow, are fixed at their steady state values.

6.2.6. Control production rate and product quality, using MPC

In this Stage, an MPC is built on the top of the resulting control structure. The main objective is to improve the control of the production rate and product quality by adjusting the setpoint of the important loops (strongest manipulated variables) in the plant. The control structure implemented is the best control structure obtained in step 6.2.4, Candidate 1-4, from Table 6.11. The resulting control structure is evaluated, using nonlinear process simulations. The tuning used for these simulations was obtained from linear calculations. Proportional-integral controllers are used in the nonlinear process simulation. The tuning parameters for these controllers can be found in Appendix V.

Transients of 8 measurements (Production rate, Product quality, %O_2 reactor feed, absorber pressure, reactor exit temperature, separator temperature, vaporizer pressure, temperature, tray 5 temperature) are calculated for each disturbance and setpoint change. The model predictive controller is build using the function scmpcnl in Matlab. This function designs an MPC controller for constrained problems and simulates closed loop systems with hard constraints. This MPC is tested using the nonlinear model simulations. In other words, the input values calculated by the MPC are fed continuously into the nonlinear simulation for the Tennessee Eastman Plant. The scmpcnl function uses the plant model in Simulink format. The tuning parameters for the MPC are the following:

1) The control horizon (M). This is the number of control moves
2) Length of prediction horizon (P)

3) Penalty weighting for changes in manipulated variables (uwt)

4) Penalty weighting for setpoint tracking (ywt)

The MPC is tuned by trial and error using the following guidelines:

The control action becomes more aggressive when: P decreases, M increases, and uwt decreases.. In this work, the same weight (ywt) is given to both controlled variables (production rate and product quality). P and M are used to give an initial tuning while uwt is used to obtain a fine tuning. Different values of uwt are given to the manipulated variables depending on how fast these variables can be manipulated, and the desired control performance.

Figures 6.2, 6.3, and 6,4 show the nonlinear simulations for a 20% increase in the production rate, DTB(1) and DB(2).

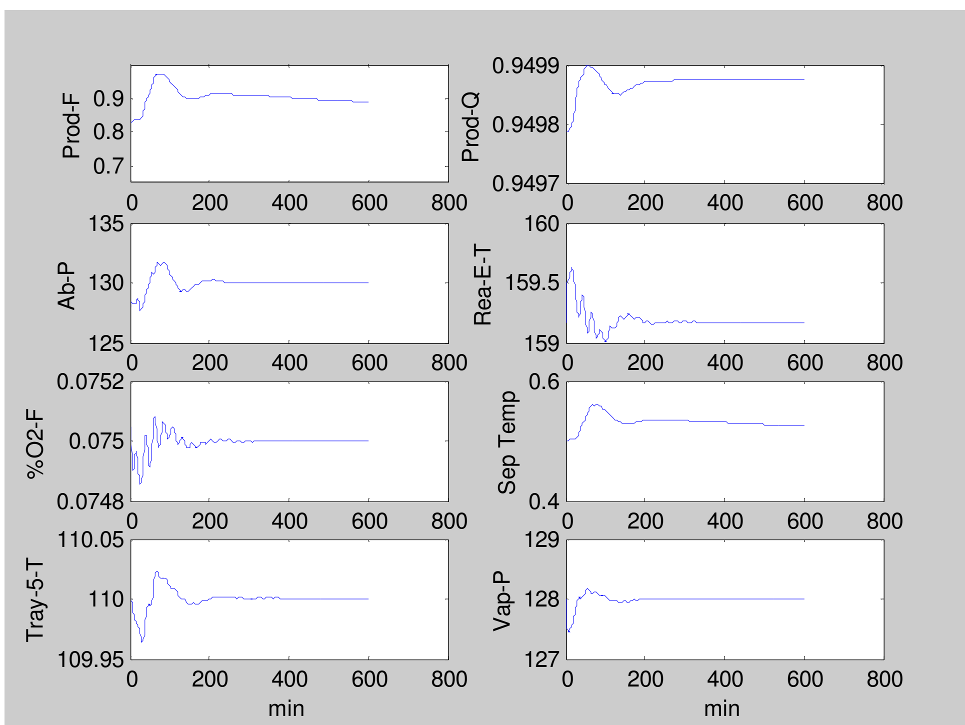


Figure 6.2 20% Setpoint change in the Product flow

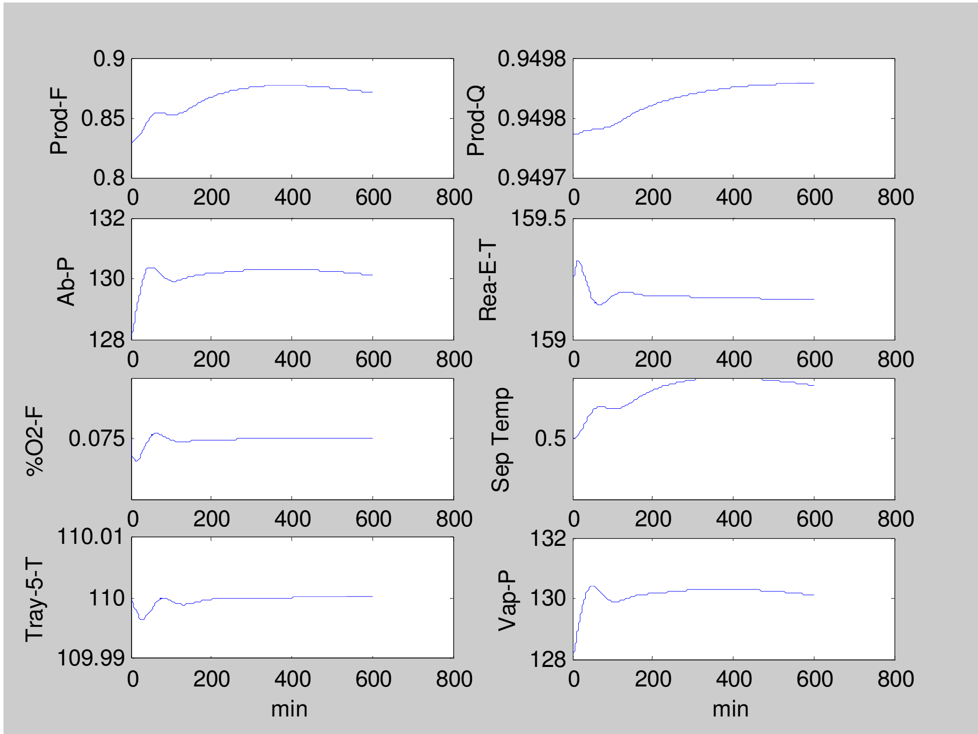


Figure 6.3 DTB(1) Change Composition of Ethane in Feed from 0.001 to 0.003 mol fraction

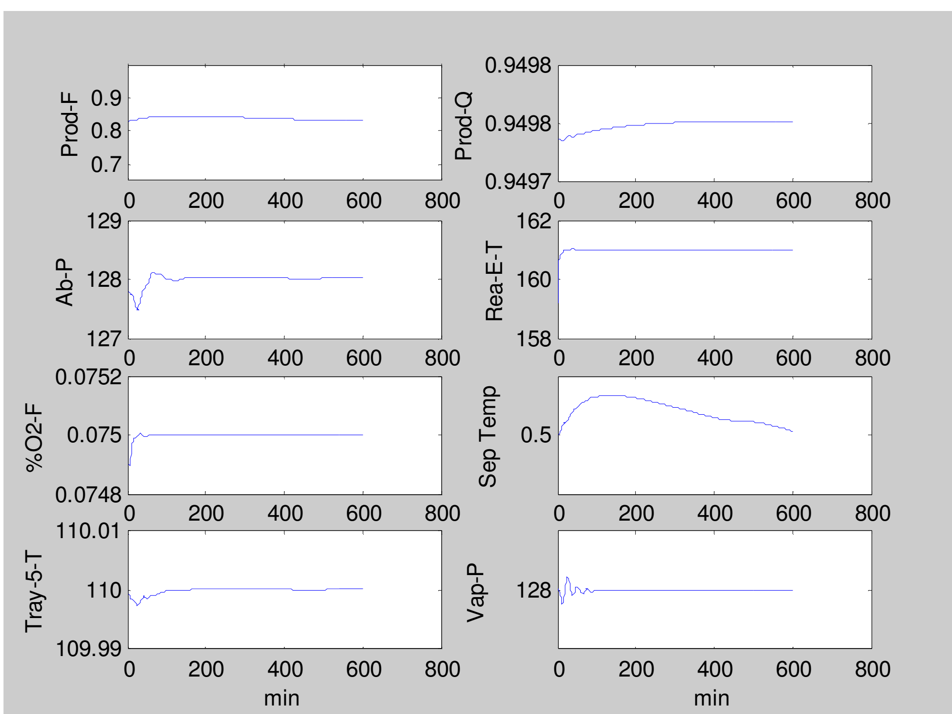


Figure 6.4 DTB(2) 6 Increase in Reactor Temperature

Chapter 7: Optimal Control of Inerts

7.1. Introduction

Inerts are chemical components that are generally present in chemical processes. They can be introduced into the process through impure feed streams, or they are generated by irreversible chemical reactions. In general, inerts do not significantly affect the process. However, the inerts become very important when there are recycle streams in the process. The reason is that the inerts can accumulate and cause undesirable site effects, such as a rapid increment of the reactor pressure that might cause the shut down of the plant. Therefore, it is necessary to eliminate the inerts at some point in the process. In general, the inerts leave the system through the purge flow. In some cases, the loss that occurs through the purge is very significant because reactants and products also leave the process through the purge. The purpose of this study is to develop a general methodology to improve the control of the inerts in a process, when the amount of inert that enters into the process is changing. This methodology considers the economics of the plant by avoiding unnecessary purge.

In general, the inventory of inerts in the process is controlled by manipulating the purge flow. For instance, the composition of inerts in the process is measured by an analyzer in the purge flow; this measurement is compared with a fixed set point value for the composition of the inert; then the purge flow is adjusted to account for this difference. In general, the setpoint of the inert composition in the process is a fixed value that can be obtained through optimization. However, when the amount of inert that enters into the process changes, it would not necessarily be good to use a fixed composition of the inert setpoint for all values of inert coming into the process. Therefore, as the amount of inert that enters into the process varies, the purge flow can potentially be varied, avoiding unnecessary purge. The idea is to change the purge flow so that the total flow of the inert that leaves the system is equal to the total flow of the inert that enters. Therefore, it is necessary to know the amount of inerts that enter into the process. One of the most frequent and important problems in the control of chemical processes is to find adequate and reliable sensors to measure important variables in the plant. Some of these important variables are key compositions in the process. In general, the sensors used to measure compositions (analyzers) are very expensive and require a lot of maintenance. Therefore, their installation should be justified from an economical point of view. For this reason, many times engineers develop soft sensors to estimate the desired measurements. Sometimes these estimations are not very accurate. Therefore, if the variable being estimated is not critical then the error in the estimation might be acceptable. However, when the variable being estimated is very critical from the operational point of view or the economic point of view it is recommended to install a hard sensor.

The proposed methodology uses the amount of inert that enters into the process to solve an optimization problem that determines the maximum amount of inert (minimum amount of purge) that can be handled in the process without having to shut down the plant. Therefore, whenever there is a change in the amount of inert that enters into the process, the setpoint of the purge composition (inert composition) controller is changed, according to the optimization results to avoid unnecessary purge. This methodology is applied to the Tennessee Eastman Process, where 67% of the loss occurs through the purge. In this process there is an inert component (B) that enters into the process as an impurity trough one of the reactant feed streams (C Feed). The amount of inert that enters into the plant varies, according to two disturbances IDV(2) and IDV(8). Disturbance IDV(2) represents a step change in the B composition that enters in the C feed stream, while disturbance IDV(8) represents a random change in the composition of components A, B, and C in the C feed stream.

7.2. Optimal Control of Inerts Methodology

1) Identify the inerts in the process, whether they enter as an impurity with the feed streams and/or are generated in the process. Also, identify whether or not there is a sensor (analyzer) that measures the amount of inerts that enter in the plant, and where the inerts leave the process. In the case where there is not a sensor that measures the amount of inerts that enter into the process, this can be estimated using a Kalman Filter. In this work, the Kalman Filter Theory is used to estimate the unknown inputs [Zasadzinski, D et al. 1995].

The formulation of the problem is as follows:

$$\begin{aligned} x_{k+1} &= \mathrm{A}\,x_k + \mathrm{B}\,u_k + \mathrm{G}\,d_k + w_k \\ y_k &= \mathrm{C}\,x_k + v_k \end{aligned} \tag{7.1}$$

where $x_k \in R^n$, $y_k \in R^p$, $u_k \in R^m$ and $d_k \in R^q$ are the state, measurement, control and unknown disturbance vectors at instant *k* respectively. Matrices A, B, C, and G are known matrices. w_k and v_k are zero mean white sequence. Their covariance is given as:

$$E(w_k w_j^T) = W\delta_{kj}, E(v_k v_j^T) = V\delta_{kj} \tag{7.2}$$

where $W > 0$, $V > 0$ and δ_{kj} is the Kronecker delta. The unknown disturbance vector d_k can be estimated under the following assumptions.

1) $p \geq q$
2) $\text{rank}(CG) = \text{rank}(G) = q$
3) $\text{rank}(C) = p$

The system defined by Eq. 7.1 can be rewritten as an augmented system under the following form:

$$\begin{aligned} H\tilde{x}_{k+1} &= A\tilde{x}_k + B\tilde{u}_k + w_k \\ y_k &= C\tilde{x}_k + v_k \end{aligned} \tag{7.3}$$

where

$$\tilde{x}_k = \begin{bmatrix} x_k \\ d_{k-1} \end{bmatrix}, \quad H = [I - G], \quad A = [\mathrm{A} \;\; 0], \quad \tilde{B} = \mathrm{B} \quad \text{and} \quad \tilde{C} = [\mathrm{C} \;\; 0]. \tag{7.4}$$

From this point A, B, C, x_k, x_{k+1}, and u_k are defined as the augmented values. The estimate based on the measurements up to k is

$$\hat{\tilde{x}} = \begin{bmatrix} \hat{x}_{k/k} \\ \hat{d}_{k-1/k} \end{bmatrix} \tag{7.5}$$

and the estimation error covariance matrix is

$$P_{k/k} = E(\hat{x}_{k/k} - x_k)(\hat{x}_{k/k} - x_k)^T \tag{7.6}$$

$P_{k/k}$ is partitioned as follows:

$$P_{k/k} = \begin{bmatrix} P_{k/k} & P_{k/k}^{xd} \\ P_{k/k}^{dx} & P_{k-1/k}^{d} \end{bmatrix} \tag{7.7}$$

where

$$P_{k/k}^{x} = E(\hat{x}_{k/k} - x_k)(\hat{x}_{k/k} - x_k)^T \tag{7.8}$$

is the state estimation error covariance matrix,

$$P_{k-1/k}^{d} = E(\hat{d}_{k-1/k} - d_{k-1})(\hat{d}_{k-1/k} - d_{k-1})^T \tag{7.9}$$

represents the unknown input estimation error covariance matrix, and

$$P_{k/k}^{xd} = \left(P_{k/k}^{dx}\right)^T = E(\hat{x}_{k/k} - x_{k-1})(\hat{d}_{k-1/k} - d_{k-1})^T \tag{7.10}$$

is the cross state and unknown input estimation error covariance matrix.

The augmented system given in Eq. (7.3) is used for the derivation of the unknown input optimal filter. By using the generalized Kalman filter theory, we obtain the following optimal state estimator for the augmented system:

$$\hat{\tilde{x}}_{k+1/k+1} = \tilde{P}_{k+1/k+1}\left(\tilde{E}^T\left(W + \tilde{A}\tilde{P}_{k/k}\tilde{A}^T\right)^{-1}\left(\tilde{A}\hat{\tilde{x}} + \tilde{B}u_k\right) + \tilde{C}^T V^{-1} y_{k+1}\right) \tag{7.11}$$

Following the approach developed in Darauach et al. (1995) the estimation of the state and the unknown input are given by:

$$\hat{x}_{k+1/k+1} = \bar{x}_{k/k} + G\hat{d}_{k/k+1} + K_{k+1}^{x}\left(y_{k+1} - C(\bar{x}_{k/k} + G\hat{d}_{k/k+1})\right) \tag{7.12}$$

$$\hat{d}_{k/k+1} = K_{k+1}^{d}\left(y_{k+1} - C\bar{x}_{k/k}\right) \tag{7.13}$$

with

$$\bar{x}_{k/k} = A\hat{x}_{k/k} + Bu_k, \qquad K_{k+1}^{x} = \left(\bar{P}_{k/k}^{-1} + C^T V^{-1} C\right)^{-1} C^T V^{-1} \tag{7.14}$$

and

$$K_{k+1}^{d} = P_{k+1/k+1}^{dk} C^{T} V^{-1} \quad (7.15)$$

where the covariance matrices are computed recursively by:

$$\overline{P}_{k/k} = A P_{k/k}^{x} A^{T} + W \quad (7.16)$$

$$P_{k+1/k+1}^{x} = \left(\overline{P}_{k/k}^{-1} + C^{T} V^{-1} C - \overline{P}_{k/k}^{-1} G \left(G^{T} \overline{P}_{k/k}^{-1} G \right)^{-1} G^{T} \overline{P}_{k/k}^{-1} \right)^{-1} \quad (7.17)$$

$$P_{k/k+1}^{d} = \left(G^{T} C^{T} \left(V + C \overline{P}_{k/k} C^{T} \right)^{-1} C G \right)^{-1} \quad (7.18)$$

$$P_{k+1/k+1}^{d} = P_{k/k+1}^{d} G^{T} P_{k/k}^{-1} \left(P_{k/k}^{-1} + C^{T} V^{-1} G \right)^{-1} \quad (7.19)$$

2) Develop a model to express the change of inerts in the process. In this case, this formulation is used in the Tennessee Eastman plant to determine the amount of inert B that enters into the process with the C feed. This is a simplified model to represent the essential process characteristics without introducing unnecessary details. The model assumptions are: 1) the amount of B (moles of B) that enters into the plant with the C feed can be estimated, 2) the composition of B in the system is uniform, i.e. the composition of B in the reactor feed and that in the purge are identical.

