2009

Framework for operability assessment of production facilities: an application to a primary unit of a crude oil refinery

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ACKNOWLEDGEMENTS

I would like to thank my research advisor, Dr. Jose Romagnoli for his patience, guidance and support over the course of this research. I will always be indebted to him. He was a constant inspiration, and his assistance and suggestions were very helpful towards the completion of this work. I would also like to thank the members of my exam committee, Dr. John Flake and Dr Francisco Hung for their efforts in reviewing and evaluating my research. I thank Dan Mowrey, Omar Galan and Rob Willis for their helpful insights and valuable suggestions throughout the course of this research.

I would also thank the entire PSE group. It has been nice to work with you all and I won’t forget the memorable moments that we shared together. I also gratefully acknowledge the financial support from the Chemical Engineering Department for providing me a financial scholarship and support to finish my course.

I would also acknowledge my friends Diwakar, Velavan, Raghava, Vikram and Shilpa for their wonderful help and assistance during the course of the project. Finally, I would also thank my family and friends for their support and encouragement.
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ABSTRACT

This work focuses on the development of a methodology for the optimization, control and operability of both existing and new production facilities through an integrated environment of different technologies like process simulation, optimization and control systems. Such an integrated environment not only creates opportunities for operational decision making but also serves as training tool for the novice engineers. It enables them to apply engineering expertise to solve challenges unique to the process industries in a safe and virtual environment and also assist them to get familiarize with the existing control systems and to understand the fundamentals of the plant operation.

The model-based methodology proposed in this work, starts with the implementation of first principle models for the process units on consideration. The process model is the core of the methodology. The state of art simulation technologies have been used to model the plant for both steady state and dynamic state conditions. The models are validated against the plant operating data to evaluate the reliability of the models. Then it is followed by rigorously posing a multi-optimization problem. In addition to the basic economic variables such as raw materials and operating costs, the so-called “triple-bottom-line” variables related with sustainable and environmental costs are incorporated into the objective function. The methodologies of Life Cycle Assessment (LCA) and Environmental Damage Assessment (EDA) are applied within the optimization problem. Subsequently the controllability of the plant for the optimum state of conditions is evaluated using the dynamic state simulations. Advanced supervisory control strategies like the Model Predictive Control (MPC) are also implemented above the basic regulatory control. Finally, the methodology is extended further to develop training simulator by integrating the simulation case study to the existing Distributed Control System (DCS). To demonstrate the effectiveness of the proposed methodology, an industrial case study of the primary
unit of the crude oil refinery and a laboratory scale packed distillation unit is thoroughly investigated. The presented methodology is a promising approach for the operability study and optimization of production facilities and can be extended further for an intelligent and fully-supportable decision making.
CHAPTER 1

BACKGROUND, PROJECT GOALS AND THESIS STRUCTURE

1.1 Introduction

The developments in technologies is expanding the boundaries and broadening the domain of what is technically and economically feasible to achieve in the application of model activities in manufacturing plants. The recent advancements have broadened the definition and the role of process simulations. In the engineering domain, the use of process simulations is promptly becoming an integral part of the plant operations. The field of simulation has widened from simple automation of design calculations to being the centre of ‘integrated engineering workflows’ that assist a variety of decision making tasks, from preliminary design to plant troubleshooting (Sundaram, 2005). The different simulation environments can now be seamlessly integrated with control hardware/software to offer broad spectrum of benefits. They allow the development of model-based strategies that enable greater sophistication of manufacturing operations.

Manufacturing processes are facing more challenges today than ever before as a result of increased competitiveness and varying energy demands. In addition, increasingly stringent fuel regulations, growing concern over global warming, environmental emissions and unconventional feed stocks have created complex and sometimes conflicting challenges for plant operation. The considerable developments that have taken place in process control, aimed towards a tighter integration between design and control to reduce capital and operating costs also add to the complexity. Companies must design and operate chemical processes effectively and efficiently so they may survive in today’s highly competitive world. It is very important for a process engineer to respond quickly and efficiently not only to the challenges in the plant operation but
also to the business change. They should be trained to make apt business decisions and also to take timely action to any deviation from the normal behavior of the process or in an emergency situation while meeting the objectives of designing and operating efficient, safer and profitable process plants. Therefore, there is a need of methodologies and training tools to assist the plant engineers in their tasks to assess different processing configurations of process plants, optimize the unit for a given configuration with constraints on unit capacities and product pattern and to understand the fundamentals of plant operation.

1.2 Motivation

Chemical processes in particular the petroleum refining processes are becoming highly integrated and interactive. The process heat integration and optimization for the efficient use of energy & resources to increase the bottom-line have made the processes more complex. The complex and multivariable nature of such processes make the design and operation of plant wide control systems a non-trivial task. Therefore there is a need for an integrated approach that support the process engineers in general decision making processes.

Existing production facilities present an interesting challenge from the operability point of view. The optimal operating conditions for a given processing unit are not unique, they are subjected to the constant fluctuations in the raw material quality and sustained unknown disturbances in the process and also there are a priori limitations related with the capacity and performance of equipment units involved in the process. Considering the above limitations and environmental effects, it is possible to put forward a methodology that embraces the optimization and control of an existing production facility. On the other hand, in the past, the corporations sought to develop young engineers through intensive training and apprenticeship but the bottom line thinking of today no longer allows such an approach. The complex plant operations and reduced training duration necessitate developing an effective training tool not only to understand
the fundamentals of the plant operations but also to improve the ability to optimize the plant performance within the same environment.

Developments in open-software architectures and information technology have enabled to integrate synergically different software components from heterogeneous sources to solve complex model-based problems. The accurate and realistic simulations allow engineers to use the integrated simulation environments to identify operational and physical constraints in a safe, theoretical environment. It facilitates a systematic, troubleshooting of problems and also to explore opportunities to improve and optimize the plant performance. Such integrated environment provides two fold advantages mainly to analyze advanced operational procedures and operator/student training.

1.3 Background

Over the past decades the use of simulations has been widely accepted in chemical engineering for design and analysis of processes. The commercial process simulation has proven to be an important tool for plant design and operations. However the greater share of process modeling was the steady state simulation and there were only limited applications of dynamic simulations and were only restricted to individual unit operations such as a distillation column or heat exchanger etc. Historically the computation speed and the storage capacity have limited the use of dynamic simulations. Some of the early industrial applications of dynamic simulations for process analysis and controllability have been discussed by Bretelle and Macchietto, 1993; Bretelle et al., 1994 and Pantelides and Oh, 1996. Most dynamic models were developed by describing the system of algebraic and differential equations, using the basic principles such as the heat and mass balance concepts and thermodynamic equations. One of the advantages of deriving such a model was the insight it provided into the fundamental behavior and structure of the process. With the recent advances in the computer technology there have been a number of
significant achievements in the design of simulation environments expanding the role of simulations in the manufacturing operations. The process simulations are now considered as state of art for the design, analysis and optimization of chemical processes. There are several process simulation software packages available in today’s market. The most widely used simulators are Aspen HYSYS®, Aspen Plus®, and UNISIM®.

Dynamic simulations are becoming predominant in the design and evaluation of plant wide control aspects (Manenti et. al, 2006). They are proving as an effective tool for implementing advanced process control projects (Alsop et. al, 2006). In general, plant-wide control refers to the control of an entire plant, involving many interacting unit operations (Luyben et al., 1999). Plant-wide control strategies play an important role in the design procedure, as the processes are required to be integrated. Thus the importance of investigating the dynamic and steady state performance of plants has been realized and lead to the concept of ‘simultaneous design’. Several researchers have focused their work on integration of process design with plant control and operation. (Russel et al., 2000, Bernardo et al., 2001 and Himmelblau et al., 1996)

The continual emphasis on energy efficiency and environmental protection, together with increasing market competition has driven process engineers to develop methodologies for optimal design and operation of chemical processes. Process design teams are forced to integrate their processes to satisfy economical, environmental objectives, while at the same time maintaining the process within a satisfactory operational performance. However, process integration creates unforeseen operational problems (Glemmestad et al., 1999 and Papalexandri et.al, 1994) and also poses a complex optimization problem. The optimization problem is no longer a problem of single objective function but has to satisfy multiple objectives that are potentially conflicting. There are several publications on the applications of multi objective optimization problems in chemical engineering. (Hwang et al., 1980, Clark et al., 1983 and Grauer et al., 1984)
1.4 Project Goals and Objectives

From the previous discussions, it is clear that process engineers are challenged with making timely decisions while meeting the business objectives of designing and operating efficient, safer and profitable process plants. This dictates the need for systematic methodologies to assist the production engineers to analyze the process behavior, to optimize and operate the plant in a safe and efficient manner. Consequently, the main objective of this work is to create a model-centric framework that supports various manufacturing operations and also to develop an overall integrated approach allowing all the objectives to be formulated and accounted for during the design and operation of the process plants. This thesis presents a general proposed framework for such a methodology that incorporates economical, environmental and operational performances for assessing various levels of process integration for a given process. Furthermore and more importantly, constitutes the first step (operation layer) towards a multilayer approach for enterprise wide optimization.

1.5 Thesis Organization

This thesis consists of a total of eight chapters and is organized according to the objectives described above:

♦ Chapter 2 presents a brief summary of the proposed integrated framework for operability assessment and optimal plant operation. This framework is divided into main sub-frameworks where each of them will be presented in the followed Chapters 3, 4, 5 and 6. These chapters focus on the fundamentals and detailed background of each sub-framework in the methodology using a demonstrative example of a packed distillation unit.