The model used to describe the change of inert B in the process is as follows:

$$M \frac{dX_{B}}{dt} = n_{B} - X_{B_s} Purge - Purge_{s} X_{B} \quad (7.20)$$

where

X_{B} = Composition of inert B in the system (mole fraction)

n_{B} = amount of B that enters in the system with the C Feed (moles)

$Purge$ = Purge flow (moles/hr)

M = Total gas holdup (moles)

Since both X_B and Purge flow are time varying, the model is linearized and then translated into a state space form. The Kalman Filter algorithm is implemented in Matlab, and it uses the composition of B in the purge, the purge flow, and the total gas holdup to determine the amount of inert B that enters into the process (unknown inputs). This estimation is done for disturbances IDV(2) and IDV(8). Figure 7.1 shows the change of the following variables: product flow, product composition, purge flow, inert composition in the purge stream, reactor pressure, C Feed flow, composition of B in the C Feed, and the estimated value for B in the C feed change for disturbance IDV(2).

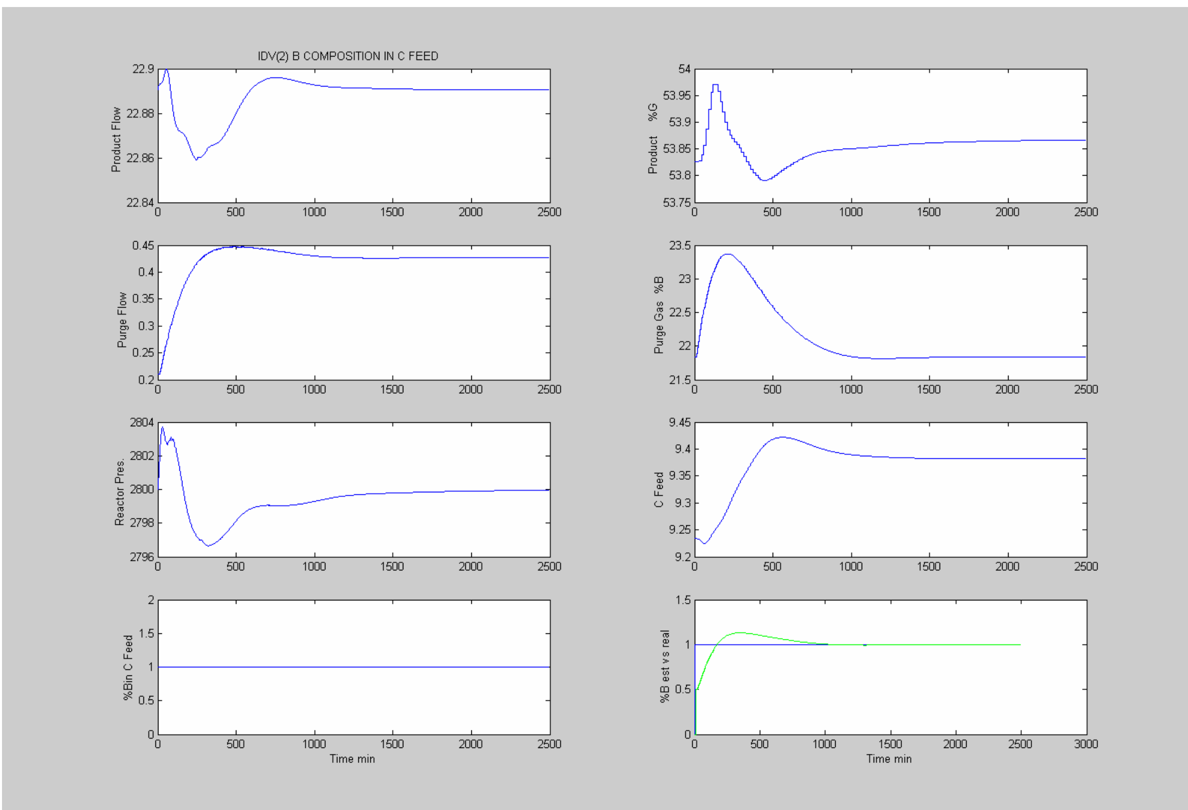


Figure 7.1 Estimation for $X_{B\ in\ C\ Feed}$ for IDV(2)

The last plot in Figure 7.1 shows the %B in the C feed estimated (curve line) vs the real value of the %B in the C Feed (straight line) for disturbance IDV(2). This plot shows that the estimation reaches the real value, but it is delayed. The reasons for this delay are: 1) the dynamics of the process (the time constant for the process is very large) and 2) the inaccuracy of the model. Therefore, it takes a long time for the analyzer in the purge to measure the effect of a change of B in the C Feed.

Figure 7.2 shows the same variables as Figure 7.1 but for disturbance IDV(8). The last plot in Figure 7.2 shows the comparison between the real composition of B in the C feed versus the estimated value. The real composition is one with greater variation. From this plot, it can be seen that the estimation of the % B in the C feed is not accurate. This inaccuracy is due to the fact that the time constant of the process is very large and the frequency of the change of B in the C feed is much larger than the frequency at which the composition of B is changing in the purge

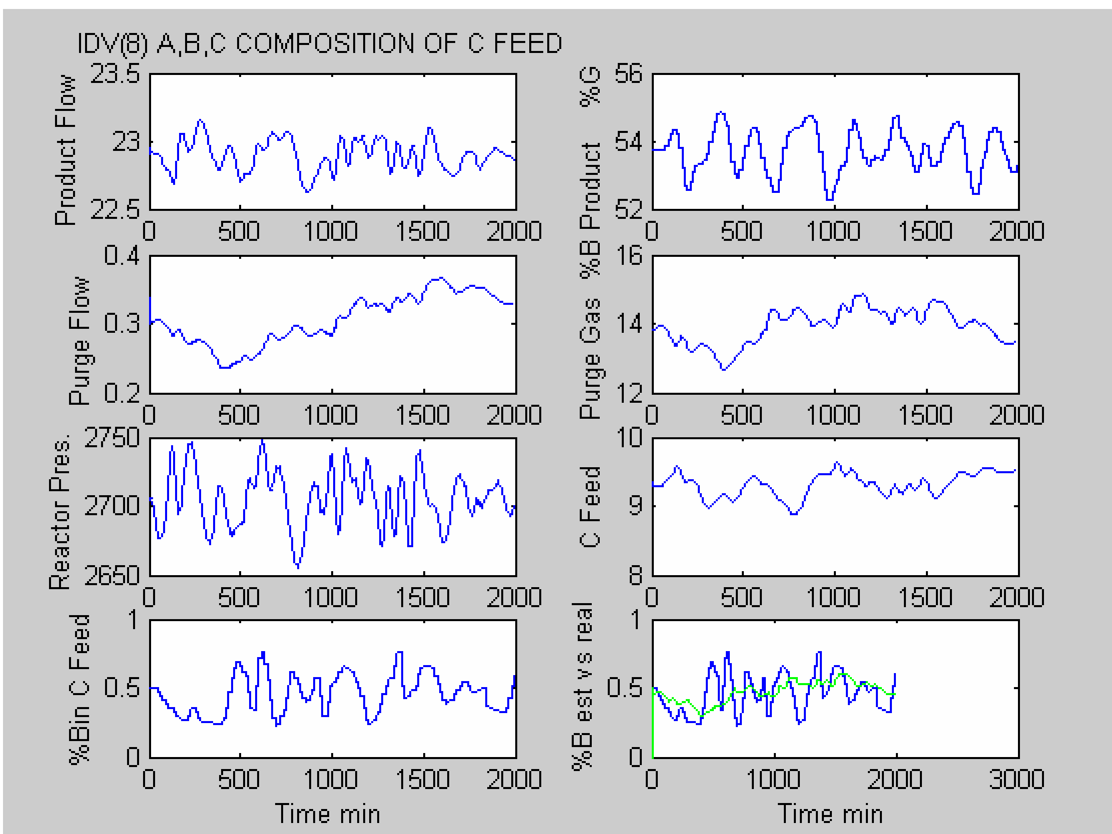


Figure 7.2 Estimation for $X_{B\ in\ C\ Feed}$ for IDV(8)

The estimation of B in the C feed was also calculated for the situation when there is no change in the %B entering the process. For this case the estimation is more accurate and can be seen in Figure 7.3. From this Figure it can be seen that there is a very small difference between the real value and the estimated value.

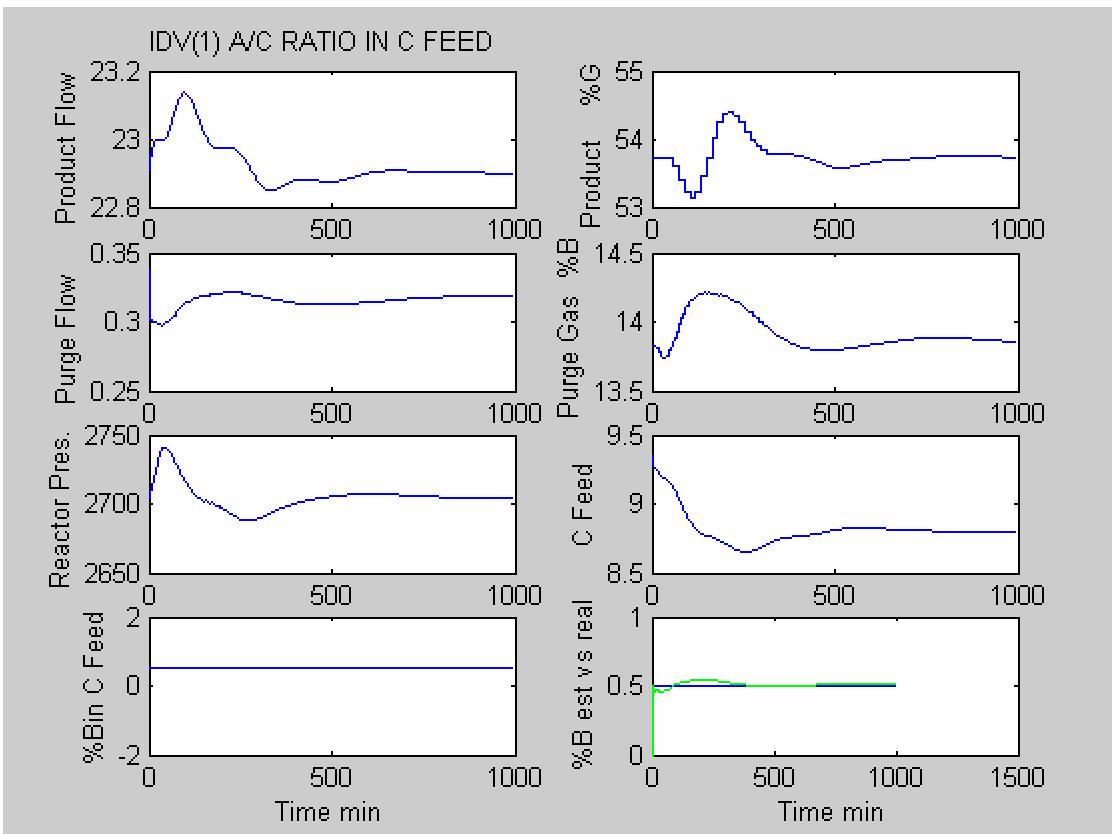


Figure 7.3 Estimation for $X_{B\ in\ C\ Feed}$ for no disturbance

The Kalman Filter formulation for unknown input estimation was tested on other models that have a smaller time constant than the Tennessee Eastman model. The results obtained for these cases were excellent and ruled out (eliminate) the possibility of problems with the estimation formulation used. Therefore, this formulation should not be used for processes with large time constant (slow dynamics), for example the Tennessee Eastman plant.

2) Determine the maximum amount of inert (minimum amount of purge) that can be handled in the plant without having side effects such as the accumulation of inert in the process that might cause shut down of the process. Once the amount of inert that enters in the plant is known the next step is to do an optimization to maximize the steady state amount of inert in the purge or minimize the steady state value of the purge flow, subject to the steady state values of the state variables and to keep the controlled variables at their set point.

7.3. __Formulation of the Optimization Problem__

The formulation for this problem is based in one presented by Ricker (1995)

Given a model of the process as:

$$\begin{aligned} \frac{dx}{dt} &= \dot{x}(t) = f\left(x,u,t\right) \\ y(t) &= h(x,t) \end{aligned} \tag{7.21}$$

where

$x(t)$ = vector of n state variables

$u(t)$ = vector of n_u manipulated variables

y(t) = vector of n_y measurements

$f(x,u,t)$ = non linear function that contains the model of the process (mass and energy balances, multicomponent equilibrium, physical properties, etc). It also includes disturbances.

$h(x,t)$ = non linear function that includes random measurement noise.

The optimization problem that is being solved is to determine the steady state value of the states *x(0)* and the manipulated variables *u(0)* that maximize the amount of B in the purge ($X_{B\ purge}$) while satisfying certain constraints:

$$\max_{x,u} X_{inert\_purge} \tag{7.22}$$

subject to

$f(x,u,0) = 0$

$0 \le u_i(0) \le 1000 \forall_i = 1, n_y$	Bounds for manipulated variables
$0 \le x_i \forall_i = 1, n$	Bounds for state variables
$g(x,u,0) \le 0$	*g* nonlinear vector function that specifies the target values for key variables in the plant, such as controlled variables and variables that have limited of operations that might cause shut down of the plant.

For the Tennessee Eastman Plant the formulation of the problem is as follows:

$$\max_{x,u} X_{B\_purge} \tag{7.23}$$

Find the steady state value for the state and the manipulated variables that maximize the amount of the inert in the purge, subject to the following nonlinear equality constraints:

$\dot{x}_{(1:38)} = 0$	Steady state value of the state variables
$\dot{x}_{38+i}(0) = u_i(0) \forall_i = 1,12$	Steady state value of manipulated variables
$g_1 = y_8 - y_{8\_sp}$	Control reactor level
$g_2 = y_{12} - y_{12\_sp}$	Control separator level
$g_3 = y_{15} - y_{15\_sp}$	Control stripper level
$g_4 = y_7 - y_{7\_sp}$	Control reactor pressure
$g_5 = y_{29} - y_{29\_sp}$	Control composition of A in purge
$g_6 = y_{18} - y_{18\_sp}$	Control stripper temperature
$g_7 = y_{17} - y_{17\_sp}$	Control production rate
$g_8 = y_{22} - y_{22\_sp}$	Control condenser cooling water
$g_9 = y_{40} - y_{40\_sp}$	Control product composition

This optimization problem is solved using the function “fmincon” in Matlab. The maximum amount of inert B (X_{B_purge}) in the purge is calculated for different values of IDV(2) (amount of inert (B) that enters into the plant with the C Feed ($X_{B\_C\_Feed}$)). The composition of inert B in the C feed is increased from 0.5 to 1.0 with increments of 0.1. Table 7.1 shows the maximum composition of B in the purge and its corresponding purge flow for the different compositions of B n the C feed.

Table 7.1 Maximum amount of B in the Purge $X_{B\ purge}$

$X_{B\ C\ Feed}$ IDV(2)	Max $X_{B\ purge}$	Purge Flow
1.0	24.7513	0.3738
0.9	24.3503	0.3413
0.8	23.9737	0.3071
0.7	23.5081	0.2734
0.6	23.0812	0.2382
0.5	22.5353	0.2028

After the optimization problem is solved, it is important to check the stability of this solution. To do so, the plant model is linearized around the steady state obtained from solving the optimization problem. Then, the eigenvalues of this linearized model are checked for stability. If there are positive eigenvalues, the optimization problem needs to be solved again until the plant is stable. In this case, the starting point for the new optimization problem is the result obtained from the previous optimization problem. Every time a new solution is reached the plant model is linearized around the steady state obtained, and the eigenvalues are calculated to check for stability. This process is repeated until the solution is stable. The maximum $X_{B\ purge}$ obtained from optimization is tested using the nonlinear simulation. The maximum composition of inerts that can be handled in the plant is used as a reference (setpoint) value for the inert composition controller in the purge. When the composition of inert that enters into the process changes, this value is fed forward to change the setpoint of the composition of inert in the purge (inventory control). The idea is to minimize the amount of purge and, therefore, the amount of reactant and products that leave the process through the purge. Therefore, every time the amount of inert that enters the plant changes, the setpoint of the inert composition in the purge controller is adjusted, according to the values obtained from the optimization problem. This methodology should be used when the maximum composition in the purge ($X_{B\ purge}$) changes considerably (more than 5%), with changes in the amount of inert that enters into the plant ($X_{B\ C\ Feed}$). If not, the setpoint for the inventory control can be a fixed value.

The values obtained in Table 7.1 for maximum $X_{B\ purge}$ are the limit values that can be handled by the plant. Therefore, it is not convenient to work with these exact values as reference values (setpoint) for the inert inventory control. The reason is that any transient and/or inaccuracy in the model can put the plant operation over the limit, causing the shut down of the plant. Therefore, these values should be lowered (approximately 10%) to avoid operating too near the limit which might cause a shut down of the plant.

In order to determine the economic benefits of using this methodology two simulation of the Tennessee Eastman plant were done. The only difference between these simulations is that one uses the $X_{B\ in\ purge}$=21.83 suggested by Ricker (1995) (Figure 7.4) while the other uses the max $X_{B\ in\ purge}$=24.7 (Figure 7.5) obtained from this methodology.

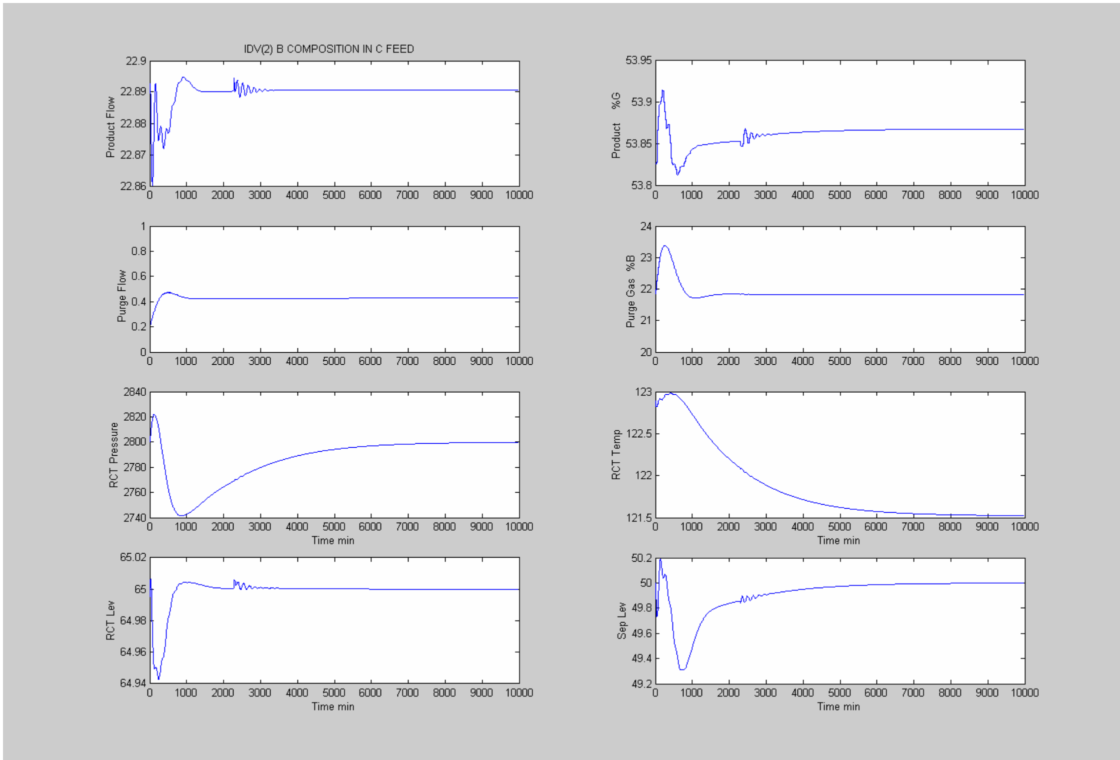


Figure 7.4 Plant Simulation for IDV(2) using $X_{B\ in\ purge}$=21.83

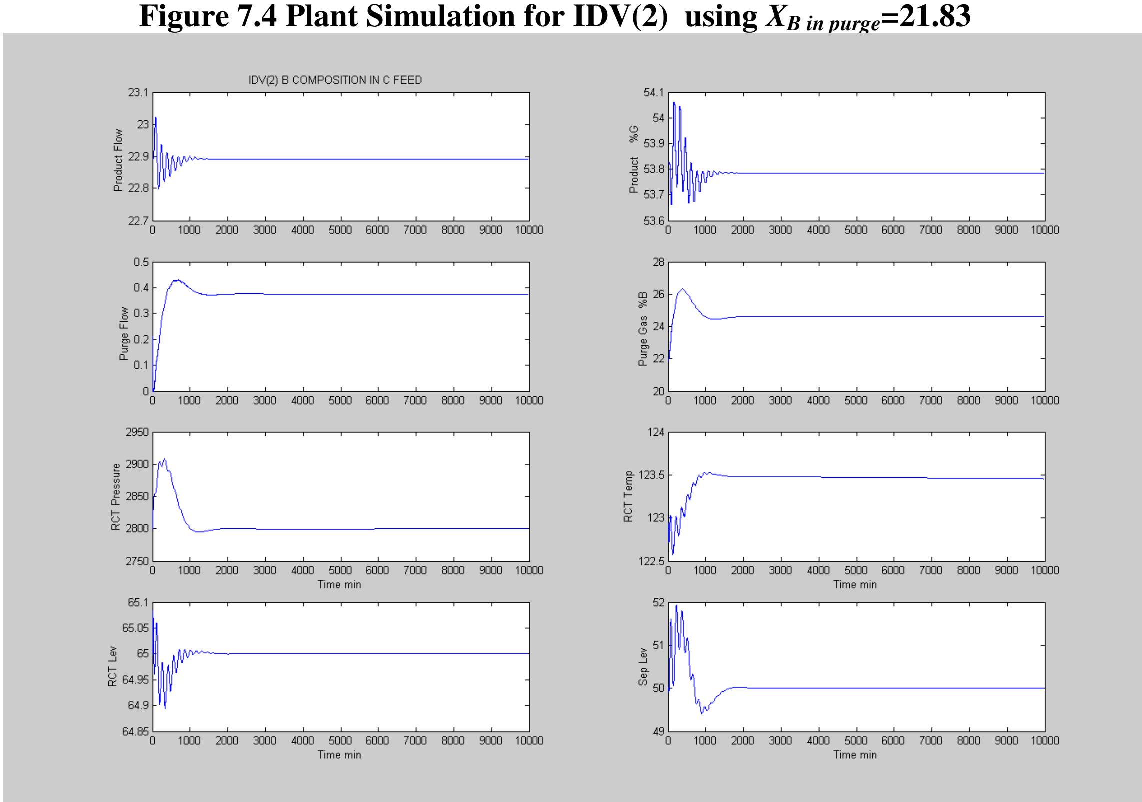


Figure 7.5 Plant Simulation got IDV(2) using max $X_{B\ in\ purge}$=24.7

Comparing the results obtained from both simulations it can be seen that the purge flow is reduced from 0.42 to 0.38 (approximately 9.5%) by using the max $X_{B\ in\ purge}$. In addition, the process operating costs for these simulations were calculated using Downs and Vogel (1993) equation and cost values for reactants and products. The operating cost (OP) for these simulations was calculated for the steady state values. For the first simulation ($X_{B\ in\ purge}$=21.83) the operating cost is OP1=180.24 \$/hr and for the second simulation ($X_{B\ in\ purge}$=24.7) OP2=173.29 \$/hr. By using this methodology, there is approximately 4% savings in the operation cost

Figure 7.6 shows the control of inert B in the purge using the Kalman Filter estimation for XB in C Feed. The setpoint of inert controller in the purge (max $X_{B\ in\ purge}$) is adjusted according to Table 7.1. However, the values of max $X_{B\ in\ purge}$ were lowered 5% to avoid operating at the limit.

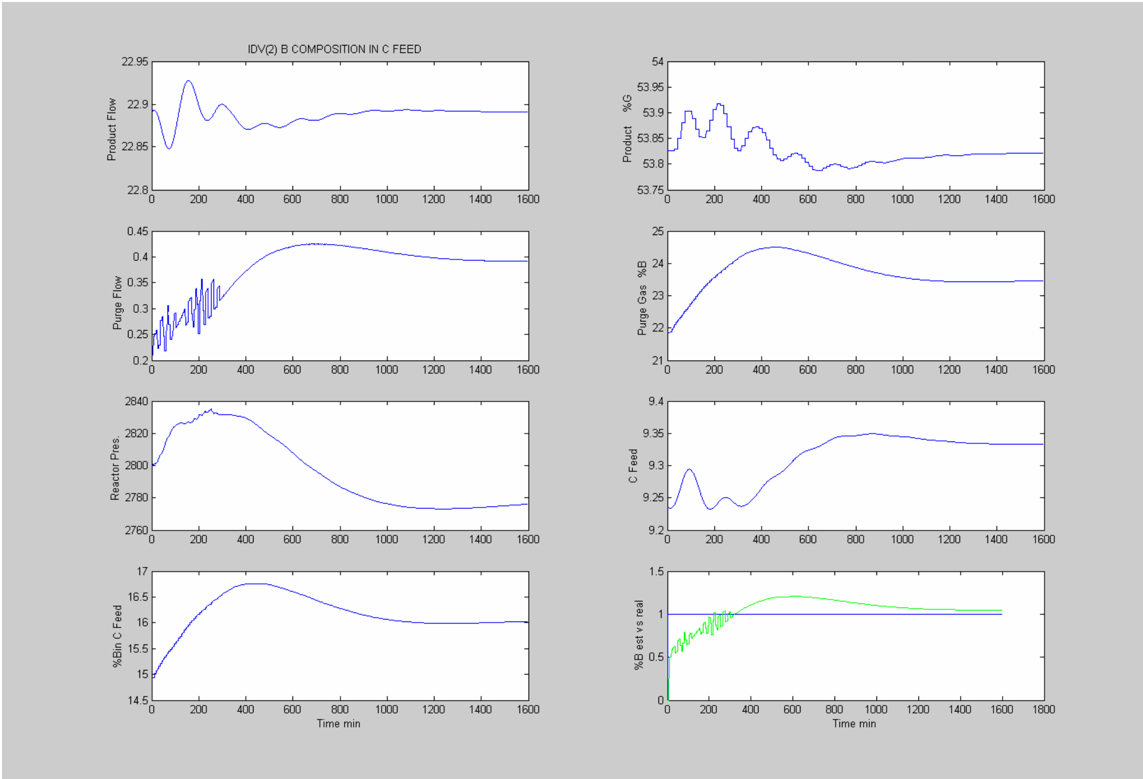


Figure 7.6 Control of inventory of inert using Kalman Filter estimation

Figure 7.6 shows that it is possible to use the estimation of the amount of inert that enter in the plant (using Kalman Filter) to control the amount of purge in the process. However, in the case of the Tennessee Eastman plant it is better to use a hard analyzer because of the dynamics of the process.

7.4. <u>Summary</u>

In this section a new methodology to have optimal control of inerts is presented. This methodology aims to reduce the losses that occur trough the purge by solving an optimization problem to determine the maximum amount of inert that can be handled in the plant without having shut down of the plant due to inert accumulation. To use this methodology it is needed to have an analyzer that measures the concentration of inert within the process as well as an analyzer that measure the amount of inert that enters in the process. If there is not an analyzer that measure the amount of inerts that enters in the plant; this amount can be estimated by developing a soft sensor based on Kalman Filter. If the plant has a slow dynamics and the only analyzer available is in the purge it might be needed to install a real analyzer to measure the composition of inert that enters into the process. Once this composition is known, an optimization problem is solved to determine the maximum amount of inert or minimum amount of purge that can be handled in the plant without having the plant shut down. This optimization problem is solved every time the amount of purge that enters in the process changes. Then the setpoint of the composition of inert in the purge is changed accordingly with the results of the optimization. This methodology should be used when the maximum composition in the purge (*XB* purge max) changes considerably (more than 5%), with changes in the amount of inert that enters into the plant (XB C Feed). This methodology is tested to the Tennessee Eastman plant were the operating cost was reduced approximately 4%. As a conclusion, the optimal control of inert is a practical approach to reduce the costs related to purge.

Chapter 8: Conclusions and Future Work

Summary and Future work

This dissertation presents a systematic procedure to determine measurements and manipulated variables that affect key economic variables in the plant, such as production rate and product quality. This methodology can be used as a tool by process control engineers, not only to identify key variables that should be controlled to improve economics in the plant, but also to design, test, and compare performance of the different control strategies. The main characteristics of this methodology are as follows:

1) It uses a linear time invariant (LTI) state space model of the plant and optimal control theory, to determine key variables in the plant that affect production rate and product quality. To do so, an optimal static output feedback controller is calculated. The control objective is to control production rate and product quality, using other variables in the plant. The information about the interaction and the effect of the variables on production rate and product quality is determined by analyzing and comparing the relative values of the elements of the OSOFC.
2) It aims to improve economics in the plant because of the following:

   a) It improves the control performance of production rate and product quality. Therefore, the plant can be operated close to the operational limits.

b) The calculation of the OSOFC is done for specific disturbance rejection and setpoint changes. Therefore, the resulting control structures are best suited for these cases.

c) It considers economics in the plant by including some of the operational costs (i.e. cost of raw material lost trough the purge and product as weighing elements for production rate and quality in the objective function.

3) It is a hierarchical design procedure that divides the plantwide control problem into sub-problems (stages), more manageable pieces that are easy to solve.

4) It is an automated tool that can be use to design control structures to improve economics in the plant by improving control performance of key economic variables. 4) It has a MPC built on top of the resulting control structure, to control production rate and product quality by manipulating the setpoint of key variables in the plant.

5) The final control structure is tested, using the nonlinear model of the plant.

The methodology presented is successfully applied to two well-known process models: the Tennessee Eastman Model [Downs, 1993] and the Vinyl Acetate Model [Luyben, 1998], obtaining similar or even better results than the ones proposed in the literature. In the case of the Tennessee Eastman Plant, the key variables obtained, using the proposed methodology, are similar to the variables obtained, using Tyreus' Thermodynamic-based approach. The resulting control strategies have demonstrated their efficiency, since the production rate can be easily increased and held to more than 50% of the steady state value. They are also able to reject disturbances IDV1 and IDV2. Tyreus is the only author who demonstrated the performance of his control strategy by increasing the setpoint of the production rate by 50%. To do so, Tyreus ramped the setpoint of the key variables that he identified in a five hour period. The resulting control structure has proven to be more efficient than Tyreus'. It accomplish the same production rate change in a shorter period of time. In addition, it uses less purge flow than Tyreus' control structure, demonstrating in this way its economic benefits. Although, this methodology is based on LTI systems, all the generated control structures were tested, using the nonlinear model of the plant.

This dissertation also presents a systematic methodology to improve the control of the inerts in the process. This methodology not only improves the control of inerts but also the economics in the plant by avoiding unnecessary purge. It is used when the amount of inert that enters in the plant is unknown and changes over time. The main characteristics of this methodology are as follows:

1) It uses the amount of inert that enters in the plant to solve an optimization problem that determines the maximum amount of inert (minimum amount of purge) that can be handled in the process, without having to shut down the plant.
2) It adjusts the purge flow so that the total flow of inert that leaves the process is equal to the total flow of the inert that enters it. To do so, the setpoint for the inert inventory control (which, in general, is controlled by adjusting the purge

flow) is modified, according to the optimization results. Therefore, every time the amount of inert that enters in the process varies, the setpoint of the purge composition (inert composition) controller is changed.

3) It requires an analyzer that measures the amount of purge at some point in the process (i.e. reactor exit or purge flow) as well as an analyzer that measures the amount of inert that enters in the process. This methodology addresses the case where there is no measurement of the amount of inert that enters in the plant. It does that by estimating this amount using a Kalman Filter or by installing a real analyzer. 4) It should be applied when the changes in the composition of purge that enters into the process changes considerably (more than 5%).

This methodology was successfully applied to the Tennessee Eastman Plant, where the amount of inert that enters in the stream C is unknown and changes for different disturbances. By using this methodology, in the Tennessee Eastman Plant, there is approximately 4% savings in the operation cost. In this case the amount of inert was estimated using Kalman Filter. However, a real analyzer should be used when the following situations occur simultaneously: 1) there is only one analyzer that measures the amount of inert in the process; 2) this measurement is located far from the amount that that is being estimated; and 3) the plant has slow dynamics.

In conclusion, the optimal control-based measurements and manipulated variables selection methodology is a practical approach, to help control engineers in the selection of key variables that affect economic variables in the plant. In addition, it can be used to pair these key variables by designing control structures to improve the control performance and , therefore, the economics in the plant. This methodology solves an approximation to an optimal economic problem. First, it improves the control performance of key economic variables in the plant (production rate and product quality). Therefore, tighter control of these economic variables is achieved and the plant can be operated closer to operational constraints. Second, it minimizes purge which is a variable that generally causes significant costs in the plant.

Future work

Even though this methodology has proven to give excellent results, there are several features that can be improved to make it more robust. For instance, this methodology is scaling dependent. In this work, several simulations were performed using different scaling factors. The scaling factors used were normal operational ranges for the process variables. The results obtained for the different scaling factors were similar because, in almost all cases, the same set of key measurements and manipulated variables were obtained. However, the order of importance for the key variables sometimes varied. Some results of the effects of the scaling factor in the OSOFC can be seen in Appendix VII. More work is recommended on the scaling effects, to identify key variables in the plant and their degree of importance. To do so, a sensitivity analysis can be performed to evaluate the effects of the scaling on the important measurements and manipulated variables.