♦ Chapter 3 gives an overview of the simulation environment. This chapter introduces the basic concepts and applications of the process simulation. It also discusses the basic steps
involved in developing both the steady state and dynamic state models

♦ Chapter 4 focuses on the process optimization problem and also discusses the increasing environmental awareness in the field of process engineering. The optimization framework developed is discussed thoroughly along with software architecture used to develop the optimization tool.

♦ Chapter 5 addresses the need for advanced process control methodologies and the concepts of the model predictive controller. In brief, this chapter discusses the proposed sub-framework that deals with plant-wide control and dynamic evaluations concerns.

♦ Chapter 6 discusses the importance of the training simulators. This chapter describes the stepwise procedure in the implementation of the training simulators using the demonstrative case study discussed in the previous chapters.

♦ Chapter 7 demonstrates the applications of the proposed framework to an industrial case study of the crude distillation unit which comprises the preflash unit, atmospheric/vacuum distillation unit and the preheat trains. This chapter shows in a transparent way the stepwise procedure of the framework and its contribution to assessment and in improving the of the plant performance.

♦ Chapter 8 summarizes the major issues discussed throughout the thesis and consequently draws the general conclusions. This chapter reviews the contributions of the thesis and highlights the possible directions of future research by some recommendations.
CHAPTER 2

METHODOLOGY

2.1 Introduction

Process industries today are facing newer challenges with increasing environmental regulations and global competitiveness, compelling to integrate different processes together for efficient use of energy and resources. In today's environment, there is a need for every advantage to ensure the sustainable success of the business and consequently, a need to optimize and operate the process units more efficiently while satisfying the process constraints. Process simulation is the most effective way to improve process design and operation, which can lead to reduced emissions, more throughput, better quality yields and safer operations. Simulation models are playing an increasing role in plant operations.

The main principle of this approach is to develop a general decision making tool that helps the process engineers in evaluating the chemical processes for operational and environmental performances. The framework represents an overall stepwise procedure that takes into account all formulated aspects of optimal design considerations, including economical, environmental, heat integration, controllability and dynamic performance issues. The proposed framework offers several benefits to the manufacturing industries and since it is developed using the standard tools it is a very cost effective approach. It provides a safe and theoretical environment to study ‘what-if’ scenarios and also to perform sensitivity analyses to identify the optimal design based on operating and business targets. It can be used to evaluate the effect of feed changes, upsets, and equipment downtime on process safety, reliability, and profitability. It facilitates study of advanced operational procedures, assist in developing and implementing the advanced supervisory controls and also aid in environmental impact assessment.
2.2 Proposed Approach

The model-based methodology proposed in this work, starts with the implementation of first principle models for the process units on consideration. Secondly the steady-state simulation of the process is developed and validated against the plant data to evaluate the reliability of the model. Then it is followed by rigorously posing the optimization problem, that is, objective function and constraints. In addition to the traditional economic objectives like raw materials and operating costs, the so-called triple-bottom-line constraints related with sustainable and environmental costs are also incorporated into the objective function. This is intended to complement the existing cost estimating practices with environmental costs for improved decision-making. The methodologies of Life Cycle Assessment (LCA) and Environmental Damage Assessment (EDA) are applied within the optimization problem. The LCA evaluates the environmental impact of a process from the raw material to a final product. The EDA can supply the necessary information about the damage caused by the process to the environment. At this stage, the influences of exogenous disturbances are not taken into account since these are mathematically feasible solutions only. Subsequent to the optimal solution, the controllability of the plant is evaluated using the dynamic state simulations in order to ensure plant safety management procedures, safe and efficient plant operation.

The assessment of process controllability is of critical importance in view of the fact that optimal set points may be difficult to maintain under sustained disturbances or process variability. Another equally critical concern is implementing model predictive control strategy (MPC) which can handle constraints and presents good robustness features against model mismatch and perturbations. The proposed framework is extended further to develop training environment by integrating the process simulation with the Distributed Control Systems (DCS) through the standard OPC interface. The primary objective of the training simulator developed in
this work is to familiarize students with the basic plant operations and also to make them understand the control philosophy. It provides a realistic control room environment for effective training. The use of such simulators enhances learning by integrating the theoretical concept of textbooks with the physical nature of the lab. This approach is motivating, provides hands-on experience, facilitates understanding the practical implications and limitations of the theory, and helps prepare students for the challenges of the professional world. Trainees are therefore able to develop good decision making skills as they experience and respond to different operating situations.

The present framework is implemented in Aspen HYSYS® and a user friendly front end in MS Excel® where the-state-of-art optimizer is implemented. The process model is linked to Honeywell’s Experion Process Knowledge System (PKS) ®, through the OPC interface program. To demonstrate the effectiveness and the components of methodology, an industrial case study of the primary unit of the crude oil refinery and a laboratory scale of packed distillation unit is thoroughly investigated. Figure 2.1 illustrates a schematic structure of the proposed framework, showing the different steps, the inter-linking of the software packages used as well as the flow of data between them. The proceeding chapters in this thesis will describe in detail the main sub-frameworks, namely simulation environment, optimization model and related environmental aspects, model predictive control strategy.

2.3 Multi-Layer Control Strategy

The availability of modern industrial computer control system architectures has made possible the expansion of the functionalities of the plant control systems, broadening the domain of what is technologically and economically feasible to achieve in the application of computers to control industrial systems computers to control industrial systems. The conventional role of process control in industrial plants has been the implementation of control strategies through closed-loop
automation. Today, this still remains to be the primary function of a control system. However, as discussed before, the advances in computer technology allowed the expansion of functionalities that can be simply referred to as *information management* at the plant wide scale. The processing and reporting of plant information can be crucial for plant operations as well as planning activities.

![Proposed framework diagram](image)

**Figure 2.1 Schematic representation of proposed framework**

Romagnoli and Palazoglu, 2005 established the objectives of a control system in modern manufacturing as: a) to enforce plant control strategy; b) to report plant performance and c) to provide a proper window to the process. These activities are carried out using the control system technology that consists of a number of functionalities, performing in a coordinated manner. It is noted that the functionalities included in the control system strongly depend on the complexity of the control actions as well as the analysis and reporting demands of the plant operators, the
engineers and the managers. The control strategy then can be described through a hierarchical decomposition, referred to as the Control Layers or Hierarchical Control. The goal of these control layers is to manage the inherent complexity in the industrial control architecture. They are conceived not only to address the primary role of the control system but also to be able to accomplish the expanded role of modern control for advanced manufacturing.

Following Romagnoli and Palazoglu, 2005 a natural decomposition for a typical control application could be described in terms of different levels of control such as:

**Level 1 Control:** This is the basic control layer utilized during the startup of the plant and allows the plant to be operated around the design conditions. It is the foundation of the plant control system and the controllability of the process depends on it.

**Level 2 Control:** It is implemented sometime after the plant is in operation and a reasonable level of consistency in operation is reached. This layer is aimed at the integration of the production process and to improve process efficiency and profitability. A typical application is in handling production rate changes in an optimal and coordinated fashion. This layer is particularly important in integrated processes where coordination of different sections of the plant is essential.

**Level 3 Control:** This layer is associated with the handling of abnormal operational conditions. Some of the basic functionalities are implemented from the beginning of the plant operation since they may be needed during normal operational procedures. A typical example is a basic alarm system for the plant. However, more advanced functionalities would be implemented after the plant is fully operational. An example of this could be the implementation of an advanced alarm management system.

The proposed framework allows the development and implementation of such a multilayer control strategy for advanced operation, optimization and control of the existing or
new production facilities. Figure 2.2 illustrates schematically the multi layer advanced control architecture implemented in this project using the software/hardware integration methodology described in previous section.

![Multi-Layer control Architecture](image)

**Figure 2.2 Multi-Layer control Architecture**

The bottom of the control hierarchy is the basic process control such as the single loops and simple cascades that appear on P&IDs and provide the operator with the first level of regulatory control. Simple processes can operate in a fairly stable fashion with basic process control. Unfortunately, most process units in refineries and chemical plants are very complex, highly interactive and therefore necessitate the advanced process control strategies like model predictive controllers, feed forward etc. which form the upper layer in the control hierarchy above the basic regulatory control.

This layer determines the optimum set point trajectories of the plant given the production requirements and operational constraints, and maintains the process operating near optimum efficiency by constantly adjusting the set points and responding to plant disturbances. Moving up
the control hierarchy is the supervisory level which optimizes the operation of the process. In most cases the systems of this level manipulate the set points of the advanced controllers and pass information to the process operator responsible for the status of the unit. The uppermost layer in the control hierarchy is developed for decision support system with functionalities such as data processing, reconciliation, process monitoring, fault diagnosis and detection of abnormal operating conditions etc. This layer comprises of the expert system, developed to support safe and consistent plant operation. It acts as high level supervisory and attempts to optimize the overall plant. The systems become complex due to interactions between the various unit operations. It is difficult to formulate a comprehensive set of rules that deal with all process scenarios and therefore requires skilled human intervention. Systems of this level are seldom used for direct process control, but rather for providing advice to the process operators.
CHAPTER 3

SIMULATION ENVIRONMENT

3.1 Introduction

Process simulation has been playing a significant role at each stage of the process life cycle starting from feasibility studies, through detailed engineering design, personnel training and plant operation. Simulation studies have become an indispensable tool for process engineers to gain insight into the operation of manufacturing systems, or to observe their fundamental behavior. First-principles simulation models have also a proven track record in real time optimization (RTO) in many process industry segments.

The ability to mathematically model a process and its unit operations from first principles arguably dates back to the advent of the first computers powerful enough to perform complex computing operations. The first equation-oriented simulator, known as Speed-Up, was proposed and outlined by Sargent and Westerberg (1964). The processing and modeling times involved then were hardly suited to study the transient behavior of the process. However with the current state of art information technology, there has been a significant development in the field of modeling and simulation. The use of modular software development approach, distributed communication protocols, multilevel abstract modeling, interoperability capabilities, and an open library/repository for providing a consistent set of simulator modules have broadened the functionality and use of simulation environments.

Simulations are broadly classified into two types based on the behavior of the process model with respect to time: Steady state and Dynamic State. The steady state simulation is now considered to be the state of the art for preliminary studies and plant design in the process industry. Nevertheless, the increasing market competition, more stringent environmental
regulations, and reduced net profit margins are pushing enterprises towards process dynamic simulation. There are a number of commercial process simulators available today. In this work, Aspen HYSYS® is used for both steady state and dynamic state simulation of the processes being analyzed. Aspen HYSYS® support modeling applications across the entire life-cycle of a plant, from steady-state design to offline engineering studies to on-line operational models. It offers a comprehensive library of unit operation models including distillation, reactions, heat transfer operations, rotating equipment, controller, and logical operations in both the steady state and dynamics environments. CAPE-OPEN compliant models are also fully supported. Further, Aspen HYSYS models can be linked to Microsoft Excel® and therefore can be used to automate the engineering workflow.

3.2 Simulation Software Architectures

The architecture of any simulation program is determined by the computation strategy used in the software package. The following section describes the three fundamental approaches that are commonly used to solve the system of equations (DAE/ODE) describing the process.

- **Sequential-Modular:** In the Sequential-Modular approach the computation is performed unit-by-unit following a calculation sequence. This approach is dominant in steady state simulation software. The incoming streams have to be either specified as inputs, or initialized as tear streams for units involved in a recycle. In such cases, the final steady state solution is obtained by iterative calculations. Tear streams are modified after successive iterations by applying an appropriate convergence algorithm. Finally the computation is terminated when both the units and the tear streams satisfy the specified convergence criteria, usually the closure of the material and heat balance. In this approach, the model is obtained by means of conservation equations for mass, energy and momentum. The final problem is represented by a system of non-linear algebraic
equations. The difference between the total number of non-redundant variables in the system and the number of independent algebraic equations gives the degrees of freedom. These are usually specifications that a user must supply to run a simulation.

- **Equation-Oriented:** In Equation-Oriented (EO) approach all the modeling equations are assembled in a large sparse system producing Non-linear Algebraic Equations (NAE) in steady state simulation, and stiff Differential Algebraic Equations (DAE) in dynamic simulation. The solution is obtained by solving simultaneously all the modeling equations. The advantages of the equation-solving architecture include flexible environment for variable specifications and better handling of recycles, and no need for tear streams. However, intense programming and substantial computing resources are required. This approach is more suited in dynamic simulation and real time optimization.

- **Simultaneous-Modular:** This approach is combination of both Sequential-Modular and Equation-Oriented. Rigorous models are used at unit level, which are solved sequentially, while linear models are used at flowsheet level, solved globally. The linear models are updated based on results obtained with rigorous models.

### 3.3 Steady State Simulation

The steady state simulations have been used extensively for the design, analysis and optimization of chemical processes. They also provide data for process flow diagrams in terms of material and energy balances. Steady-state models use equations defining the relationships between elements of the modeled system and attempt to find a state in which the system is in equilibrium. These models are therefore independent of the time. Such models are used at the early stages of a study for conceptual design, feasibility studies, detailed engineering and at the initializing steps for dynamic simulations which are used for evaluating the transient behavior of the system.
These models usually consist of blocks of unit operations interconnected by the user and
of physical property data for the chemical components of input streams specified by the user.
Modern simulators allow the user to graphically configure the model as the process flow diagram
as compared to other software packages like MATLAB®. The simulator's easy-to-create
flowsheet environment allows process engineers to concentrate on engineering, rather than
computing operations like developing the heat and mass balance equations. A minimum amount
of information is required to input from the user in order to run the simulation. In addition they
also offer advanced features, such as rigorous column calculations, sizing and rating of heat
exchangers and separators, within the flowsheet for a wide variety of processing applications.
Most simulation programs provide features like pure component data library, thermodynamic
methods, development of non library components (pseudo components), physical and transport
properties, simulated laboratory test, unit operation calculations, and a user interface for program
input and output. The various components facilitate simulation tools an extremely powerful
approach to steady state modeling.

In this methodology the steady state model of the process is used mainly for the
optimization and to evaluate the plant performance. The following steps are used in developing a
steady state simulation model. In general other software packages also follow similar approach
for building the plant model.

1. Selecting the unit set
2. Defining Simulation basis
3. Defining the feed streams
4. Installing and defining the unit operations like preheat exchangers, distillation columns
5. Installing the downstream unit operations

For better explanation of developing the simulation model of the process, simulation of
laboratory scale packed distillation unit is considered in the following section. The distillation unit is modeled in Aspen HYSYS® simulation software. The process considered is being installed in Unit Operations lab in the department of chemical engineering, LSU. This is a small pilot unit designed to demonstrate the process of continuous fractional distillation. Distillation is the most extensively used separation technique in the petrochemical industry and can contribute to substantial part of plant operating costs. The process requires enormous amounts of energy, both in terms of cooling and heating requirements.

3.3.1 Process Description

The distillation unit is designed to separate high purity methanol as the top product. The feed stream (Methanol – 48.4 %, 2-propanol – 16.3 % and water 35.1 % mole basis) at approximately 80° F is preheated to around 145° F by exchanging heat with hot ethyl glycol stream in a feed preheater and enters the packed distillation column. The unit is equipped with a total condenser, a partial reboiler, and a pump-back reflux system. The distillation column is 3” in diameter and constructed of Type 304 stainless steel. It contains two packed sections, each of which is 3’ 0” high and contains 2’ 8” of PROPAK1 0.24” protruded stainless steel packing. The feed is introduced between the two packed sections through a central feed distributor. The overhead from the column is sub cooled below 100° F in a condenser using cooling water as cold stream. The sub cooled liquid is then collected in a reflux drum and a portion of which is fed back to the column as the overhead reflux and the remaining is sent as a product via a distillate cooler to the storage tank. The bottom flow from the column is split in two streams, one stream is sent to the thermosyphon reboiler and the other is sent to storage via a bottom cooler.

3.3.2 Selecting the Unit Set

HYSYS has the default unit sets like the SI, Field units. However the unit set used in the simulation can be customized. Either you can modify the units of a particular property or can
create a new unit. For the above problem, the field units are used.

3.3.3 Defining the Simulation Basis

Defining a simulation basis, include selecting the components and the thermodynamic fluid package. HYSYS uses the concept of the fluid package to contain all necessary information for performing flash and physical property calculations. This approach allows you to define all information (property package, components, interaction parameters, reactions, tabular data, hypothetical components, etc.) inside a single entity. Multiple fluid packages can be used within the simulation by assigning them to different flow sheets and linking the flow sheets together. The selection of a suitable thermodynamic package is fundamental to process modeling for accurate predictions. Selection of an inappropriate model will result in convergence problems and erroneous results. Effects of pressure and temperature can drastically alter the accuracy of a simulation given missing parameters or parameters fitted for different conditions. The selection is based on the nature of process, compositions, pressure, temperature ranges, phase systems involved and availability of data.

One of the main assets of HYSYS is its strong thermodynamic foundation. The built-in property packages in HYSYS provide accurate thermodynamic, physical and transport property predictions for hydrocarbon, non-hydrocarbon, petrochemical and chemical fluids. If a library component cannot be found within the database, a comprehensive selection of estimation methods is available for creating fully defined hypothetical components. For the above process, methanol, water and propanol are added from the pure component library and the Uniquac-ideal model is used in defining the simulation basis.

3.3.4 Defining Feed Streams

Once the components and the thermodynamic package are selected the feed streams are defined by specifying the process conditions and the composition. In order to define a stream in
HYSYS it is required to specify two process variables (temperature, vapor fraction, pressure etc.), flow rate and composition. The other conditions of the stream are estimated by HYSYS. The information in Table 3.1 is used to define the feed stream to the preheater.

<table>
<thead>
<tr>
<th>Table 3.1 Feed stream specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
</tr>
<tr>
<td>Pressure</td>
</tr>
<tr>
<td>Flowrate</td>
</tr>
<tr>
<td>Feed Composition</td>
</tr>
</tbody>
</table>

* Composition is expressed in mole % [Methanol, Propanol, and Water]

3.3.5 Installing and Defining Unit Operations

The commonly used unit operations are

- Mixer
- Heat Exchanger
- Heater
- 3-phase separator
- Separator
- Refluxed absorber

For each unit operation it is required to specify certain parameters to satisfy the number of degrees of freedom. Each parameter specification will reduce the degrees of freedom by one. The number of active specifications must equal the number of unknown variables to solve. The following section describes the modeling procedure of the heat exchanger and the packed distillation column which are used later in the case study. The detailed modeling procedure of each section in the unit is described in Aspen HYSYS® operations guide.