Another important aspect that can be the object of future work is to improve the algorithm used to calculate the OSOFC. Since all the variables in the plant are considered in this methodology, this can be a computationally intensive, especially when highly correlated variables are considered simultaneously. Several simulations demonstrated that when variables that are linearly dependant are considered simultaneously, the algorithm did not converge, or that the convergence was very slow. Currently, this problem is solved by carrying out a correlation and a condition number analysis, to eliminate highly correlated variables and to improve the conditioning of the problem. However, more study on the use of different algorithms such as gradient-based methods (DFP method) for faster convergence in the calculation of OSOFC is recommended.

In addition, economic aspects such as the costs of the reactant, purge, steam and product flows, and work require by process equipments could be taken into consideration to find a control structure that satisfies the economic objectives (to reduce the operation cost) in the plant. An alternative to weighing the product flow and quality could involve using cost as the objective function. The Tennessee Eastman plant can be used to illustrate this idea. In the Tennessee Eastman Plant the objective function based on operating cost has the following form:

Total operation cost= *(purge cost)(purge rate) + (product stream cost)(product rate)*
+(compressor cost)(compressor work)+(steam cost)(steam rate)

Operating costs for this plant are mainly determined by the loss of raw materials. Raw materials are lost in the purge gas, the product stream and by means of the two side reactions. The total operating cost is determined by adding the cost of raw material and the products leaving in the purge stream, the cost of raw material leaving in the product stream, and using an assigned cost to the amount of byproduct formed. Cost of the compressor work and steam to the stripping column are also included [Downs and Vogel, 1993].

$$Cost = (y_{purge\ comp\ cost})(y_{purge\ rate}) + (y_{product\ comp\ cost})(y_{product\ rate}) + (y_{compressor\ cost})(y_{compressor\ work}) + (y_{steam\ cost})(y_{steam\ rate})$$

where

$y_{purge\ comp\ cost}$: (mole fraction of component in purge) (molar cost)

$y_{product\ comp\ cost}$: (mole fraction of component in product) (molar cost)

To use cost as the objective function the molar cost of reactants, products and inerts could be included in the Q matrix. These cost elements can be included as off diagonal element that correspond with the flows (purge and product) and their related compositions. In this case the cost of the compressor work and steam work can be neglected because they are relatively small compare to the costs of the components

.

Appendix I

Correlation Analysis

In this work, the interaction between measure ements is determined by analyzing the correlation of the measurements in each of the left singular vectors of the U matrix. To do so, the model for measurements are calculated as follows:

$$y_i = \sum a_{i,j} \mu_j \qquad \text{A1.1}$$

where $a_{i,j}$ is an element of the left singular vectors by the singular values (U*Σ) from the SVD analysis. Then the correlation coefficient between the measurements can be calculated as

$$r_{i,j} = \varepsilon(y_i y_k)/(\sigma(y_i)\sigma(y_k)) \qquad \text{A1.2}$$

where ε is the expected value, σ is the variance, and i,k refer to different rows. The correlation matrix has elements

$$r_{i,k} = \sum_j a_{i,j} a_{k,j} / \sqrt{(\sum_j a_{i,j}^2 * \sum_j a_{k,j}^2)} \qquad \text{A1.3}$$

The elements of the correlation matrix are known as coefficients of determination $(r_{i,k}{}^2)$. These elements measure the variation of the measurement i that is explained by measurement k. Therefore, to determine the correlation between two measurements, the elements of the correlation matrix in each column are analyzed. If $r_{i,k}{}^2$ is close to 1 then y_i and y_k are correlated. If there is more than one measurement that has a value of $r_{i,k}{}^2$ close to 1, in the same column, this means that these measurements have interaction between them.

After this correlation analysis we found that the following groups of variables are correlated

Correlation Analysis and Condition number Analysis for the Tennessee Eastman Plant

Group # 1: Reactor Pressure, separator pressure and stripper pressure

Group # 2: Separator temperature, stripper temperature, stripper steam flow, recycle flow and reactor feed.

Group # 3: Composition of E in the reactor feed and composition E in the purge

Group # 4: Composition of F in the reactor feed and composition of F in the purge

Group # 5: Composition of G and H in the purge

Condition Number Analysis of the C Matrix

Table A1.1 shows how the condition number of the C matrix is affected when highly correlated measurements are included together in the C matrix.

Table I-I Condition Number Analysis of C Matrix

Measurements included	CN of the C matrix
Reactor pressure	982.0030
Reactor and separator pressure	1.6637e+004
Reactor and stripper pressure	1.3718e+004
Reactor, separator and stripper pressure	2.3442e+012
Composition of G in the purge	9.0452e+004
Composition of H in the purge	5.9808e+004
Compositions of G and H in the purge	7.5591e+016

Correlation Analysis and Condition number Analysis for the Vinyl Acetate Process

The correlation analysis shows that the following groups of variables are correlated:

Group 1: Vaporizer Pressure and Absorber Pressure

Tray 5 Temperature, VAc, H2O, and HAc Column Bottom Composition, H2O Gas Recycle, VAc Gas Recycle, H2O Reactor Feed, HAc Reactor Feed,

Group 2: O_2 Gas Recycle Composition and O_2 Reactor Feed Composition

C_2H_6 Gas Recycle Composition and C_2H_6 Reactor Feed Composition

VAc Gas Recycle Composition and VAc Reactor Feed Composition

C_2H_4 Gas Recycle Composition and C_2H_4 Reactor Feed Composition

CO_2 Gas Recycle Composition and CO_2 Reactor Feed Composition

Group 3: VAc Gas Recycle Composition, HAc Gas Recycle Composition, VAc Reactor Feed

Group 4: Reactor Exit Flow, Organic Product Flowrate

Table I-II Condition Number of C Matrix

Measurements included	**CN of the C matrix**
CN-AM	1.3033e+018
CN-AM - HAc Column Bottom Composition HAc Gas Recycle Composition H2O Reactor Feed Composition HAc Reactor Feed Composition Organic Product Flowrate	2.0554e+004

Appendix II

The OSOF LQR calculation procedure is outlined as follows:

Inputs:

- A scaled state space model (A, B, C, D)
- Weight matrices (Q, R, g_{ij})
- Initial autocorrelation states (X)
- Selection of one of the following LQR numerical algorithms:
  1) Basic Moerder's algorithm
  2) Toivonen's algorithm
  3) Ectended Moerder's algorithm
  4) Extended Toivonen's algorithm
- Selection of one of the following methods of generating an initial stabilizing K Procedure:
  1) Ramdom selection method
  2) Minimization of the maximum eigenvalue of A-BKC method
  3) Petkovski and Rakic's method

Procedure:

- Conditions to run the program:
  1) C has to be full range
  2) R should be positive definite
  3) C^TQC should be positive semi-definite
  4) $\sqrt{Q}C, A$ should be detectable when A is not stable
- Calculate the OSOF controller K using Equation 3.8
  An effective iterative solution algorithm specifically for the output feedback LQR design problem was presented in [Moerder and Calise 1985]. It is given as follows:

  1) Set $\boldsymbol{k = 0}$
  Determine a gain $\boldsymbol{K_0}$ so that $\boldsymbol{A\text{-}BK_0C}$ is asymptotically stable

  2) Set $\boldsymbol{A_k = A\text{-}BK_kCN_x}$

  Solve for $\boldsymbol{P_k}$ and $\boldsymbol{S_k}$ in: $\boldsymbol{0 = A_k^TP_k + P_kA_k + C^TK_k^TRK_k^TC + Q}$
  $$\boldsymbol{0 = A_kS_k + S_kA_k^T + X}$$
  Set $\boldsymbol{J_k = trace(P_kX)}$

  Evaluate the gain update direction: $\boldsymbol{\Delta K = R^{-1}B^TPSC^T(CSC^T)^{-1} - K_k}$
  Update the gain by: $\boldsymbol{K_{k+1} = K_k + \alpha\Delta K}$
  where $\boldsymbol{\alpha}$ is chosen so that $\boldsymbol{A\text{-}BK_{k+1}C}$ is asymptotically stable and $\boldsymbol{J_{k+1} = trace(P_{k+1}X) <= J_k}$
  If $\boldsymbol{J_{k+1}}$ and $\boldsymbol{J_k}$ are closer enough to each other, go to 3, otherwise, set $\boldsymbol{k = k + 1}$ and go to 2
  3.- Set $\boldsymbol{K_{opt} = K_{k+1}}$ and $\boldsymbol{J_{opt} = J_{k+1}}$
  end

Output:

- The OSOF controller K
- The optimal cost J

Details in the generation of the initial K, convergence, algorithms used and programming can be found in Chen (2002)..

Diagonal optimal static output feedback controller (OSOFC)

Chen (2002) proposed 2 alternatives to obtain the diagonal OSOFC:

1) To force the off-diagonal elements in the OSOF controller to be 0 by using large g_{ij}'s that correspond to the off-diagonal elements. The problem with this alternative is that the computation speed is much slower than using zero g_{ij}'s in Equation 3.8.
2) To generate a diagonal initial OSOFC and keep it diagonal when updating it by solving the coupled design equations. The algorithm used for obtaining the diagonal OSOFC is extended from the basic OSOFC explained in Appendix I.

In this work we used the second alternative. A brief description of how the diagonal OSOFC is given as follows

Inputs:

- A scaled state space model (A, B, C, D)
- Weight matrices (Q, R, g_{ij})
- Initial autocorrelation states (X)
- Design parameters (selection of the LQR algorithm and the methods of generating an initial stabilizing K)

Procedure:

- Calculate the diagonal OSOFC
    1) Generate the initial stabilizing K_i, in which all the off-diagonal elements are zeros.
    2) Solve the P_i and S_i based on K_i and calculate J_i.
    3) Use optimization to find a K^* in which all the off-diagonal elements are zeros, such that $\left\| RKCSC^T - B^T PSC^T \right\|_2$ is minimized.
    4) Let $\Delta K = K^* - K_i$ and $K_{i+1} = K_i + \alpha\lambda\Delta K$, where λ is a random number between -0.5 and 0.5. This step should be repeated until $A-BKC$ is stable.
    5) Calculate J_{i+1}.
    6) If $J_{i+1} > J_i$, go to step 4, else if ΔK is small enough, go to step 7, else go to step 2.
    7) Output $Ki+1$

Output:

- The diagonal OSOFC K
- The optimal cost J

Details on the tuning algorithm used can be found in Chen (2002).

Appendix III

Results for Method 1 and Method 2

In this Appendix results form methods 1 and 2, presented in Chapter 4, to determine the set of measurements and manipulated variables that affect production rate for the Tennessee Eastman Plant are presented.

Method 1:
This method does not include the production rate (xmeas17) in the set of available measurements. It does not penalize *K* from Equation 4.3.

Optimal_K =

7	8	9	5	6	11	18	20	23	24	25	26
-0.0044	-0.0042	0.0092	0.0004	-0.0156	0.0140	-0.0035	-0.0600	-0.0653	0.0080	0.0216	0.0251
-0.0014	-0.0033	0.0022	-0.0002	-0.0102	0.0026	0.0011	-0.0215	-0.1228	-0.0136	-0.0389	0.0127
0.0001	0.0005	-0.0001	0.0001	0.0013	-0.0002	-0.0003	0.0017	0.0202	0.0029	0.0083	-0.0013
-0.0003	0.0101	0.0023	0.0016	0.0209	0.0123	-0.0112	0.0076	0.4470	0.0724	0.2014	-0.0249
-0.0000	-0.0001	0.0000	-0.0000	-0.0003	-0.0001	0.0001	-0.0004	-0.0036	-0.0005	-0.0013	0.0003
0.0041	-0.0014	-0.0041	-0.0000	0.0134	-0.0423	0.0094	0.0478	-0.0043	-0.0102	-0.0131	0.0037
0.0028	-0.0006	0.0046	0.0012	0.0148	-0.0624	0.0109	0.0261	0.1141	0.0194	0.0891	0.0273
-0.0002	0.0001	0.0002	-0.0000	-0.0008	0.0026	-0.0006	-0.0028	-0.0016	0.0003	-0.0003	-0.0005
-0.0060	0.0008	0.0139	0.0017	-0.0070	0.0225	-0.0120	-0.0713	0.2308	0.0622	0.1738	0.0165
0.0020	-0.0008	-0.0062	-0.0015	-0.0066	0.0173	0.0047	0.0143	-0.2592	-0.0558	-0.1657	-0.0067
0.0213	0.0219	0.0428	0.0068	0.0908	0.1762	0.0538	0.2534	1.2691	0.2453	0.7136	0.1190

27	28	29	30	31	32	33	34
0.0810	0.0178	0.0491	0.0281	0.0558	0.0087	0.0568	-0.0055
0.0243	0.0049	0.0008	0.0121	0.0268	0.0042	0.0439	0.0024
-0.0009	-0.0002	0.0003	-0.0017	-0.0037	-0.0005	-0.0065	-0.0007
0.0061	0.0041	0.0827	-0.0074	-0.0277	-0.0054	-0.1065	-0.0184
0.0005	0.0001	-0.0008	0.0000	0.0002	0.0001	0.0010	0.0001
-0.0135	-0.0088	-0.1977	-0.0749	-0.1344	-0.0095	-0.0850	-0.0013
0.0634	0.0017	-0.3203	-0.1226	-0.2276	-0.0133	-0.1623	-0.0141
0.0004	0.0006	0.0115	0.0044	0.0080	0.0006	0.0051	0.0001
0.1137	0.0263	0.0990	0.0231	0.0384	0.0068	-0.0093	-0.0212
-0.0823	-0.0150	0.0817	0.0505	0.0932	0.0036	0.1005	0.0226
0.3861	0.0794	0.8438	0.3248	0.6159	0.0527	0.5768	0.0864

Method 2:

This method includes the production rate (xmeas17) in the set of available measurements. It penalizes the production rate measurements in the K of Equation 4.4 by using large corresponding weighting g_{ij} elements.

Optimal_K =

7	8	9	5	6	11	17	18	20	23	24	25
-0.0043	-0.0042	0.0091	0.0004	-0.0156	0.0139	0.0003	-0.0035	-0.0599	-0.0656	0.0080	0.0215
-0.0014	-0.0032	0.0022	-0.0002	-0.0102	0.0025	-0.0000	0.0011	-0.0215	-0.1229	-0.0136	-0.0389
0.0001	0.0004	-0.0001	0.0001	0.0013	-0.0002	0.0000	-0.0003	0.0018	0.0202	0.0029	0.0083
-0.0003	0.0100	0.0023	0.0016	0.0209	0.0122	0.0006	-0.0111	0.0078	0.4469	0.0723	0.2012
-0.0000	-0.0001	0.0000	-0.0000	-0.0003	-0.0001	-0.0000	0.0001	-0.0004	-0.0036	-0.0005	-0.0013
0.0041	-0.0014	-0.0041	-0.0000	0.0134	-0.0421	-0.0004	0.0093	0.0476	-0.0042	-0.0102	-0.0130
0.0027	-0.0006	0.0046	0.0012	0.0148	-0.0622	-0.0005	0.0109	0.0259	0.1142	0.0194	0.0892
-0.0002	0.0001	0.0002	-0.0000	-0.0008	0.0026	0.0000	-0.0006	-0.0028	-0.0017	0.0003	-0.0003
-0.0060	0.0007	0.0139	0.0017	-0.0069	0.0223	0.0007	-0.0119	-0.0710	0.2305	0.0621	0.1736
0.0019	-0.0007	-0.0062	-0.0015	-0.0066	0.0174	-0.0004	0.0047	0.0142	-0.2591	-0.0557	-0.1655
0.0212	0.0215	0.0427	0.0068	0.0907	**0.1755**	0.0031	0.0535	**0.2528**	**1.2690**	**0.2450**	**0.7127**

26	27	28	29	30	31	32	33	34
0.0252	0.0811	0.0178	0.0485	0.0279	0.0555	0.0087	0.0566	-0.0055
0.0127	0.0244	0.0049	0.0007	0.0121	0.0268	0.0042	0.0439	0.0024
-0.0013	-0.0009	-0.0002	0.0003	-0.0017	-0.0038	-0.0005	-0.0065	-0.0007
-0.0248	0.0060	0.0040	0.0821	-0.0077	-0.0281	-0.0054	-0.1067	-0.0183
0.0003	0.0005	0.0001	-0.0008	0.0000	0.0002	0.0001	0.0010	0.0001
0.0036	-0.0135	-0.0088	-0.1969	-0.0746	-0.1339	-0.0095	-0.0848	-0.0013
0.0272	0.0634	0.0017	-0.3193	-0.1222	-0.2270	-0.0133	-0.1619	-0.0141
-0.0005	0.0004	0.0006	0.0114	0.0044	0.0080	0.0006	0.0051	0.0001
0.0165	0.1135	0.0262	0.0981	0.0228	0.0378	0.0067	-0.0095	-0.0211
-0.0068	-0.0821	-0.0149	0.0820	0.0506	0.0933	0.0036	0.1005	0.0226
0.1190	**0.3857**	0.0792	**0.8401**	**0.3240**	**0.6144**	0.0526	**0.5764**	0.0863

As can be seen both methods give the same results

Appendix IV

This Appendix contains additional results for other control candidates of the Tennessee Eastman Plant. First, the results for the downs drill analysis, for the different candidates identified in Chapter 5 (Table 5.5) are presented in Table IV-I. Then, control structures identified for each of these candidates are shown in Table IV-II, followed by the tuning parameters used for these candidates (Table IV-III). In addition, since the TE process needs to operate in three different operation modes, it is desirable to determine a control structure that is feasible for each mode. Therefore, this appendix shows results for other operating modes.