Heat Exchanger

Heat exchangers can be modeled in Aspen HYSYS using either a shell and tube or a
cooler/heater configuration. There are different rating models available like

- The End Point model
- The Weighted model
- Steady State Rating model
- Dynamic Rating – basic and detailed model

The End point model uses the standard heat exchanger duty equation defined in terms of overall heat transfer coefficient, area available for heat exchange, and the log mean temperature difference. This model treats the heat curves for both heat exchanger sides as linear. For simple problems where there is no phase change and Cp is relatively constant, this option may be sufficient to model the heat exchanger. In this model, the overall heat transfer coefficient, U is and the specific heats of both shell and tube side streams are assumed to be constant. The preheat exchanger in the PDU is modeled using the End point model. In addition to defining the inlet stream of the shell side (i.e. ethyl glycol), the pressure drop across both the sides of the exchanger and the tube side exit temperature are specified in order to solve the heat exchanger.

**Packed Distillation Column**

Installing the column is the most difficult step in building the simulation model. It consists of a series of equilibrium or non-equilibrium flash stages and has many parameters. It is a special type of sub flow sheet that contains equipment and streams, and exchanges information with the parent flow sheet through the connected internal and external streams. HYSYS has a number of pre-built column templates that can be installed and customized by changing attached stream names, number of stages, draw and return stages and default specifications, and adding side equipment. Each prebuilt column has unique degrees of freedom which have to be satisfied by defining the active specifications. The active specifications should be equal to the number of degrees of freedom in order to run the column.
There are more than 25 available specs like column reflux ratio, column component flow rate and column component fraction, stage temperatures or duty specifications. The reflux ratio is defined as the ratio of the liquid returning to the tray section divided by the total flow of the products. Component flow rate allows specifying the flow rate of any component, or the total flow rate for any set of components for the flow leaving any stage. Component fraction allows specifying the mole, mass or volume fraction in the liquid or vapor phase for any stage. It is necessary to choose the specifications wisely in order to avoid the convergence failures. Avoid using conflicting specifications, and try using ranged spec rather than a fixed specification.

Aspen HYSYS has no provisions to simulate a packed column as such. The column solves using theoretical stages of separation. Therefore, a HETP approach is used in defining the equivalent number of theoretical plates for the packing being used. HETP is the "Height Equivalent to a Theoretical Plate" and is defined as the height of the packed column divided by the number of theoretical/ideal stages. As a starting point, manufacturer suggested HETP factor is used to estimate the number of ideal stages. Since the actual HETP is dependent on several factors such as the viscosity, surface tension, the operating regime etc., the HETP factor is slightly adjusted to match the simulation results with the actual process conditions such as the temperature and pressure profile.

The distillation column is simulated using a prebuilt distillation unit operation template having a condenser operating in total reflux mode and a reboiler. Using the HETP method the equivalent number of theoretical stages are estimated for the given packing configuration and then adjusted to match the operating conditions. The actual thermosyphon reboiler is modeled using the prebuilt kettle type reboiler available in HYSYS. Table 3.2 gives the summary of the calculations used in the modeling. In addition to the pressure specifications across the column, the pre built column has two degrees of freedom. The reflux ratio and reboiler duty are being
used as active specifications to run the simulation. The alternate variables that can be selected as active specifications are product flow rate, reflux flow rate, product purity etc. The condenser outlet is specified at be 86°F to consider the sub cooling effect of the condenser.

**Table 3.2 Column specifications data**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Manufacturer HETP *</td>
<td>2.5 in</td>
</tr>
<tr>
<td>Modified HETP</td>
<td>2.66 in</td>
</tr>
<tr>
<td>Ht of packing</td>
<td>60 in</td>
</tr>
<tr>
<td>No. of theoretical plates</td>
<td>60/2.66 ~ 24</td>
</tr>
</tbody>
</table>

*for n-heptane – methylcyclohexane system operating at similar condition

**Adding downstream unit operations**

As discussed before HYSYS uses sequential modular approach, the plant is modeled unit by unit in sequence. Therefore it is required to solve the distillation column before modeling any downstream units like the product coolers. The distillate and the bottom product cooler and the overhead condenser can be modeled as a cooler instead of a heat exchanger to simplify the model. The specifications used are the exit temperature and the pressure drop for each system. The overview of the steady state simulation model is as shown in Figure 3.1.

**3.3.6 Model Validation**

The simulation model is the core of the methodology because it resembles the actual process. Any irregularities or mismatch in the model is reflected throughout the methodology and there is ample scope to arrive at the wrong conclusions. Therefore model validation is the important step in order to identify the accuracy of the model. This will also allow all current and future users of the simulation model to assess the significance of the apparent model inaccuracies, and better understand any limitations in extrapolating the model. The results obtained from the simulation model are compared with the actual plant data. The Table 3.3 summarizes the comparison between the actual and simulation results of the process.
Figure 3.1 Main flowsheet of the steady state model

Table 3.3 Steady-state model validation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Actual plant</th>
<th>Steady state model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Top Temperature(°F)</td>
<td>153.5</td>
<td>154.5</td>
</tr>
<tr>
<td>Bottom Temperature(°F)</td>
<td>171.0</td>
<td>170.5</td>
</tr>
<tr>
<td>Reflux flow(GPH)</td>
<td>2.21</td>
<td>1.90</td>
</tr>
<tr>
<td>Reflux Temperature(°F)</td>
<td>86</td>
<td>86</td>
</tr>
<tr>
<td>Feed Temperature(°F)</td>
<td>145</td>
<td>145</td>
</tr>
<tr>
<td>Distillate Flow(GPH)</td>
<td>1.3</td>
<td>1.42</td>
</tr>
<tr>
<td>Bottom Flow(GPH)</td>
<td>1.8</td>
<td>1.66</td>
</tr>
<tr>
<td>Distillate Composition</td>
<td>[0.91,0.05,0.04]</td>
<td>[0.89,0.04,0.80]</td>
</tr>
<tr>
<td>Bottom Composition</td>
<td>[0.18,0.24,0.58]</td>
<td>[0.20,0.22,0.58]</td>
</tr>
<tr>
<td>Feed Composition</td>
<td>[0.49,0.16,0.36]</td>
<td>[0.49,0.16,0.36]</td>
</tr>
</tbody>
</table>

* Composition is expressed in mole % [Methanol, Propanol, and Water]

3.4 Dynamic State Simulation

The use of dynamic simulations has grown significantly over the last decade. In this context, dynamic process models are becoming key tools to improve unit yields, plant stability,
safety and controllability. These simulations allow the user to predict the dynamic behavior of the process and also assist in evaluation/design of the control strategies (Bezzo et al., 2004). The dynamic simulations are being used in development of training simulators and validation of safety systems.

Dynamic models can be categorized as empirical and first principle models. Empirical models are based on black box model approach. The model consists of a number of regressions of the input/output responses. Examples of empirical modeling techniques include multivariable regression, neural networks and fuzzy logic systems. For processes where the underlying physical science is not sufficiently understood or if the process always operates within a well understood operating, empirical modeling techniques can be used successfully. However such models do have limitations in handling a wide range of operating conditions and pose issues if the process moves outside the operating conditions for which the model was regressed. On the other hand, the first principle models are those developed from the fundamental equations for the mass, energy and momentum balances; diffusive and heat transport; chemical kinetics and reaction mechanisms; thermodynamics and phase equilibrium. The process is described in terms of Ordinary Differential Equations (ODE) or Algebraic Equations. Numerical integration techniques are used to solve these equations over time to predict the dynamic behavior of the process in response to various planned or unplanned disturbances to the process.

HYSYS Dynamics™ Option provides a dynamic simulation capability fully integrated with the HYSYS environment, a steady-state model can be leveraged into a dynamic model which offers rigorous and high-fidelity results with a very fine level of equipment geometry and performance detail. A dynamic model can either be developed from the steady state model or directly in the dynamic mode with no prior steady state model.

The following are the important steps involved in transitioning from the steady state to
dynamic state model

1. Equipment sizing
2. Defining pressure flow specifications
3. Installing controllers
4. Analyzing the results

3.4.1 Equipment Sizing

Appropriate equipment sizing is important for dynamic state simulation. The vessel hold-up will not only affect the system's transient response but also affects the pressure calculations that are associated with the unit operation. Sizing is necessary so that the dynamic capacitance of the unit operations is available to the simulator. It is not necessary to have all the details of the mechanical design of the equipment. Some good estimates of the gas and liquid holdups are sufficient to predict the realistic dynamic responses.

HYSYS Dynamics permit a two-tiered approach to simulation with numerous options to supply different levels of equipment design and performance information. HYSYS Dynamics provides modeling capabilities aimed at both process design and detailed design activity. For the design activity simulation, the basic design information is used and HYSYS Dynamics estimates reasonable defaults for the detailed equipment information. The dynamics model can be further expanded by incorporating detailed equipment and performance information.

3.4.2 Control Valve Sizing

A critical part of developing dynamic simulation is control valve sizing. This means setting the percent valve opening and the pressure drop over the valve at steady-state design conditions. Most valves are designed to be 50% open at design conditions. The design pressure drop of a valve is a tradeoff between dynamic controllability and steady state economics, the higher the valve pressure drop, the more the flow through the valve can be changed and better is
the control. However, larger valve pressure drops require pumps and compressors with high
discharge pressures, which mean higher energy consumption.

3.4.3 Defining Pressure Flow Specifications

Before a transition from steady state to dynamic occurs, the simulation flow sheet should
be set up so that a pressure drop exists across the plant. This pressure drop is necessary because
the flow in HYSYS Dynamics is determined by the pressure drop throughout the plant. Aspen
HYSYS offers an advanced method of calculating the pressure and flow profile of a simulation
case in Dynamics mode. Almost every unit operation in the flowsheet can be considered a
holdup or carrier of material (pressure) and energy. A network of pressure nodes can therefore be
conceived across the entire simulation case. The Pressure-Flow (P-F) solver considers the
integration of pressure flow balances in the flowsheet. The pressure and/or flow of a material
stream can be specified in the flowsheet. To satisfy the degrees of freedom of the pressure-flow
matrix, you must input a certain number of pressure-flow specifications. The volume balance
equations, resistance equations, and pressure-flow relation equations make up a large number of
equations in the pressure-flow matrix. In general, one pressure-flow specification is required per
flowsheet boundary stream. A flowsheet boundary is one that crosses the model boundary and is
attached to only one unit operation

3.4.4 Installing Controllers

HYSYS is capable and have inbuilt template of the following Control operations:

- Split Range Controller
- Ratio Controller
- PID Controller
- MPC Controller
- DMCplus Controller
A controller can also be added before switching to the Dynamic mode but it is recommended to add them after. Controllers can be added to the Flowsheet using the same methods as for other unit operations. Once the Controller has been added to the Flowsheet:

- Make the necessary connections for the Process Variable Source and Output Target Object.
- Select the Minimum and Maximum values for the Process Variable.
- Size the valve - controller range. This is not necessary if a valve was chosen as the Output Target Object.
- Select Controller Action, Reverse or Direct.
- Input Controller Tuning Parameters.
- If desired, choose the mode of the controller, Off, Manual, or Automatic

While installing the controller, the manipulated variable may be specified as an actual control valve position or a material/energy stream directly without building any valve. If a material/energy stream is chosen as an operating variable, the maximum and minimum value of the stream (range) should be specified. HYSYS varies the corresponding specification according to the calculated controller output. The 0% corresponds to the Minimum value and 100% valve output corresponds to maximum value of the variable.

The use of specifying the operating variable as the material and energy streams simplify the dynamic model since there is no need to simulate the physical control valve. If a material stream is chosen as an operating variable, the material stream’s flow becomes a P-F specification in the dynamic simulation case. The maximum and minimum flow of the material stream is specified by clicking the Control Valve button on the parameter page tab of the controller property view. The plant can be simulated more accurately by modeling the hardware elements of the control loop. It also has an option of selecting different control algorithm like positional
and velocity form algorithm: the value of the manipulated variable is calculated and used directly in positional form. In the velocity form of the PID, on other hand, we compute and use the change in the manipulated variable. The choice of positional vs. velocity forms will have an impact on such issues as initialization, bump less transfer. In this study the default settings of the controller are used.

Control schemes are configured within the same environment from a pre-built suite of function blocks. As mentioned in the steady state model, the condenser is modeled for subcooled conditions i.e. there is no vapor from the reflux drum. However HYSYS Dynamics is not capable of simulating such a condenser system with only a liquid exit stream and no vapor. It is required that a separator/tank model in HYSYS has both vapor and liquid exit streams. Therefore in this model, an inert stream, nitrogen at approximately same process conditions is introduced into the system. The vapor exit stream from the tank is very small and is mainly nitrogen thus not affecting the other process conditions and other unit components. Figure 3.2 and 3.3 gives an overview of the main flowsheet and column sub flowsheet in dynamic simulation and Table 3.4 below summarizes the basic regulatory controllers installed.

**Controller Tuning**

It is necessary to adjust the controller parameters according to the nature of the process. This tailoring of the controller to achieve the optimum control performance is known as controller tuning. Tuning a controller has severe impact on the process performance, for example tuning a controller too sluggish will not handle the process upsets, and also at the same time will take too long to reach the set point or the desired performance. On the other side, aggressive tuning will result in the overshoot or plant instability. Therefore the process performance deteriorates when the controller is poorly tuned; this deterioration may be reflected, for example, increase in energy costs and environmental emissions and in decrease of the plant capacity.
Figure 3.2 Main flowsheet of dynamic simulation

Figure 3.3 Column sub flowsheet of the dynamic simulation
Table 3.4 Basic regulatory controllers installed in the distillation unit

<table>
<thead>
<tr>
<th>Variable of Primary Interest</th>
<th>Controller</th>
<th>Manipulated Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overhead Temperature (in effect, Composition)</td>
<td>TC</td>
<td>Reflux Flow</td>
</tr>
<tr>
<td>Bottoms Temperature (in effect, Composition)</td>
<td>TC</td>
<td>Reboiler Duty</td>
</tr>
<tr>
<td>Reflux Drum Level (Total Reflux)</td>
<td>LC</td>
<td>Distillate Flow</td>
</tr>
<tr>
<td>Reboiler Level</td>
<td>LC</td>
<td>Bottoms Flow</td>
</tr>
<tr>
<td>Feed flow rate</td>
<td>FC</td>
<td>Feed Flow</td>
</tr>
<tr>
<td>Feed Inlet Temp.</td>
<td>TC</td>
<td>Ethyl Glycol Flow</td>
</tr>
</tbody>
</table>

The overall effect will be an increase in operating costs and a reduction in overall competitiveness. Therefore proper tuning of a controller is important to reduce the process variability and to improve the efficiency. There have been numerous approaches available for controller tuning today. The first tuning method for defining the setting up controller parameters was defined in 1934 for a proportional-derivative (PD) controller and subsequently, tuning rules were defined for PI and PID controllers. HYSYS Dynamics has inbuilt auto tuning algorithm however the results obtained from this method could not provide adequate control for the application. In this study, the controllers are tuned using the control station® software. There are other tuning software available such as the APCON tool available in Mat lab which uses the closed loop tuning method i.e. Zeigler–Nichols method.

The foremost step in this tuning process is to develop a process model that defines the relationship between the manipulated variable (input) and the process variable (output) response. In an open loop, a step change in the manipulated variable is introduced and the response of the controlled variable is recorded over the time. In general this curve is referred to as the process characteristics curve and can be represented using the first order plus time delay (FOPDT) model. The response data is recorded in an Excel (CSV) format and is exported to Control Station® software to fit the process data and to obtain the process model along with the tuning
parameters. If the tuning parameters obtained by this process fail to provide satisfactory control due to presence of process interactions, they can be used as the initial estimates and are then tuned by trial and error method.

Figure 3.4 shows the process data fit using FOPDT model for the bottom temperature controller in the control station design tool. Figure 3.5 shows the model parameters and the PID tuning parameter for the same controller.

![Image of process data fit in control station design tool](image)

**Figure 3.4 Process data fit in the control station design tool**

<table>
<thead>
<tr>
<th>Process Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process Gain, $K$</td>
<td>0.11</td>
</tr>
<tr>
<td>Overall Time Constant, $\tau$</td>
<td>2.70</td>
</tr>
<tr>
<td>Dead Time, $\theta$</td>
<td>0.0999</td>
</tr>
<tr>
<td>Sum of Squared Error (SSE)</td>
<td>0.0044</td>
</tr>
<tr>
<td>Goodness of Fit (R²)</td>
<td>0.9997</td>
</tr>
</tbody>
</table>

![Table of PID tuning parameters](image)

**Figure 3.5 Tuning parameters recommended by the Control Station**

The advantages of using the Control station software is the ease to adjust the controller performance based on the nature of the process. It is equipped with a performance slide bar to adjust the controller performance from conservative to aggressive or anything in between. This is done by a user specified closed loop time constant. For a conservative PID the recommended value for the user specified closed loop time constant is about 50% of the process time constant.
The data can be analyzed and plots for mean, standard deviation, and variance can be viewed. The data can be modeled with a library of dynamic forms including first order plus dead time (FOPDT), FOPDT integrating, second order plus dead time (SOPDT), SOPDT integrating, SOPDT with Lead Time, and SOPDT under damped.

3.4.5 Analyzing the Results

Once all the unit operations are added and the dynamic performance specifications are specified, the dynamic solver is started and allowed to run for certain time interval to propagate all the values. The results are analyzed by adding desired strip charts. Further analysis can be done be exporting the history values into the Microsoft Excel. The response plots for a set point change in the top and bottom temperature controller are as shown below in Figure 3.6 and 3.7

![Figure 3.6 Response plot for a set point change in top temperature](image1)

Figure 3.6 Response plot for a set point change in top temperature

![Figure 3.7 Response plot for a set point change in bottom temperature](image2)

Figure 3.7 Response plot for a set point change in bottom temperature
3.5 Application Areas and Benefits

In the engineering domain, the simulation practices are playing an increasingly critical role in the plant design, operations, planning and optimization. Process companies are using a various synergistic engineering technologies in combination with steady state process simulation, such as process synthesis, economic evaluation, dynamic modeling, and advanced control strategies.

3.5.1 Process Design

The modern design strategy consists of developing not only a unique design but also alternative case studies from which the optimal design case is refined, integrated and optimized with respect to high efficiency of raw materials and energy, ecologic performance and operability properties. Though steady state simulations are more prominent in detailed plant design and feasibility studies, certain process decisions require the knowledge of the transient response and interactive behavior of the process. Therefore the dynamic simulation studies are also performed in conjunction with steady state simulation for sizing of critical units. For instance the sizing of intermediate hold up tanks can have significant impact on the process operability of the downstream units. While larger tanks give better control and operability performance, they do cost additional capital and are often source of environmental emissions and safety problems. For critical applications dynamic simulations can be used to properly minimize surge capacity while providing sufficient attenuation of process disturbances.