Table IV-I Downs Drill Analysis for TE Process

Candidate	Component	Self-Reg	Why Self-Reg	Manipulated Var	Measurement
Candidate 4	A	No		A Feed	%A RCT Feed, %A Purge
	B	Yes	Purge-RCT P		
	C	No		C Feed	%C RCT Feed,%C Purge
	D	No		D Feed	%D RCT Feed,%D Purge
	E	Yes	E Feed-RCT L		
	F	Yes	RCT CW-RCT T		
Candidate 5	A	No		A Feed	%A RCT Feed, %A Purge
	B	Yes	Purge-RCT P		
	C	No		C Feed	%C RCT Feed,%C Purge
	D	No		D Feed	%D RCT Feed,%D Purge
	E	No		E Feed	%E RCT Feed,%E Purge
	F	Yes	RCT CW-RCT T		
Candidate 6	A	No		A Feed	%A RCT Feed, %A Purge
	B	No		Purge	%B RCT Feed,%B Purge
	C	No		C Feed	%C RCT Feed,%C Purge
	D	No		D Feed	%D RCT Feed,%D Purge
	E	Yes	E Feed-RCT L		
	F	Yes	RCT CW-RCT T		

Candidate	Component	Self-Reg	Why Self-Reg	Manipulated Var	Measurement
Candidate 7	A	No		A Feed	%A RCT Feed, %A Purge
	B	Yes	Purge-RCT P		
	C	No		C Feed	%C RCT Feed,%C Purge
	D	No		D Feed	%D RCT Feed,%D Purge
	E	Yes	E Feed-RCT L		
	F	Yes	RCT CW-RCT T		
Candidate 8	A	No		A Feed	%A RCT Feed, %A Purge
	B	Yes	Purge-RCT P		
	C	No		C Feed	%C RCT Feed,%C Purge
	D	No		D Feed	%D RCT Feed,%D Purge
	E	No		E Feed	%E RCT Feed,%E Purge
	F	Yes	RCT CW-RCT T		
Candidate 9	A	No		A Feed	%A RCT Feed, %A Purge
	B	No		Purge	%B RCT Feed,%B Purge
	C	No		C Feed	%C RCT Feed,%C Purge
	D	No		D Feed	%D RCT Feed,%D Purge
	E	Yes	E Feed-RCT L		
	F	Yes	RCT CW-RCT T		

Table IV-II Plantwide Control Structure Candidates for the TE Process

No.	RCT P	RCT L	RCT T	Sep. L	Str. L	% A	%B	% C	% D	%E	Sep T	MPC Prod & %G
4	Purge	E	RCT CW	Sep. Bot.	Stri. Bot.	A		C	D		CCW	RCT T, %D, Sep T, RCT L, %A, %C,
5	Purge	CCW	RCT CWT	Sep. Bot.	Stri. Bot.	A		C	D	E		
6	CCW	E	RCT CWT	Sep. Bot.	Stri. Bot.	A	Purge	C	D		RCT T	RCT P, Sep T, %D %A, %C
7	Purge	E		Sep. Bot.	Stri. Bot.	A		C	D		CCW	
8	Purge	CCW		Sep. Bot.	Stri. Bot.	A		C	D	E		
9	CCW	E		Sep. Bot.	Stri. Bot.	A	Purge	C	D		RCT T	

Table IV-III Tuning Parameters for Tennesse Eastmant Plant

Mode #	R P	R L	R T	Sp L	St L	%A	%C	%D	Sp T
Mode 1	-12.14	6.97	2.64	-0.50	-0.50	7.11	2.59	2.26	2.55
Mode 2	-10.29	7.64	1.90	-0.50	-0.50	11.51	2.47	1.50	2.74
Mode 3	-14.33	7.60	4.25	-0.50	-0.50	4.61	2.18	4.08	1.96
All Modes	-12.5	7.6	2.6	-0.5	-0.5	7.1	2.3	2.2	2.5

Control Structure for Candidate 4 for Operation Modes 2 and 3

Chapter 5 shows results for candidate 4 (from Table 5.5) for operating mode1. To determine the control structure for the same candidate for operation modes 2 and 3, the same procedure is applied. Stages 1 (preparation), 2 (control structure for safety variables), and 3 (control structure for inventory variables) from the procedure are the same for each operation mode. Stage 4 (control structure for production rate and quality) is the key stage in determining the control structure because this stage is the one that gives information about the strongest measurements and manipulated variables to control production rate and product quality. If stage 4 gives the same strongest measurements and manipulated variables for operation modes 2 and 3 as the ones given in mode 1, then the same MPC design is used for these modes. Since there are three different set of tuning parameters (one for each mode), trial and error is used to find a single set of tuning parameters that works for the three operation modes.

In the case that a different set of strongest measurements and manipulated variables are obtained for any mode then, 1) the scaling factor should be evaluated since the OSOF solutions depends on how measurements, manipulated variables and states are scaled; and 2) the multiple steady state operation design procedure, proposed by Chen et. al. (2003), is applied. The only limitation of this method is that if specific forcing is desired then, the forcing must have the same effect on each state for each operating mode.

Results for Candidate 4 Operation Mode 2

Table IV-IV OSOFC Matrix   Mode2

Control Objective: to Control Product Rate and Quality

SP	RF	**SpT**	**StT**	CpW	BF	E F	F F	BP	EP	FP	**GP**	Σrow
%A	0.108	0.523	-0.804	0.072	-0.002	-0.004	-0.016	0.017	-0.015	-0.007	-0.222	**1.792**
RP	0.092	-0.639	0.127	0.023	0.045	0.033	0.028	-0.018	0.040	0.006	0.212	1.264
%C	0.125	-0.337	-1.685	0.001	0.014	0.018	0.009	0.012	-0.030	-0.017	0.067	**2.313**
%D	0.176	-2.409	0.399	0.159	0.026	-0.130	0.019	0.024	0.066	0.065	0.873	**4.344**
R T	-0.467	6.284	-2.642	0.031	-0.250	-0.838	-0.154	0.052	-0.103	-0.171	-1.760	**12.75**
CCW	-0.494	4.293	-2.688	-0.316	-0.085	-0.805	-0.024	-0.140	-0.079	-0.243	-0.950	**10.12**
R L	-0.165	2.887	-1.006	-0.072	0.013	0.220	0.024	-0.088	0.046	-0.124	-0.941	**5.585**
S L	-0.111	0.251	-0.451	-0.103	0.019	-0.237	-0.020	-0.083	0.019	-0.042	-0.131	1.467
St L	0.016	-0.438	0.344	0.038	0.006	-0.073	-0.011	-0.049	0.038	0.006	0.151	1.171
Σcol	1.754	**18.06**	10.15	0.815	0.460	2.358	0.304	0.483	0.436	0.681	5.306	

Table IV-V Optimal Static Output Feedback Controller (OSOFC)

Man Var	**S T**
%A	-0.028
RP	0.004
%C	-0.008
%D	0.001
RCT T SP	0.124
CCW SP	**0.484**
RCT L SP	0.019
Sep L SP	-0.005
Stp L SP	-0.000

Table IV- VI OSOFC Matrix Mode 3

Control Objective: to Control Product Rate and Quality

SP	RF	**SpT**	**StT**	CpW	BF	E F	F F	BP	EP	FP	**GP**	Σrow
%A	0.032	-0.111	-0.228	0.058	-0.007	-0.013	-0.000	-0.003	0.017	-0.001	0.062	**0.532**
RP	0.024	-0.208	-0.025	0.037	0.008	-0.017	0.002	-0.007	0.011	-0.000	0.080	0.419
%C	0.026	-0.117	-0.181	0.044	-0.003	-0.021	-0.000	-0.004	0.002	0.000	0.064	0.461
%D	0.166	-1.588	0.191	0.222	0.067	-0.122	0.007	-0.027	0.011	0.006	0.604	**3.010**
R T	0.211	-0.957	-0.285	0.270	0.010	0.005	-0.001	0.004	0.012	0.009	0.402	**2.166**
CCW	-0.155	0.030	-0.217	-0.106	-0.012	-0.168	0.016	-0.099	0.109	-0.020	0.007	**0.939**
R L	-0.086	0.708	-0.155	-0.103	-0.050	0.077	-0.002	-0.015	0.027	-0.006	-0.277	**1.506**
S L	-0.041	0.142	-0.071	-0.042	-0.019	-0.014	-0.001	-0.010	0.009	-0.003	-0.081	0.433
St L	-0.044	-0.038	0.081	-0.048	0.010	-0.017	-0.001	0.001	0.010	-0.000	-0.020	0.270
Σcol	0.786	**3.899**	1.434	0.929	0.186	0.453	0.030	0.169	0.208	0.045	1.598	

Table IV-VII Optimal Static Output Feedback Controller (OSOFC)

Man Var	**S T**
%A	-0.006
RP	-0.001
%C	0.000
%D	0.009
RCT T SP	0.145
CCW SP	**0.514**
RCT L SP	0.001
Sep L SP	-0.003
Stp L SP	-0.000

Next figures (IV-I, IV-II, IV-III, V-IV, IV-V, IV-VI, IV-VII, IV-VIII , and IV-IX), show the nonlinear simulations for Candidate 4 for setpoin change (to achieve maximum production rate) and disturbance rejection for operation modes 1, 2, and 3 using the tuning parameter that work for all modes.

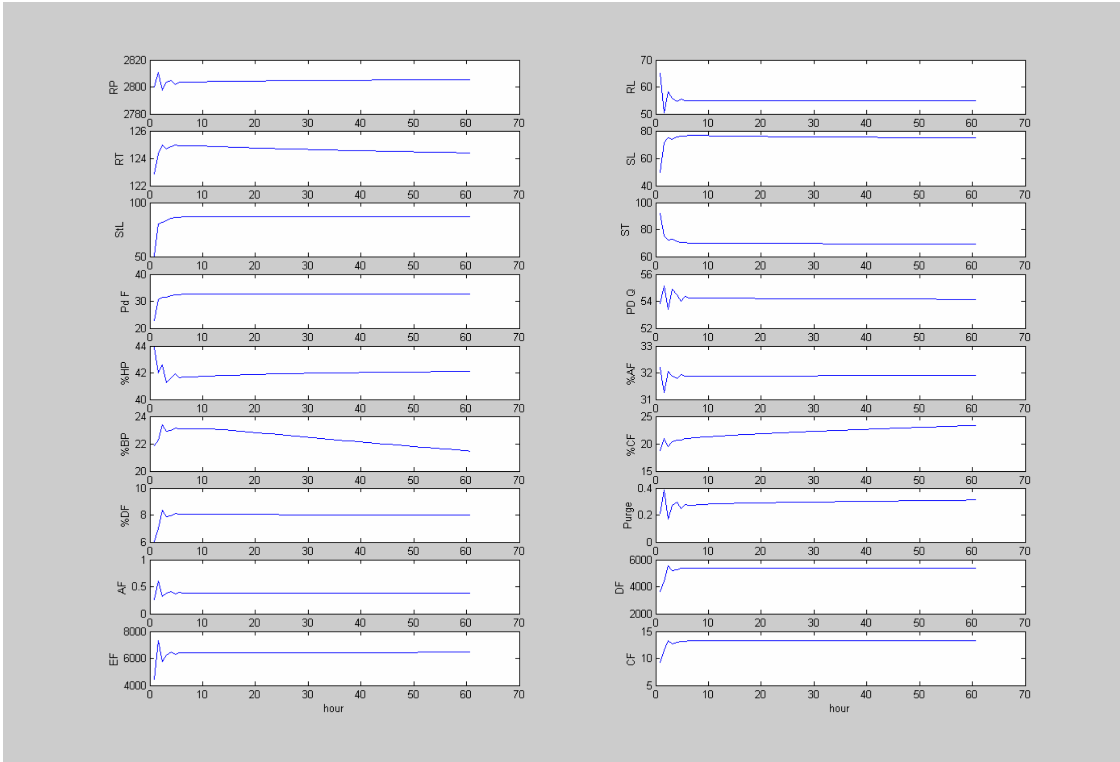


Figure IV-I Maximum Production Rate for Operation Mode 1 (Candidate 4-6)

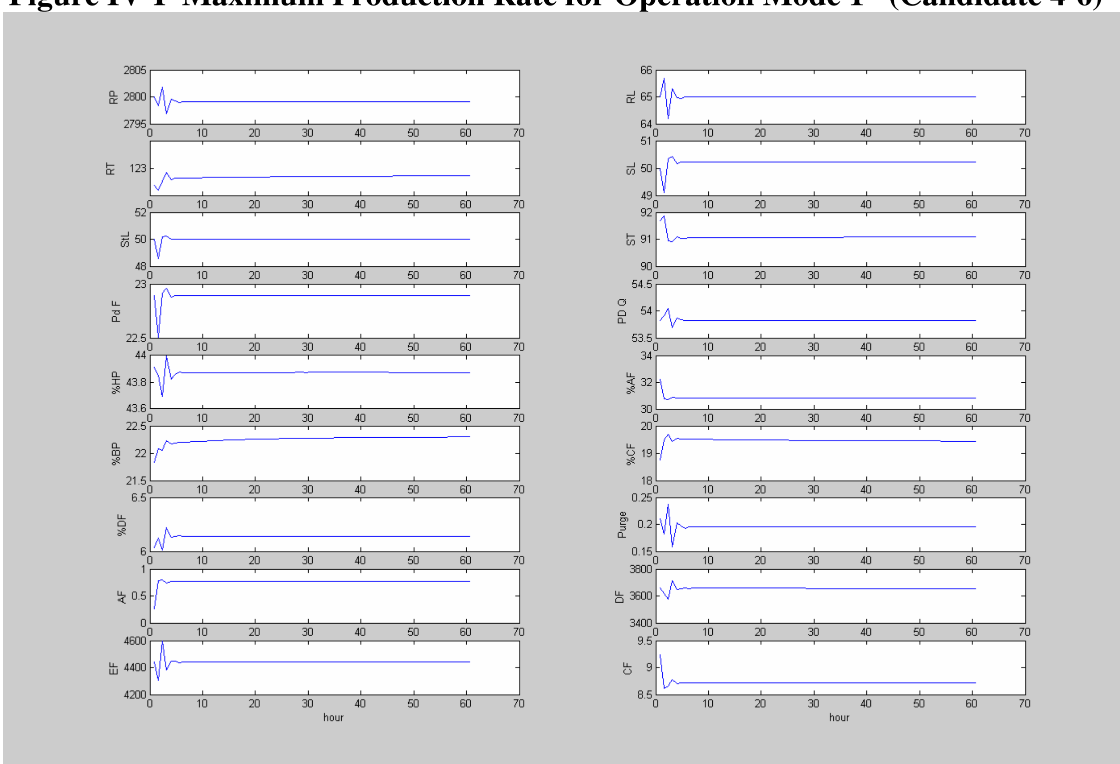


Figure IV-II IDV(1) for Operation Mode 1 (Candidate 4-6)

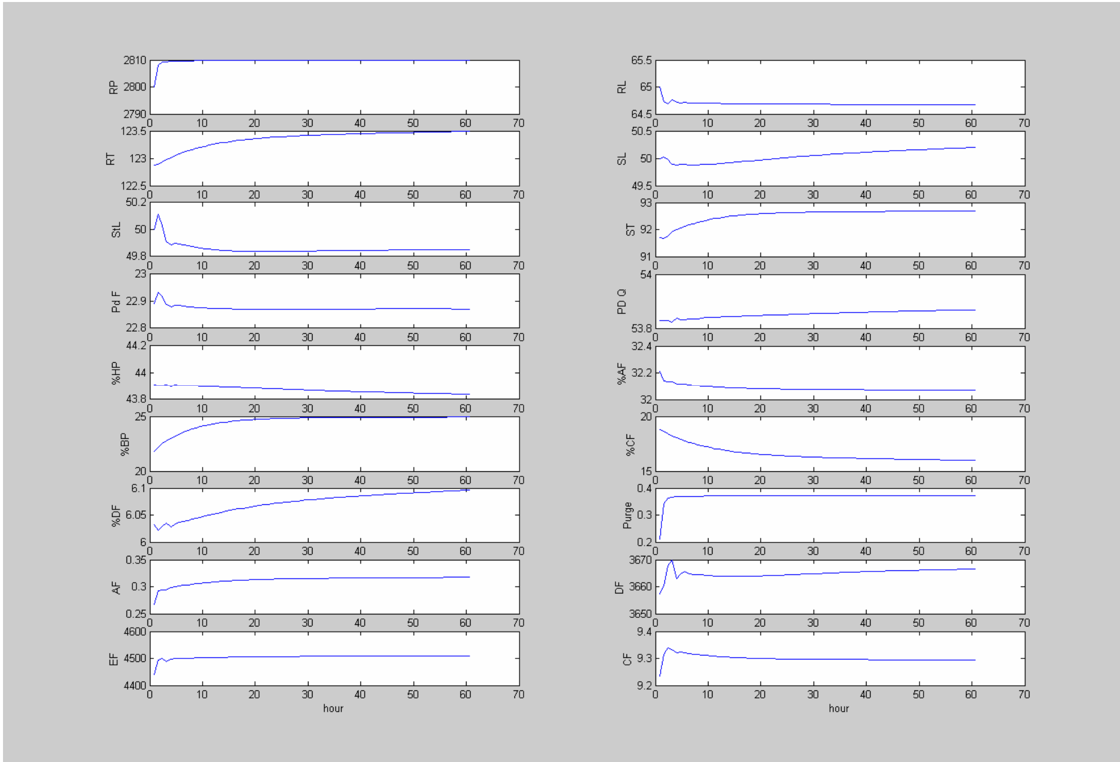


Figure IV-III IDV(1) for Operation Mode 1 (Candidate 4-6)