3.5.2 Process Control and Operability

Thorough understanding of the process is the first step in the design of a control strategy. The ability of the plant to adapt itself to external disturbance both planned and unplanned is the key to bottom-line. Planned disturbances are mainly product switchovers, changes in the production targets whereas the unplanned disturbances are feed composition fluctuations,
changes in ambient conditions and the utility loads. The use of dynamic simulation can identify
the important operability and control issues leading to a better process design and a smoother
operating plant. They can also be used to determine the critical variables that have a significant
impact on the key process parameters which affect the profitability of the plant.

Dynamic simulations can also be deployed to develop, evaluate, test and tune novel
control strategies for both new and existing processes. Empirical modeling techniques in
advanced process control strategies (APC) such as model predictive control algorithms are now
standard in the process industry. Such control methods require information of transient responses
of the process from known disturbances for their design and implementation. Process
identification step or step testing is done through extensive plant testing which is very expensive
and time consuming. The use of rigorous, validated dynamic models in conjunction with limited
plant testing can be used in model identification step and thus reduce the time and cost of the
process identification step. They can also be employed to test and evaluate its performance prior
to plant implementation.

3.5.3 Safety Studies

Process simulations can play a pivotal role in identifying potentially hazardous scenarios
and the changes in the design and operation procedures to mitigate or avoid them. They can be
used to evaluate, test and quantify the performance of these emergency and relief systems.
Distillation column relief system evaluations and compressor surge control are typical
applications of process simulation. These models can be used to perform the hazop study or
‘what if’ analysis.

3.5.4 Online Applications and Operator Training

Although operator training has taken many forms over the years, the use of rigorous, high
fidelity dynamic model of the process, with direct connection to or emulation of the DCS
operational screens and control algorithms is highly demanding since it would emulate a life like simulation of the control room. In addition such integrated environment facilitates testing of DCS configuration and control strategy prior to putting it online for real operation. The dynamic model is linked to the DCS control system and is run, emulating the actual operating process and used to test the control algorithms responses to various disturbances. Configuration errors in the DCS control strategies can be quickly identified and control loops can be tuned prior to actual plant startup, leading to much smoother and quicker plant startups, leading to substantial economic benefits. They can also used to estimate the key process operating data such as compositions that cannot be easily measured directly. Dynamic models running online, accepting process operating data and ‘shadowing’ the actual operation of the plant in real time, can act as ‘soft sensors’ for those critical process data.
CHAPTER 4
PROCESS OPTIMIZATION

4.1 Introduction

The field of optimization pervades in engineering, science, and business. A wide variety of problems in the design, construction, operation, and analysis of chemical plants can be resolved by optimization. In plant operations, improved performance means better profits. Traditionally, the chemical processes are optimized based on a single objective function which is frequently accounted for the economic performance. Chemical plants were designed primarily to maximize reliability, product quality and profitability. Issues such as toxic emissions, waste disposal and process safety have often been treated as secondary factors. Chemical engineering economics are well defined and developed in literature, where a number of methods are primarily focused on the profitability of designed processes (Peters and Timmerhaus, 1991; Turton et al., 1998; Biegler et al., 1997). The failure of such traditional economic analysis methods to address environmental issues is well-documented (Jackson and Clift, 1998). The reason for such relatively simple optimization problems was due to the lack of advanced computing technology and also because of lack of stringent environmental policies.

Today, with the rising environmental concerns, and soaring global oil prices, manufacturing plants are forced to integrate different processes and to adopt new approaches to design and operate. Such practices subsequently present new dilemmas for decision making and thereby pose a complex optimization problem and have to simultaneously satisfy environmental, economic and social goals. This invariably needs some tradeoff between these objectives. The following section briefly describes the new optimization tool developed along with the improved objective function used for optimization of plant control operations. This methodology allows process engineers to introduce the environmental costs in the process analysis for improved
decision-making, by the prediction of environmental damage for different scenarios of study. The results obtained from this technique not only boost the profits by obtaining optimal design and operating conditions but also tackle the environmental issues related to emissions.

### 4.2 Optimization Framework

As mentioned earlier the main objective of the proposed framework is to integrate process analysis with the environmental damage assessment and to formulate improved objective function for advanced optimization of the chemical plants. The methodology comprises the steps of process modeling, transference of data, evaluation of the environmental damage, and optimization. A short description of the actions concerned to each of the steps is presented in the following section.

#### 4.2.1 Process Modeling

The objective of the process modeling is to perform inventory calculations and quantify the consumption of resources (including energy and utilities) and releases to the environment as close as possible to the real operation. Therefore modeling is the most critical part of this methodology. There are several commercial simulation programs available today which offers detailed modeling and other advanced features. For this study, Aspen HYSYS is used to model the process to obtain all the mass and energy information. This step can also be used to identify the process streams and other basic information regarding their role in the process (input/output, energy/material and product/by-product). Considering the example of the Packed Distillation Unit in Chapter 3, the summary of the main production results are presented in Table 4.1.

#### 4.2.2 Integration and Data Transfer

The steady state model, predicts the mass, energy flows and all other parameters and, at the same time, these data are transferred to/from MS-Excel. The bridge code is programmed in Visual Basic Application (VBA), the computational resource to programming macros. It allows
Table 4.1 The summary of the production results

<table>
<thead>
<tr>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>--</td>
<td>Reflux Ratio</td>
<td>1.12</td>
</tr>
<tr>
<td>Btu/hr</td>
<td>Reboiler Duty</td>
<td>9000.60</td>
</tr>
<tr>
<td>Deg F</td>
<td>Feed preheat Temperature</td>
<td>145.00</td>
</tr>
<tr>
<td>GPH</td>
<td>Distillate Flow Rate</td>
<td>1.12</td>
</tr>
<tr>
<td>GPH</td>
<td>Bottom Flow Rate</td>
<td>1.97</td>
</tr>
<tr>
<td>--</td>
<td>Distillate Mole Fraction(Methanol)</td>
<td>0.90</td>
</tr>
<tr>
<td>--</td>
<td>Bottom Mole Fraction(Methanol)</td>
<td>0.28</td>
</tr>
<tr>
<td>Btu/hr</td>
<td>Condenser Duty</td>
<td>8646.63</td>
</tr>
<tr>
<td>Btu/hr</td>
<td>Feed preheater Duty</td>
<td>1156.84</td>
</tr>
</tbody>
</table>

the user to import and export any selected variables between the HYSYS model and Excel worksheet (Herrera, 2001). Microsoft Excel is used to extend the computational and optimization capability of the simulated process, particularly, within the context of the optimization framework. This extracted data provides the basis for calculation of energy consumption and environmental emissions and is further used in optimization. Figure 4.1 is the overview of the Excel spreadsheet used optimization interface. Also shown in the spreadsheet are the optimum values (column top and bottom temperature) sent to the MPC controller as set points (discussed the next chapter) to study the operability for the optimized conditions and the effects of transition.

The proposed optimization framework is proven to be very cost effective as it has been developed exploiting the capabilities of the commercial software packages like Aspen HYSYS®, Microsoft Excel (Premium solver add in) and Standard Visual Basic Applications. For every trial solution, during the optimization method, process data has to be communicated back and forth to the simulation model in order to obtain the optimum results. Therefore the linkage between the HYSYS model and Microsoft Excel is bidirectional in nature.
4.2.3 Environmental Assessment

The environmental objectives used in the framework are developed based on the Life Cycle Assessment (LCA) methodology. In recent years, LCA has given a lot of attention as an environmental indicator of chemical processes (Burgess and Brennan, 2001). The LCA is a fairly new chain-orientated tool created to evaluate the environmental performance of a product, since the extraction of raw materials, through manufacture, use and final disposal. The methodology of LCA can be divided in four steps: Goal and Scope Definition, Inventory Analysis, Impact Assessment and Interpretation (Heijungs et al., 1992; Fava et al 1993). Through all of these steps, environmental aspects regarded to consumptions of natural resource and releases to air, water and soil, are identified, quantified and expressed in terms impact indicators providing to the decision makers, the environmental profile of the process in study. The application of EDA technique provides consistent information about the type and extent of damage on environment.
The foremost step in developing the economic or environmental model is inventory calculation which includes the raw material and energy consumption. The main sources of energy consumption in any refinery or a petrochemical plant are pumps, compressors, furnaces, heaters and reboilers. The energy consumed could be either in the form of electricity, steam and fuel. The amount of pollutants and the extent of environmental damage is directly related to the consumption of resources both raw material and energy. Therefore the total energy consumed has to be accounted, to estimate the actual emissions to the atmosphere. The extracted data from the model is used to develop the environmental model for the optimization.

The following three steps are used: a) definition of the eco-vector; b) determination of scenarios and c) environmental damage assessment. The eco-vector definition requires the assignment of environmental loads (EL). In this work, Sulfur dioxide (SO2), carbon dioxide (CO2), and nitrogen oxides (NOx) were chosen as Environmental Load (EL), considering the severity of their relevance in the main environmental effects. The information related with these loads were provided by two bibliographic sources: *ETH Report* (Frischknecht, 1996), and *TEAM database* (Ecobilan Group, 1998).

The manufacturing firms adopt different strategies to meet the energy requirement which is unique for that process. It depends on several factors like plant capacity, location, and nature of the process etc. The use of scenarios during the environmental analysis allows comparing different alternatives in terms of system environment interactions. In this study, two scenarios were chosen, based on the several possibilities to obtain the steam and electricity required in the process. Once the total environmental loads associated with material and energetic streams of the overall process are estimated, the environmental related costs, included in the objective function are calculated. This information can further be used to study and categorize the impact on human health, natural resources and the ecosystem. These environmental impacts can be calculated in
terms of damage indicators by using weighting methods as discussed in Herrera et al, 2000.

Referring to the PDU example, considering that the plant requires electric power and steam, the production of which consumes natural resources and generates environmental emissions. In defining the eco vector, sulfur dioxide (SO2), carbon dioxide (CO2), and nitrogen oxides (NOx) are chosen as Environmental Load (EL), taking into account their relevance in the main environmental effects. In this study, the efficiency for Glycol Heating system is assumed to be 0.80. The net equivalent electricity consumed is then calculated in Giga Watt Hr (GWH). Then the quantity of each environmental load is estimated using the available correlation. The data in Table 4.2 has been used in computing the total environmental emissions.

<table>
<thead>
<tr>
<th>Environmental Loads</th>
<th>Fuel oil</th>
</tr>
</thead>
<tbody>
<tr>
<td>C02, Ton/GWH</td>
<td>657</td>
</tr>
<tr>
<td>SO2 Kg/GWH</td>
<td>1030</td>
</tr>
<tr>
<td>NOX Kg/GWH</td>
<td>988</td>
</tr>
</tbody>
</table>

*special report of World Energy Council, July 04

4.2.4 Optimization Model

The process optimization has been a major quantitative tool in industrial decision making. Traditionally, the process engineers were more concerned about the economical and control objectives and have ignored the environmental aspects. The main goals of the process optimization are minimizing cost, maximizing throughput, increasing yields of valuable products, and lower maintenance period. These profitability assessment techniques vary from simple measures to more advance and complex ones, such as operating expenses, operating profit, capital cost, rate of return, discounted cash flow rate of return, net present value, payback period and etc., based on the decision makers’ preferences and on the nature of the optimization problem and the selected decision variables. The conventional objective function (Eq.4.1)
includes only the costs associated with the feed, products, utilities and energy.

Profit Function = Product Revenues – Raw material costs – operating expenses. \(4.1\)

However, the rising concerns on global warming and with implementation of emissions trading programs (“cap and trade”), the environmental costs are becoming significantly higher and therefore have to be considered in the optimization criteria together with technical and economical evaluations. Therefore an improved objective function known as triple bottom line function is defined (Eq. 4.2) which would take into account the environmental effects into the optimization problem (Sengupta et al, 2007). The addition of the environmental aspects to the optimization adds to complexity of the problem because these are often conflicting with the economic objectives. This proposed framework is intended to complement the existing cost estimating practices with environmental costs for improved decision-making.

Triple bottom line = Profit function – Environmental cost - Sustainable debit + Sustainable credit. \(4.2\)

- **Sustainable debit** = Costs to the society to repair the damage to the environment by emissions
- **Environmental Cost** = Costs required to comply with environmental regulations including permits, monitoring emissions, fines, etc
- **Sustainable Credits** = Credit given to the processes that use CO2

The new objective function is based on Total Cost Assessment (TCA) methodology. This methodology is developed by team of industrial firms that is broadly applicable to many industrial sectors. It provides the framework for not only decision making process but also for estimating baseline costs that have a much broader and potentially longer timeframe. TCA is defined as the identification, compilation, analysis, and use of environmental and human health cost information associated with a business decision (TCA Manual, 2000). Therefore TCA will
contribute to improved long-term competitiveness such as reducing environmental expenses, increasing revenues, and improving future environmental performance requires paying attention to current and potential future environmental costs. Potential future costs include potentially hidden impacts on the environment, human health, and ecology, as well as internal intangible costs. When environmental accounting extends beyond conventional costs to include potentially hidden, future, contingent and image/relationship costs, manufacturing firms may find it more difficult to assess and measure certain environmental costs.

In many of these decision contexts, environmental cost information is treated as just another cost of doing business, as it is in product pricing or product mix. In certain situations, the environmental cost information may play a unique role in the decision process, for example, in waste management decisions, pollution prevention alternatives, or market-based environmental options.

The following section explains the model formulation with respect to the packed distillation unit discussed earlier. It is assumed that the feed to the process is fixed and the environmental cost is estimated as a fraction of the feed cost. It is also assumed that there are no processes utilizing the emissions in the plant i.e. there is no sustainable credits associated with the process. Therefore the improved objective function being used in the methodology is reduced to the following equation.

Objective Function = Product revenues – Utilities cost – Sustainable debit

The quantities of the pollutant that are calculated during the environmental analysis are used to estimate the associated cost. The Eq. 4.4 gives the expression used to compute the total sustainable debit for the given process conditions while Table 4.3 summarizes the information used for calculating the total sustainable debit associated with the process.

Sustainable debit = Σ Environmental load, Ton * Cost, $/Ton
Table 4.3 Sustainable debits used for various environmental loads

<table>
<thead>
<tr>
<th>Environmental Load</th>
<th>$/Ton</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO2</td>
<td>3.25</td>
</tr>
<tr>
<td>SO2</td>
<td>192</td>
</tr>
<tr>
<td>NOX</td>
<td>1030</td>
</tr>
</tbody>
</table>

Once the sustainable debit is computed, the final objective function is computed using the following equation

\[
OBJ = (20 \times X_M \times F_D + 2.62 \times F_B) - (Q_H \times 4 \times 10^{-6} + Q_C \times 0.75 \times 10^{-6}) - \text{Sustainable debit}
\]

Where, 
- \(F_D\) – Product flow rate, gal 
- \(F_B\) – Bottom residue flow rate, gal 
- \(Q_H\) – total heating duty required, btu/hr 
- \(Q_C\) – total cooling duty, btu/hr 

It should be noted that the decision variables used in the optimization should be specified as active specifications in the steady state simulation case in order for the optimizer to manipulate the variables. In addition to the constraints on the decision variables, the optimization problem is subjected to other process and environmental constraints such as those on quality, heating and cooling duty specifications. The Table 4.4 summarizes the results as well as the decision variables and the constraint imposed in the optimization problem. Table 4.5 is the summary of the product and utility costs used in the optimization problem. The results from the solver are shown in Figure 4.2. The value of the objective function is increased from 22.3$/hr to 24.7$/hr.

4.3 Software Architecture

In the proposed framework, the optimization technique, \(\varepsilon\)-constraint, is formulated with the Frontline Systems' premier spreadsheet optimization product, Premium Solver Platform®. It is a compatible upgrade of the standard Microsoft Excel solver that greatly extends its speed and
problem solving capacity. It uses improved generalized gradient method (Frontline Systems, 2000) and is capable of solving large scale nonlinear and global optimization problems. As mentioned earlier the data transfer between the HYSYS model and the spreadsheet interface is programmed in Visual Basic Application. Interaction with the HYSYS uses link and embed (OLE) Automation. OLE is a tool that enables applications to expose information/data constructed within them to other applications to support automation.

### Table 4.4 The summary of decision and constraint variables in the optimization

<table>
<thead>
<tr>
<th>Decision Variables</th>
<th>Initial value</th>
<th>Optimal value</th>
<th>Minimum</th>
<th>Maximum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reflux Ratio</td>
<td>1.12</td>
<td>1.30</td>
<td>1</td>
<td>1.6</td>
</tr>
<tr>
<td>Reboiler Duty</td>
<td>9000.60</td>
<td>10449.06</td>
<td>8500</td>
<td>15000</td>
</tr>
<tr>
<td>Feed preheat Temperature</td>
<td>145.00</td>
<td>140.00</td>
<td>140</td>
<td>148</td>
</tr>
<tr>
<td><strong>Constraints</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Distillate Flow Rate</td>
<td>1.12</td>
<td>1.43</td>
<td>0.75</td>
<td>1.5</td>
</tr>
<tr>
<td>Bottom Flow Rate</td>
<td>1.97</td>
<td>1.66</td>
<td>1</td>
<td>2.4</td>
</tr>
<tr>
<td>Distillate Mole Fraction(Methanol)</td>
<td>0.90</td>
<td>0.88</td>
<td>0.8</td>
<td>0.99</td>
</tr>
<tr>
<td>Bottom Mole Fraction(Methanol)</td>
<td>0.28</td>
<td>0.20</td>
<td>0</td>
<td>0.3</td>
</tr>
<tr>
<td>Condenser Duty</td>
<td>8646.63</td>
<td>10075.03</td>
<td>8000</td>
<td>10000</td>
</tr>
<tr>
<td>Feed preheater Duty</td>
<td>1156.84</td>
<td>1138.04</td>
<td>850</td>
<td>1250</td>
</tr>
</tbody>
</table>

The $\varepsilon$-constraint method is employed in the optimization formulation due to its ability of handling the two types of optimization problems, convex and non-convex, which is a characteristic of many chemical design problems. In the optimization framework, the objective function is normalized, over the specified range of the assigned decision variables, and scaled between 0 and 1, where 0 represents the best value and 1 represents the worst value of the objective. This scaling is usually recommended in optimization problems to ease the comparison between the formulated objectives and to avoid the computational confusion that is due to different scale objectives. Moreover, the normalized objectives will follow the same path of
optimization, maximization or minimization, and at the end of the optimization process, the restored objective values are displayed in the original scales to the decision-maker.