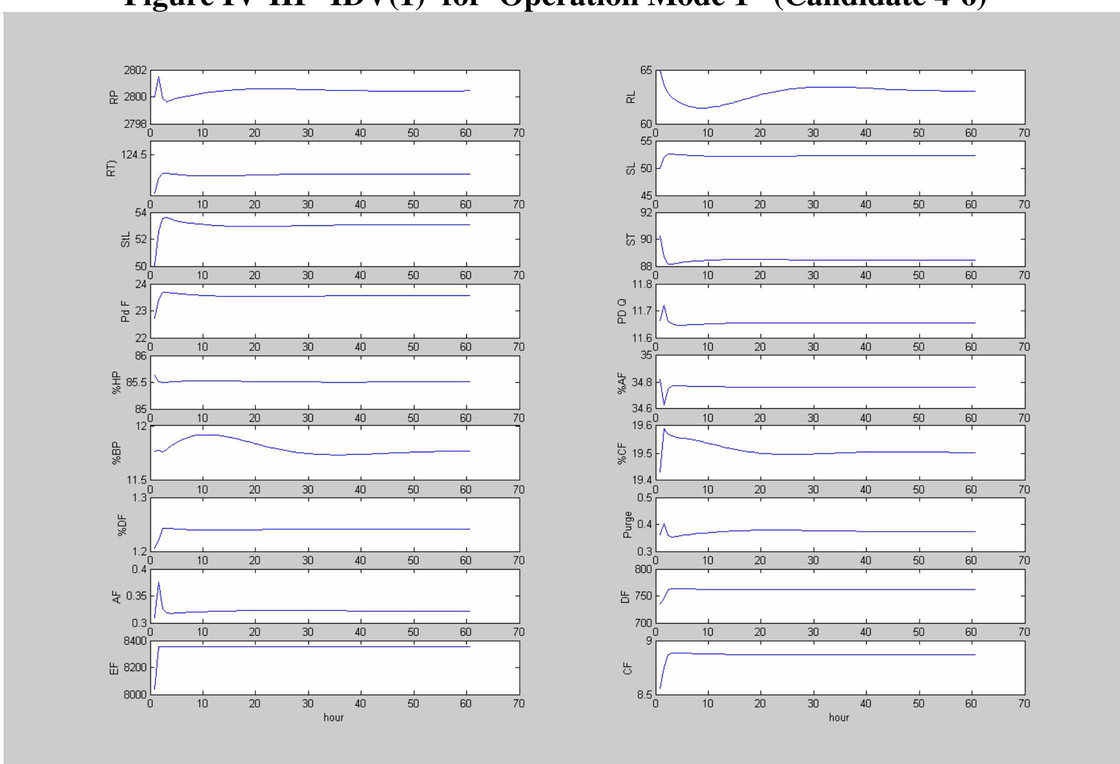


Figure IV-IV Maximum Production Rate for Operation Mode 2 (Candidate 4-6)

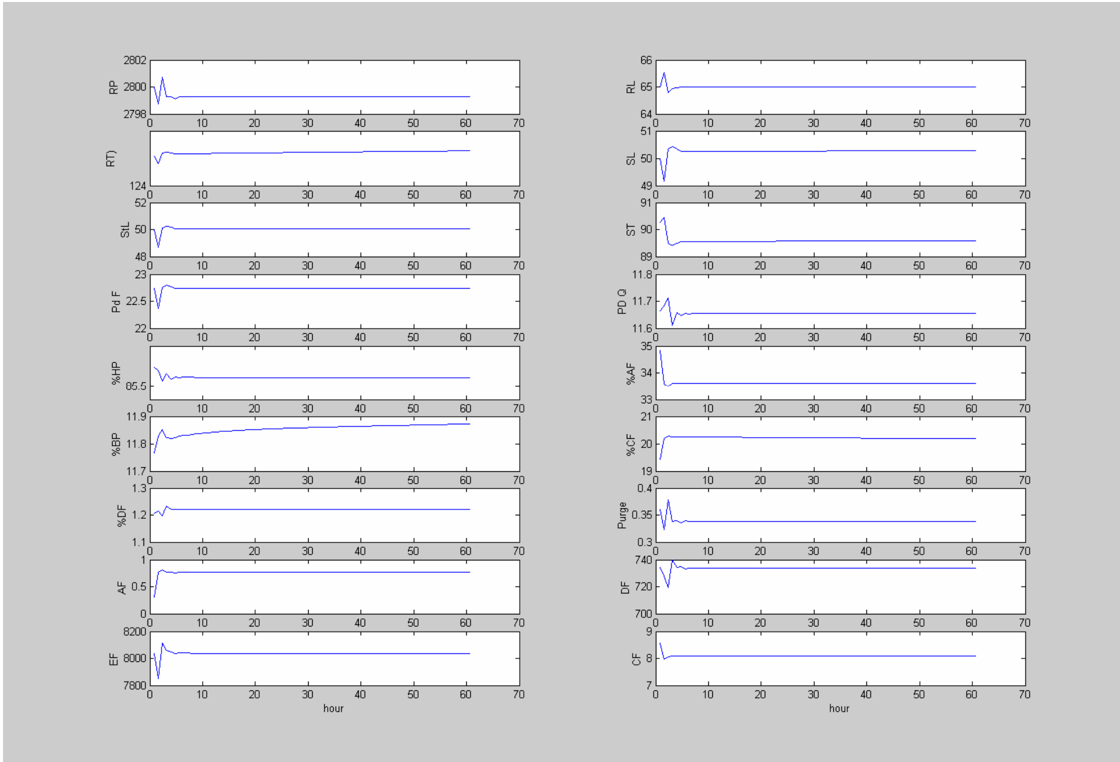


Figure IV-V IDV(1) for Operation Mode 2 (Candidate 4-6)

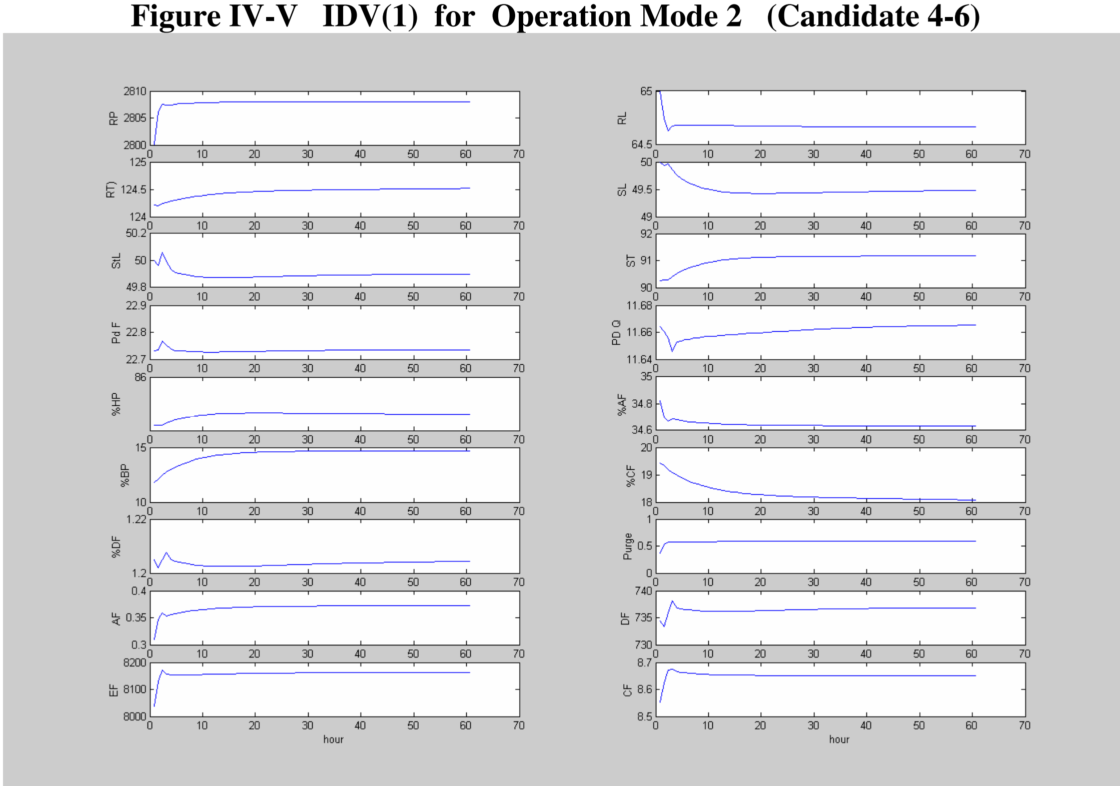


Figure IV-VI IDV(2) for Operation Mode 2 (Candidate 4-6)

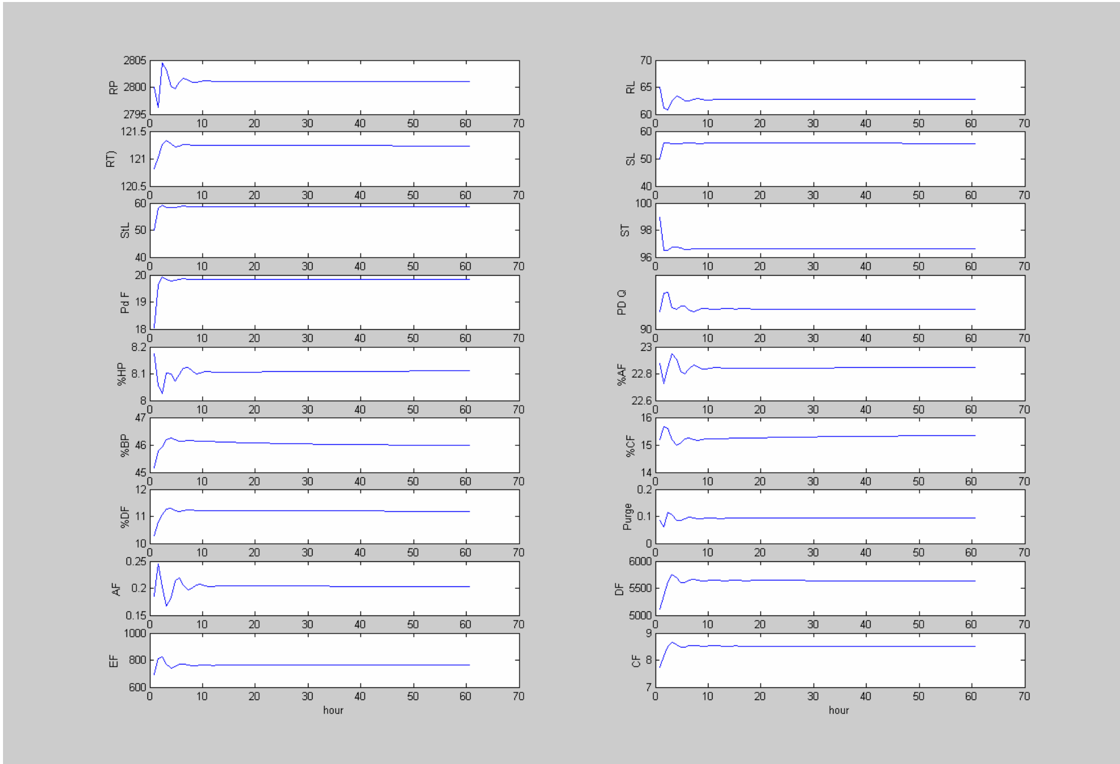


Figure IV-VII Maximum Production Rate for Operation Mode 3 (Candidate 4-6)

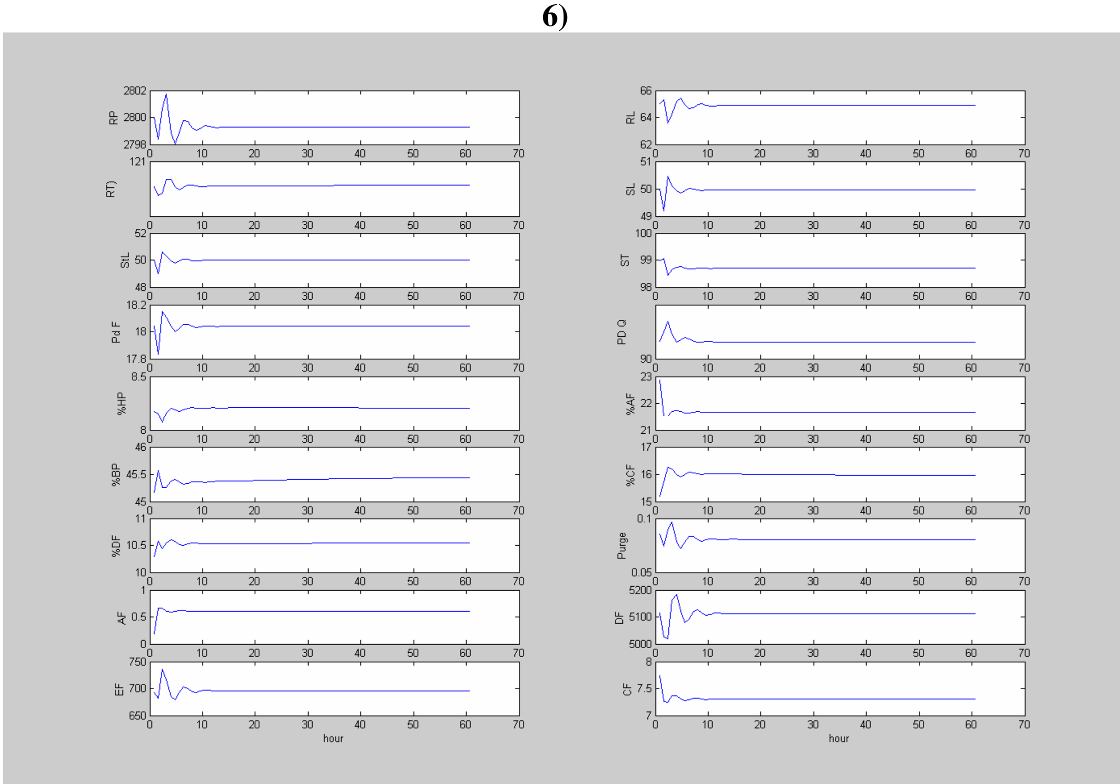


Figure IV-VIII IDV(1) for Operation Mode 3 (Candidate 4-6)

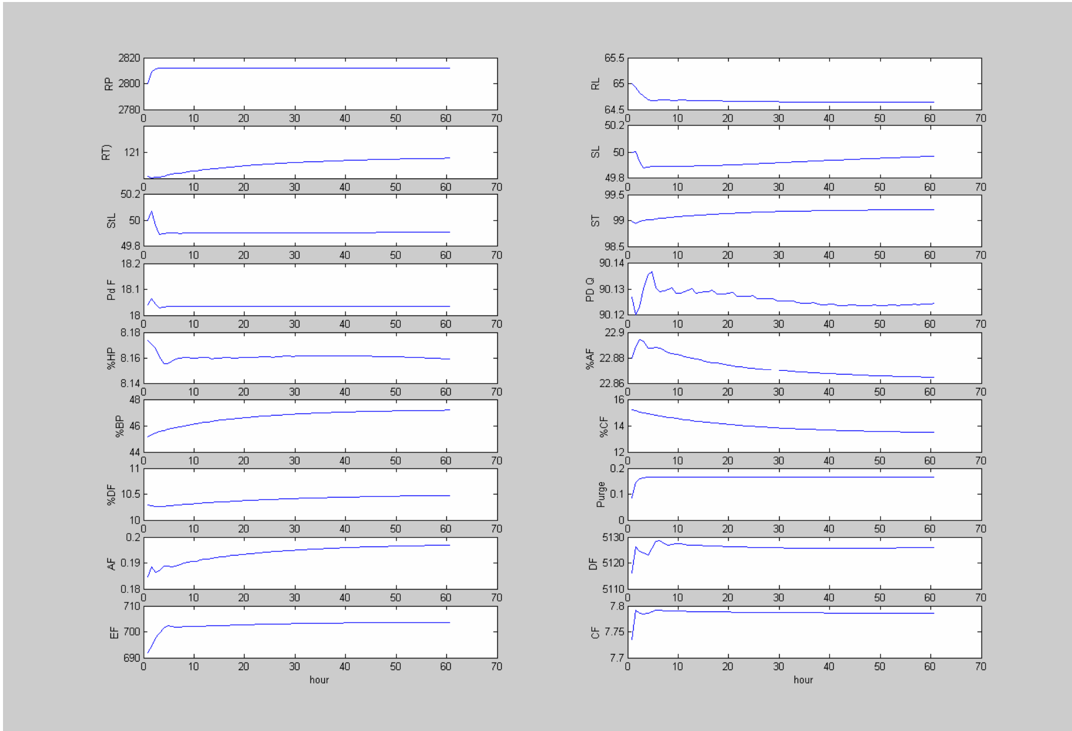


Figure IV-IX IDV(2) for Operation Mode 3 (Candidate 4-6)

Appendix V

This Appendix contains results for the Vinyl Acetate Plant. First, the results for the downs drill analysis for the different candidates identified in Chapter 6 are presented in Table V-I. Then, control structures identified for each of these candidates are shown in Table V-II, followed by the tuning parameters used (Table V-III).

Table V - I Downs Drill Analysis for Vinyl Acetate Process

Candidate	Component	Self-Reg	Why Self-Reg	Manipulated Var	Measurement
Candidate 1	O_2 (react)	Yes	O_2 Feed - %O_2		
	C_2H_4 (react)	Yes	C_2H_4 feed -Abs pressure		
	HAc (react)	Yes	HAc feed-HAc level		
	C_2H_6 (inert)	No		Purge	% C_2H_6 **in gas recycle –** reactor feed
	VAc (prod)	Yes	Column exit-Column level		
	H_2O (byprod)	No		Organic reflux	%H_2O **Column bottom -** organic product composition
	CO_2 (byprod)	No		CO_2 removal inlet	%CO_2 **in gas recycle –** reactor feed
Candidate 3	O_2 (react)	Yes	O_2 Feed - %O_2		
	C_2H_4 (react)	**Yes**		C_2H_4 feed	% C_2H_4 **in gas recycle –** reactor feed
	HAc (react)	Yes	HAc feed-HAc level		
	C_2H_6 (inert)	No		Purge	% C_2H_6 **in gas recycle –** reactor feed
	VAc (prod)	Yes	Column exit-Column level		
	H_2O (byprod)	No		Organic reflux	%H_2O **Column bottom -** organic product composition
	CO_2 (byprod)	No		CO_2 removal inlet	%CO_2 **in gas recycle –** reactor feed
Candidate 7	O_2 (react)	Yes	O_2 Feed - %O_2		
	C_2H_4 (react)	Yes	C_2H_4 feed -Abs pressure		
	HAc (react)	Yes	HAc feed-HAc level		
	C_2H_6 (inert)	No		Purge	% C_2H_6 **in gas recycle –** reactor feed
	VAc (prod)	Yes	Column exit-Column level		
	H_2O (byprod)	No		Organic reflux	%H_2O **Column bottom -** organic product composition
	CO_2 (byprod)	No		CO_2 removal inlet	%CO_2 **in gas recycle –** reactor feed

Candidate	Component	Self-Reg	Why Self-Reg	Manipulated Var	Measurement
Candidate 9	O_2 (react)	Yes	O_2 Feed - %O_2		
	C_2H_4 (react)	**Yes**		C_2H_4 feed	% C_2H_4 **in gas recycle** – reactor feed
	HAc (react)	Yes	HAc feed-HAc level		
	C_2H_6 (inert)	No		Purge	% C_2H_6 **in gas recycle** – reactor feed
	VAc (prod)	Yes	Column exit-Column level		
	H_2O (byprod)	No		Organic reflux	%H_2O **Column bottom** - organic product composition
	CO_2 (byprod)	No		CO_2 removal inlet	%CO_2 **in gas recycle** – reactor feed

Table V-II Plantwide Control Structure Candidates for the VA Process

	Candidates			
Variables	**1**	**3**	**7**	**9**
Vaporizer level	Vap steam duty	Vap steam duty	Vap liquid inlet	Vap liquid inlet
Separator level	Sep liquid exit	Sep liquid exit	Sep liquid exit	Sep liquid exit
Absorber level	Abs liquid exit	Abs liquid exit	Abs liquid exit	Abs liquid exit
Organic level	Col organic exit	Col organic exit	Col organic exit	Col organic exit
Aqueous level	Col aqueous exit	Col aqueous exit	Col aqueous exit	Col aqueous exit
Column base level	Col bottom exit	Col bottom exit	Col bottom exit	Col bottom exit
HAc tank level	Fresh HAc feed	Fresh HAc feed	Fresh HAc feed	Fresh HAc feed
Tray 5 temperature	Col reboiler duty	Col reboiler duty	Col reboiler duty	Col reboiler duty
% O_2 reactor feed	Fresh O_2 feed	Fresh O_2 feed	Fresh O_2 feed	Fresh O_2 feed
Vaporizer pressure	Vap vapor exit	Vap vapor exit	Vap vapor exit	Vap vapor exit
Absorber pressure	Fresh C_2H_4 feed	Sep vapor exit	Fresh C_2H_4 feed	Sep vapor exit
Reactor input temp	Vap heater duty	Vap heater duty	Vap heater duty	Vap heater duty
Reactor exit temp	Reactor shell temp	Reactor shell temp	Reactor shell temp	Reactor shell temp
FEHE exit temp	FEHE bypass ratio	FEHE bypass ratio	FEHE bypass ratio	FEHE bypass ratio
O_2 (react)	Self-Regulated	Self-Regulated	Self-Regulated	Self-Regulated
C_2H_4 (react)	Self_Regulated	C_2H_4 feed	Self-Regulated	C_2H_4 feed
HAc (react)	Self -Regulated	Self -Regulated	Self-Regulated	Self-Regulated
C_2H_6 (inert)	Purge	Purge	Purge	Purge
VAc (prod)	Self-Regulated	Self -Regulated	Self -Regulated	Self -Regulated
H_2O (byprod)	Organic Reflux	Organic reflux	Organic reflux	Organic reflux
CO_2 (byprod)	CO_2 removal inlet	CO_2 removal inlet	CO_2 removal inlet	CO_2 removal inlet
MPC Prod rate Prod Quality	GRP SP- Ab Pressure Separator Vapor Exit Decanter Temp SP Reactor E Temp SP	GRP SP- Ab Pressure Separator Vapor Exit Reactor E Temp SP Decanter Temp SP	Same as 1	Same as 3

Table V-III Tuning Parameters for Vinyl Acetate Model

Vap L	Sep L	Abs L	Org L	Aq L	Col L	HAc L	T 5 T	%O_2 F	Vap P
-0.2	-0.2	-0.2	-0.2	-0.2	-0.2	0.2	0.14018	0.50576	-0.3968
Abs P	R inT	REx T	FEHE T	%C_2H_6 I	%H_2O	CO_2	GR F	Vap T	
0.59966	0.22001	0.88649	0.44747	-0.77644	-1.838	-0.0628	0.7749	0.3687	

Results for Vinyl Acetate Plant using proportional only controllers

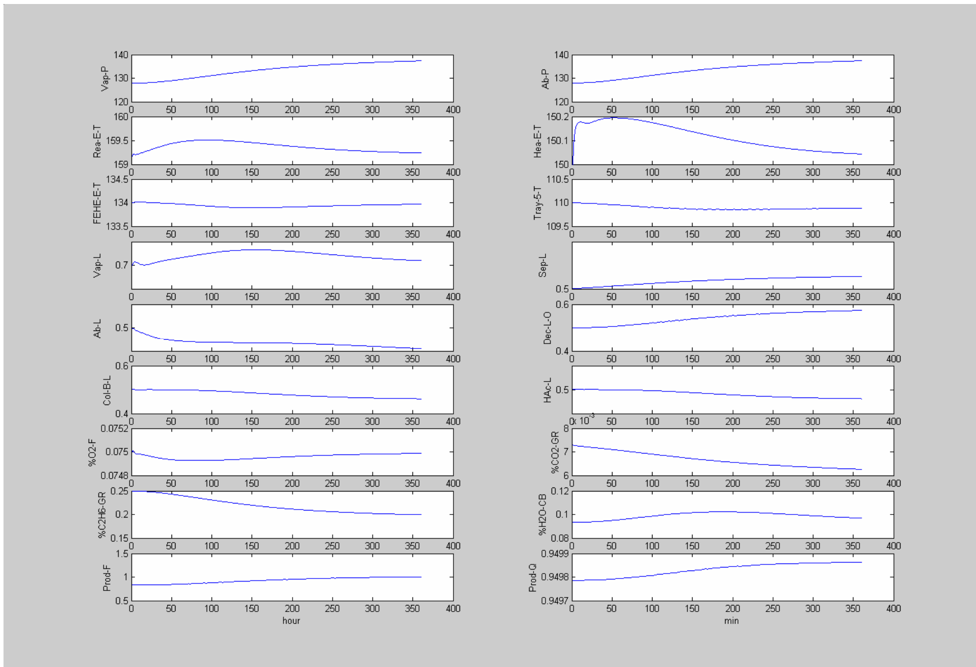


Figure V-I 20% Setpoint change in the Product flow

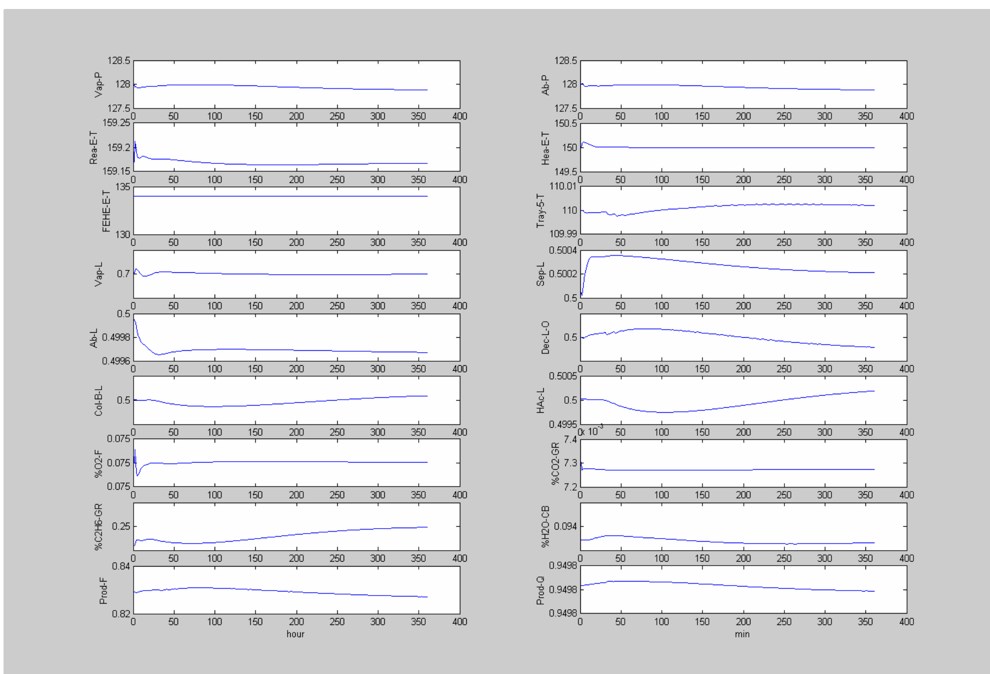


Figure V-II DTB(1) from 0.001 to 0.003 mol fraction

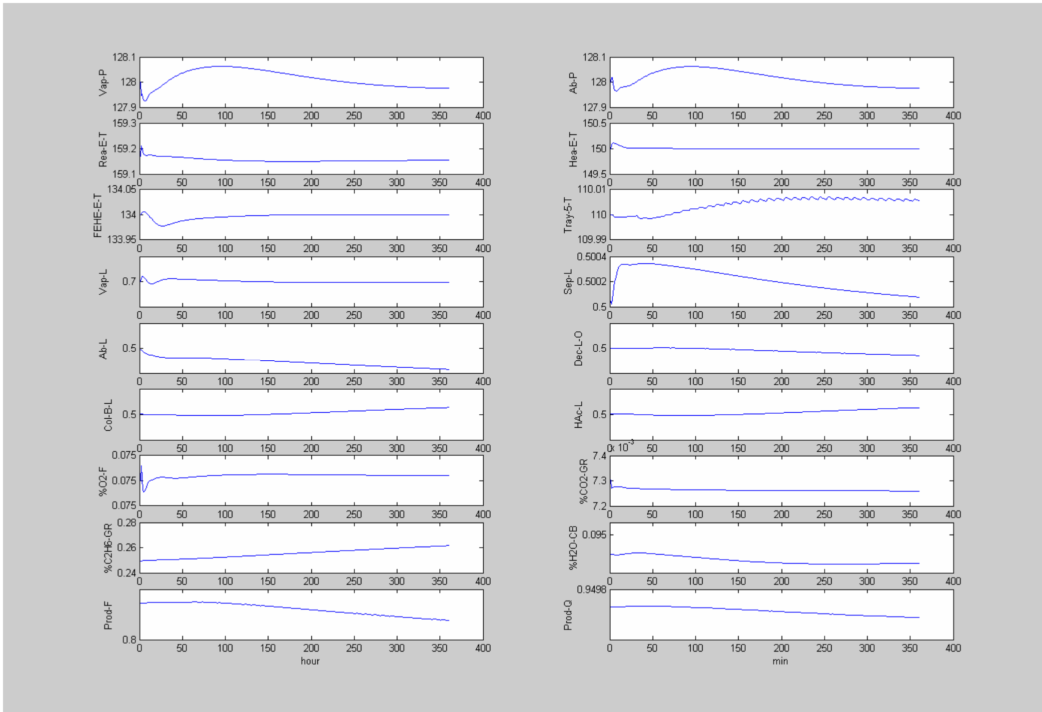


Figure V-III   DTB(2) 0.0003 mol fraction of water (impurity) in acetic acid feed stream

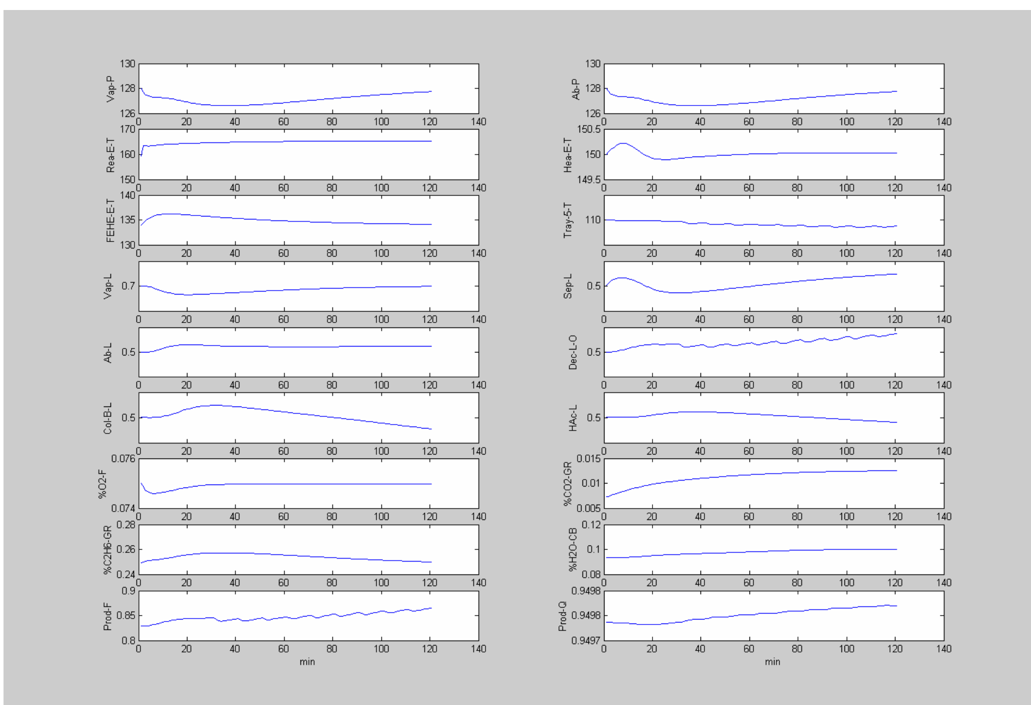


Figure V-IV   DTB(3): 6^{o}C increase in the reactor temperature

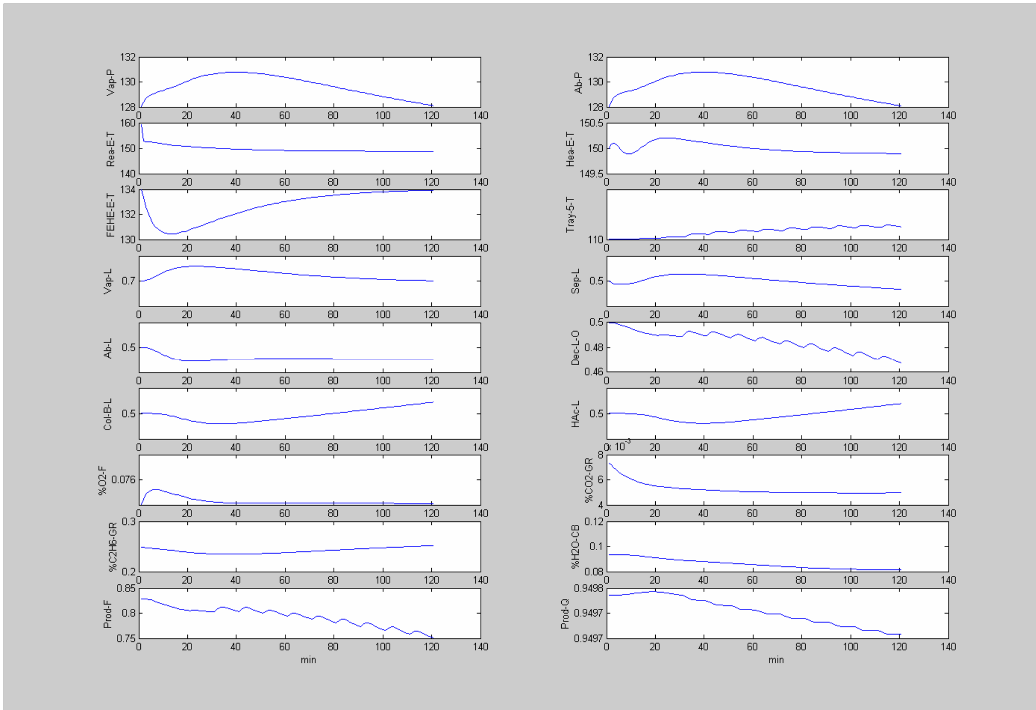


Figure V-V DTB(4): 10^{o}C Decrease in the reactor temperature

Appendix VI

Derivation to include proportional integral (PI) controller in the state space model for the plant

$$\dot{x} = Ax + Bu + Gd$$
$$y = Cx + Du + Md$$

$$\dot{x}' = ax' + b(y^{SP} - y)$$
$$u = cx' + e(y^{SP} - y)$$

$$y = Cx + D\left[cx' + e(y^{SP} - y)\right]$$

$$y(I + De) = Cx + Dcx' + Dey^{SP}$$

$$y = (I + De)^{-1}Cx + (I + De)^{-1}Dcx' + (I + De)^{-1}Dey^{SP} + (I + De)^{-1}Md$$

$$\dot{x} = Ax + B\left[cx' + ey^{SP} - ey\right] + Gd$$

$$\dot{x} = Ax + Bcx' + Bey^{SP} - Be\left[(I + De)^{-1}Cx + (I + De)^{-1}Dcx' + (I + De)^{-1}Dey^{SP} + (I + De)^{-1}Md\right] + Gd$$

$$\dot{x} = \left[A - Be(I + De)^{-1}C\right]x + \left[Bc - Be(I + De)^{-1}Dc\right]x' + \left[Be - Be(I + De)^{-1}De\right]y^{SP}$$
$$+ \left[- Be(I + De)^{-1}M + G\right]d$$

$$\dot{x}' = ax' + by^{SP} - b\left[(I + De)^{-1}Cx + (I + De)^{-1}Dcx' + (I + De)^{-1}Dey^{SP} + (I + De)^{-1}Md\right]$$

$$\dot{x}' = \left[a - b(I + De)^{-1}Dc\right]x' + b(I + De)^{-1}Cx + \left[b - b(I + De)^{-1}De\right]y^{SP} - b(I + De)^{-1}Md$$

$$\begin{bmatrix} \dot{x} \\ \dot{x}' \end{bmatrix} = \begin{bmatrix} A - Be(I+De)^{-1}c & Bc - Be(I+De)^{-1}Dc \\ b(I+De)^{-1}C & a - b(I+De)^{-1}Dc \end{bmatrix} \begin{bmatrix} x \\ x' \end{bmatrix} +$$

$$\begin{bmatrix} Be - Be(I+De)^{-1}De \\ b - b(I+De)^{-1}De \end{bmatrix} \begin{bmatrix} y^{SP} \\ \end{bmatrix}$$

$$+ \begin{bmatrix} -Be(I+De)^{-1}M + G \\ -b(I+De)^{-1}M \end{bmatrix} \begin{bmatrix} d \\ \end{bmatrix}$$

$$\begin{bmatrix} y \end{bmatrix} = \begin{bmatrix} (I+De)^{-1}C & (I+De)^{-1}Dc \end{bmatrix} \begin{bmatrix} x \\ x' \end{bmatrix} + \begin{bmatrix} (I+De)^{-1}De \end{bmatrix} \begin{bmatrix} y^{SP} \end{bmatrix} +$$

$$\begin{bmatrix} (I+De)^{-1}M \end{bmatrix} \begin{bmatrix} d \end{bmatrix}$$

Appendix VII

This Appendix contains scaling results for the Tennessee Eastman Plant. These results show the effects of the scaling factors of some measurements and manipulated variables in the Σcol (L_1-norm col) and Σrow (L_1-norm row) of the OSOFC matrix.

These results show that changes in the scaling factor of the measurements and/or the manipulated variables result in changes in the OSOFC element values, for the particular variable being scaled and other related variables. However, the dominant measurements and manipulated variables remain the same but in some cases the order of importance of these variables might vary.

Efects of the Scaling in measurement

Reactor Feed scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	Scalinf F
0.0905	***13.5773***	***2.4964***	0.8634	0.3899	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.01xms(6)**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.1*xms(6)**
9.0525	***13.5778***	***2.4964***	0.8634	0.3899	0.6813	0.1853	0.3465	0.2627	0.2652	4.6259	**1*xms(6)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.2204	0.8218	***1.1887***	***4.6739***	***7.9884***	***3.8500***	***2.4462***	0.7602	0.8350	**0.01*xms(6)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**0.1*xms(6)**
1.5732	**1.3585**	***1.4504***	***6.9032***	***9.1787***	***6.2105***	***3.3710***	**1.7625**	0.9390	**1* xms(6)**

Separator Temperature scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.9053	***6.7886***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6258	**10**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**20**
0.9053	***33.9442***	***2.4964***	0.8634	0.3899	0.6813	0.1853	0.3465	0.2627	0.2652	4.6259	**50**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
0.9145	0.6136	***0.9267***	***3.4569***	***5.6348***	***3.0137***	***1.8666***	0.7329	0.6507	**10**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**20**
2.2664	1.6413	***2.0698***	***9.1354***	***15.4821***	***7.2173***	***4.5212***	1.2067	1.4259	**50**

Stripper Temperature scaling Effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.9053	***13.5774***	***1.2482***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**10**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**20**
0.9053	***13.5777***	***6.2411***	0.8634	0.3899	0.6813	0.1853	0.3465	0.2627	0.2652	4.6259	**50**
0.9053	***13.5774***	***12.482***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**100**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.1600	0.8565	***1.0282***	***4.7586***	***7.6857***	***3.8880***	***2.4317***	0.8161	0.7263	**10**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**20**
1.5299	0.9128	***1.7652***	***5.2305***	***9.3296***	***4.5946***	***2.8258***	0.9569	1.1990	**50**
1.9920	0.9834	***2.6863***	***5.8201***	***11.384***	***5.4779***	***3.3187***	1.1330	1.7898	100

Compressor work scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.9053	***13.5773***	***2.4964***	**0.2878**	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.1*xms(20)**
0.9053	***13.5774***	***2.4964***	**0.8634**	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.3*xms(20)**
0.9053	***13.5779***	***2.4964***	**1.4390**	0.3899	0.6813	0.1853	0.3465	0.2627	0.2652	4.6259	**0.5*xms(20)**
0.9053	***13.5773***	***2.4964***	**2.8780**	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**1*xms(20)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.2239	0.8565	***1.2050***	***4.7361***	***8.0387***	***3.8885***	***2.4461***	0.7857	0.8431	**0.1*xms(20)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**0.3*xms(20)**
1.2811	0.8846	***1.2201***	***5.0170***	***8.1546***	***4.2408***	***2.6143***	0.9170	0.8459	**0.5*xms(20)**
1.3522	0.9198	***1.2386***	***5.3678***	***8.2990***	***4.6813***	***2.8248***	1.0810	0.8493	**1*xms(20)**

Composition of B in Reactor Feed scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.9053	***13.5776***	***2.4964***	0.8634	**0.1950**	0.6814	0.1853	0.3464	0.2627	0.2653	4.6259	**0.1*xms(24)**
0.9053	***13.5774***	***2.4964***	0.8634	**0.3900**	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.2*xms(24)**
0.9053	***13.5774***	***2.4964***	0.8634	**0.9749**	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.5*xms(24)**
0.9053	***13.5774***	***2.4964***	0.8634	**1.9498**	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**1*xms(24)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.2381	0.8590	1.2121	***4.8540***	***8.0017***	***4.0375***	***2.5279***	0.8379	0.8365	**0.1*xms(24)**
1.2524	0.8706	1.2125	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**0.2*xms(24)**
1.2958	0.9052	1.2137	***4.9442***	***8.3813***	***4.1461***	***2.5375***	0.8919	0.8685	**0.5*xms(24)**
1.3680	0.9630	1.2158	***5.0569***	***8.8558***	***4.2818***	***2.5497***	0.9595	0.9086	**1*xms(24)**

Manipulated Variables

%A in Reactor Feed scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.8044	***11.7080***	***2.5936***	0.7324	0.4907	0.7111	0.1798	0.3482	0.2971	0.2630	3.9671	**0.5*xms(1)**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**2*xms(1)**
1.2495	***15.0645***	***2.0996***	1.0004	0.2808	0.6394	0.1833	0.4714	0.2353	0.2881	5.1132	**4*xms(1)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
0.3919	0.9535	***1.0682***	***4.5653***	***7.8749***	***3.9768***	***1.7892***	0.8005	0.6753	**0.5*xms(1)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**2*xms(1)**
2.8660	0.7425	***1.6223***	***4.8206***	***8.1030***	***3.9688***	***2.6174***	0.8869	0.9980	**4*xms(1)**

%C Composition in reactor feed scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.9452	***13.2945***	***2.0301***	1.0990	0.2445	0.4730	0.1549	0.6191	0.2701	0.2969	4.3560	**0.1*xms(4)**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.25*xms(4)**
1.2098	***13.4706***	***2.1884***	1.0309	0.7988	1.0259	0.2510	0.3010	0.2860	0.2345	5.1250	**1*xms(4)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.3179	0.7338	0.8418	***5.2071***	***7.4031***	***3.8227***	***2.5540***	1.1663	0.7366	**0.1*xms(4)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**0.25*xms(4)**
1.2042	0.9670	***1.3119***	***4.4239***	***9.3438***	***4.6230***	***2.4882***	0.7354	0.8246	**1*xms(4)**

%D Composition in reactor feed scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.8190	***13.1109***	***2.3959***	0.8000	0.3635	0.6351	0.1758	0.3540	0.2514	0.2676	4.4363	**0.05*xms(2)**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.1*xms(2)**
1.0015	***13.0670***	***2.5626***	0.8850	0.4411	0.7069	0.1982	0.2929	0.2205	0.2305	4.4452	**1*xms(2)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.5316	0.7389	***1.4385***	***3.1954***	***8.3945***	***3.8331***	***2.7101***	0.8640	0.9036	**0.05*xms(2)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**0.1*xms(2)**
0.5816	0.9636	0.6230	***7.4716***	***6.6737***	***4.8033***	***1.4252***	0.8379	0.6713	**1*xms(2)**

Reactor Level scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.9570	***14.5946***	***2.4305***	0.8692	0.4306	0.6265	0.2031	0.3900	0.2839	0.2866	4.8493	**0.05*xms(3)**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.1*xms(3)**
0.9440	***13.5347***	***6.2456***	0.9170	0.5723	1.5929	0.1521	0.2589	0.4654	0.2637	5.0912	**1*xms(3)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.3928	0.9409	***1.3000***	***5.5534***	***9.1397***	***3.9617***	***2.0552***	0.7562	0.8211	**0.05*xms(3)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**0.1*xms(3)**
1.0791	***1.5698***	***1.3638***	***6.1393***	***7.3917***	***4.1695***	***6.5412***	0.6061	1.1773	**1*xms(3)**

Reactor Pressure scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
1.0015	***11.2722***	***3.3884***	0.9606	0.6595	0.7271	0.2275	0.3619	0.1932	0.2816	3.6035	**0.1*xms(10)**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**1*xms(10)**
0.9980	***18.7778***	***1.0725***	0.9082	0.2168	0.6696	0.0933	0.3911	0.5226	0.2023	7.0545	**10*xms(10)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
0.9177	0.1642	0.6774	***4.7534***	***8.3141***	***3.7562***	***2.4223***	0.7963	0.8755	**0.1*xms(10)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**1*xms(10)**
1.5915	***2.5519***	***1.8299***	***5.5980***	***8.2861***	***5.9053***	***3.4742***	0.9338	0.7360	**10*xms(10)**

Separator Level scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
1.0333	***13.2347***	***2.3618***	0.8531	0.6575	0.9021	0.1822	0.4580	0.2782	0.2196	4.7918	**0.5*xms(14)**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**xms(14)**
0.8939	***14.5294***	***2.6833***	0.8442	0.2605	0.6455	0.1641	0.5294	0.2786	0.3025	4.6746	**2*xms(14)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
0.8786	0.6091	***1.3391***	***4.0196***	***7.3195***	***6.1318***	***2.8147***	1.1758	0.6841	**0.5*xms(14)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**xms(14)**
1.7314	0.9353	***1.4738***	***5.3476***	***9.3557***	***3.0149***	***2.4945***	0.6159	0.8368	**2*xms(14)**

Stripper Level scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.8704	***13.4731***	***2.5534***	0.8068	0.3857	0.6585	0.1857	0.3669	0.2449	0.2689	4.4782	**0.5*xms(17)**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**xms(17)**
0.8927	***13.4886***	***2.6019***	0.8852	0.3966	0.6799	0.1842	0.3285	0.2718	0.2533	4.6524	**2*xms(17)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.2800	0.8122	***1.3169***	***4.5712***	***8.3358***	***3.6688***	***2.3786***	0.9884	0.9407	**0.5*xms(17)**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**xms(17)**
1.2397	0.8967	***1.1219***	***5.0392***	***7.8630***	***4.3830***	***2.6196***	0.8029	0.6691	**2*xms(17)**

Reactor Temperature scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.8757	***14.1089***	***2.7528***	0.8502	0.4576	0.6839	0.2030	0.3256	0.2499	0.2762	4.8341	**10**
0.9053	***13.5774***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**20**
0.8587	***13.0472***	***2.2705***	0.8364	0.3569	0.6778	0.1733	0.3882	0.2673	0.2556	4.4385	**50**

1.6785	0.8931	***1.4900***	***5.0788***	***8.3028***	***3.9109***	***2.6400***	0.7697	0.8541	**10**
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**20**
1.0302	0.8139	***1.0751***	***4.5987***	***7.8678***	***4.0821***	***2.3873***	0.8683	0.8472	**50**

Product Flow scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
1.0773	***14.815***	***2.7422***	1.2058	0.3845	0.9077	0.1941	0.3186	0.3203	0.2383	5.1726	**0.05xms(17)**
0.9053	***13.577***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.1*xms(17)**
0.4657	***12.311***	***2.5456***	0.3444	0.4198	0.5164	0.1807	0.3260	0.2060	0.2565	3.9046	**0.5*xms(17)**
0.4314	***12.149***	***2.5257***	0.3181	0.4174	0.5002	0.1821	0.3186	0.1980	0.2530	3.8392	**1*xms(17)**
0.4191	***12.083***	***2.5170***	0.3129	0.4159	0.4960	0.1826	0.3163	0.1942	0.2516	3.8133	**10*xms(17)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**0.1*xms(17)**
1.5613	0.5769	***1.4112***	***2.8928***	***9.1542***	***2.9701***	***1.8313***	0.7974	0.2816	**0.5*xms(17)**
1.5835	0.5638	***1.4090***	***2.7885***	***9.2134***	***2.9240***	***1.7841***	0.7802	0.0865	**1*xms(17)**
1.5910	0.5593	***1.4074***	***2.7569***	***9.2344***	***2.9077***	***1.7673***	0.7767	0.0009	10*xms(17)

Composition of G in the product scaling effect

RF	SpT	StT	CpW	BF	E F	F F	BP	EP	FP	GP	
0.9053	***13.577***	***2.4964***	0.8634	0.3900	0.6814	0.1853	0.3464	0.2627	0.2652	4.6259	**0.02*xms(40)**
0.4694	***2.0454***	***1.7868***	0.5343	0.1455	0.2369	0.0683	0.1702	0.1579	0.0545	0.7317	**0.1*xms(40)**
0.3691	***0.9222***	***1.8710***	0.4579	0.1015	0.2290	0.0526	0.1161	0.1624	0.0351	0.3493	**0.5*xms(40)**
0.3644	***0.8821***	***1.8738***	0.4561	0.1003	0.2336	0.0523	0.1130	0.1627	0.0348	0.3308	**1*xms(40)**

% A	R P	%C	%D	RT	CCW	RL	SL	StL	
1.2524	0.8706	***1.2125***	***4.8765***	***8.0965***	***4.0646***	***2.5303***	0.8514	0.8445	**0.02*xms(40)**
0.4831	0.2499	0.2533	***1.2614***	***1.1287***	***0.9421***	***0.7961***	0.6640	0.6223	**0.1*xms(40)**
0.4650	0.0483	0.2654	0.0945	***1.0493***	***1.2943***	0.1507	0.7524	0.5462	**0.5*xms(40)**
0.4600	0.0395	0.2643	0.0470	***1.0473***	***1.3177***	0.1268	0.7579	0.5435	**1*xms(40)**

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