Table 4.5 Summary of the product and utility cost used for the optimization

<table>
<thead>
<tr>
<th>Product Name</th>
<th>Price ($/Gal)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distillate</td>
<td>20 * $X_M</td>
</tr>
<tr>
<td>Bottoms</td>
<td>2.6</td>
</tr>
<tr>
<td>Feed</td>
<td>0.7</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Duty</th>
<th>Price ($/MMBtu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reboiler Duty</td>
<td>4</td>
</tr>
<tr>
<td>Feed Preheater Duty</td>
<td>4</td>
</tr>
<tr>
<td>Condenser Duty</td>
<td>0.75</td>
</tr>
</tbody>
</table>

$X_M$ - Mole fraction of methanol

Figure 4.2 Results from Excel spreadsheet
The selected process parameters are assigned as the decision variables of the optimization problem. These variables should be as active specifications in the HYSYS model so that the optimizer is able to manipulate the values of these variables. The optimizer searches over each process variable’s space, within the feasibility and constraints regions and export the decision variables to the model in HYSYS. During this step, the optimizer waits till the model is converged and then the new process information is imported back to the spreadsheet to recalculate the target value i.e. the objective function and the other variables. This search loop between the optimizer in Excel and the model in HYSYS continues until a global optimum point is found. The above optimization process is repeated for different bounds of the constrained objectives to develop the entire Pareto optimality set of solutions.
CHAPTER 5

MODEL PREDICTIVE CONTROL

5.1 Introduction

The scope of the control systems in process industries has been broadened from the basic regulatory control to advanced control strategies to ensure the competitive edge in the face of dynamic market conditions. In modern refining and petrochemical industries there is a strong correlation between the plant control performance and the financial performance condition of the industry. The control systems become more effective by integrating all aspects of automation and decision making such as measurements, control, optimization and the logistics. Thus the implementation of such integrated systems are demanding advanced control strategies with the ability to integrate and satisfy several criteria such as economic, safety, environmental, plant capacity, and the product quality. Such systems also facilitate in efficient use of energy resources and to reduce environmental emission.

Model Predictive Control (MPC), is the most prominent among all the exiting advanced control strategies. The use of MPC concept has now spread wide and covers a broad spectrum of industries such as food processing, metallurgy, pulp and paper and aerospace and defense industries (Qin and Bagwell, 1997). MPC is an efficient and integrated solution to complex process control problems involving inverse responses and extensive process delays. It is ideally suited for multivariable control operations where all interactions between manipulated variables (MVs) and control variables (CVs) are taken into account. MPC has the ability to operate without much expert interference for relatively long periods of time.

5.2 Background

MPC was initially developed to meet the specific control objectives of the petroleum
refineries and power plants. Over the past decade, MPC has become a standard control practice particularly in petrochemical and refinery industries (Qin and Bagwell, 1997) mainly due to its extended benefits over traditional controllers (Garcia et al., 1989). There have been several papers published in the last two decades describing the successful applications of the model predictive control algorithms in process industries (Richalet et al. 1978; Tinham, 1993; Warren, 1992 and Oguinnake, 1994).

However, the thought of ideas for MPC had started since the 1960’s (Garcia et al., 1989). The correlation between the closely related optimal control problem and linear programming were recognized first by Zadeh and Whalen, 1962. Propoi, 1963 had suggested the core of all MPC algorithms the moving horizon approach. With the rapid increase in the use of MPC, the control algorithms have gained both academic and commercial interest. The MPC fundamentals and its applications are thoroughly discussed in several textbooks (Bitmead, Gevers and Wertz, 1990; Soeterboek, 1992; Clarke, 1994; Berber, 1995; Camacho &Bordons, 1995). There are a wide variety of MPC algorithms that have been developed over past decades. The first model predictive control algorithm was Model Predictive Heuristic Control and was successfully implemented on a Fluid Catalytic Cracking Unit (FCCU) main fractionators’ column in a poly-Vinyl Chloride plant (Richalet et al. 1978).

In general, MPC refers to a family of controllers in which there is a direct use of an explicit process model to forecast the future behavior of a plant, make preemptive control moves, and optimize plant performance. The future control sequence is computed at the current time, k. The future control action is determined by posing an optimization problem with the objective of minimizing the prediction error subject to the constraints. The optimization problem is generally solved via a numerical minimization algorithm using the current plant operating conditions as the initial state but only the first control move in this sequence (at time k+1) is applied to the plant.
Therefore MPC is supposedly a perfect real-time optimal control model equipped with process integration capability (Camacho and Bordons, 1998). The name “Model Predictive Control” arises from the approach in which the control strategy is computed.

There are a number of MPC algorithms namely LMPC algorithm, the Dynamic Matrix Control (DMC) (Cutler and Ramaker, 1979), the Generalized Predictive Control (GPC) (Clarke et al. 1987), Quadratic-Program Dynamic Matrix Control (QDMC) (Cutler et al. 1983) and the Internal Model Control (IMC) (Garcia and Morari, 1982). These algorithms differ from each other in applied model structure and the solution of the cost function of the optimization problem (Henttonen 1992), (Soeterboek, 1992). However, the fundamental structure of the MPC algorithms is common for any kinds of MPC strategy. The basic elements of MPC methodology are illustrated in Figure 5.1 and can be defined as follows

**Figure 5.1 Principle of the Model Predictive Control**

- An explicit dynamic model (mostly linear empirical models) is used to predict the dynamic behavior of a plant over a certain future time interval normally known as the prediction horizon (P). At the present time k the behavior of the process over a horizon p is considered.
Using the model the process response to changes in the manipulated variable is predicted. For a discrete time model this means it predicts the output state of the process from \( y'(k + 1) \) to \( y'(k + H) \) based on all actual past control inputs \( u(k), u(k-1),...,u(k-j) \) and the current state \( y(k) \).

- The moves of the manipulated variables are determined such that the predicted response has certain desirable characteristics i.e. a sequence of control action moves \( (\Delta u(k|k-1)\ldots \Delta u(k+m|k-1)) \) to be implemented over a certain time interval, known as the control horizon (m) is calculated by optimization of specified objectives such as the deviation of predicted output from set point over the prediction horizon and the size of control action adjustments in driving the process output to target plus some operating constraints. However, as discussed before only the first move of computed control action sequence is implemented. At time \( k+1 \) the entire computation is repeated with the horizon moved by one time interval and therefore the algorithm proceeds forward in time. This strategy is often referred to as *receding horizon* strategy.

- As mentioned before the key to the MPC strategy is the plant model to predict the dynamics of the process and since no model can constitute a perfect representation of the actual process, plant measurements are used to compute the prediction error \( \varepsilon(k) \) between the plant measurement \( y(k) \) and the model prediction \( y'(k) \). The \( \varepsilon(k) \) obtained is normally used to update the future prediction. The basic block diagram of MPC is illustrated in Figure 5.2.

### 5.3 Types of Model

As discussed the model is the essential element of an MPC controller. These models are most often linear empirical models obtained by system identification. However when linear models are not sufficiently accurate because of nonlinearities, the process can be represented by...
a nonlinear model i.e. the MPC utilizes a nonlinear model directly in the control application. The issues of feasibility of the online optimization, stability and performance for both the linear and nonlinear MPC are discussed in several papers (Morari and Lee, 1999 and J. Rawlings, 1999). More detailed information about the MPC formulation, future prospects and implications from both the academic and commercial perspective are reviewed in several research papers. (Garcia et al., 1989; Camacho and Bordon, 1999; Qin and Bagwell, 2000; Maciejowski; 2002)

![Figure 5.2 The basic block diagram of Model Predictive Control](image)

5.3.1 Non Linear Models

Although the need of Nonlinear Model Predictive Control (NMPC) is well recognized and various types of NMPC strategy have been developed, the number of NMPC applications are limited (Qin and Bagwell, 1997 & 2000). This is mainly due to the difficulty in developing an accurate nonlinear process model and the computational problem associated with the Non-Linear Programming (NLP). NMPC refers to the MPC algorithm that employs a more accurate nonlinear model in control applications (Henson, 1998). NMPC strategies are mainly applied to processes such as high purity distillation column (Fruzzetti et al., 1997; Georgiou, et al., 1988)
and Ravi Srinivas et al., 1995) and semi-batch reactors where frequent product grade changes, wide operating conditions and large disturbances are common. Some of the commercial NMPC products that are available in the market are: Adersa Predictive Functional Control (PFC), Aspen Technology Aspen Target, Pavilion Technologies Process Perfecter and Continental Controls Multivariable Control (MVC).

The nonlinear models may be in the form of either an empirical data fit (e.g. artificial neural networks) or a high fidelity model based on fundamentals such as mass, species, and energy balances. The empirical method relies only on the process data available and requires no understanding of underlying physical phenomena of the system. Therefore the use of this modeling method is limited to the operating region where the model has been identified. Various kinds of empirical models have been utilized in NMPC design. These include Hammerstein model (Fruzzetti, et al., 1997), Volterra model (Maner et al., 1996), and collocation model (Jang and Wang, 1997). The models developed using the fundamental laws are normally in the form of differential and algebraic equations such as the ordinary differential equations (ODE) or partial differential equation (PDE). This kind of model is globally valid due to its natural characteristic, however, the derivation of first principles model is normally expensive and difficult to maintain (Piche et al., 2000) and often yield a model of very high order due to rigorous modeling (Lee, 1998). Many of NMPC studies based on the fundamental model had been reported within last decade (Patwardhan and Edgar, 1990; Ricker and Lee, 1995; Zheng, 1997).

5.3.2 Linear Models

Historically, the models of choice in early industrial MPC applications were time domain, input/output, step or impulse response models (C. R. Cutler and B. L. Ramaker, 1980), J. Richalet et al, 1978 and D. M. Prett and R D. Gillette, 1980) due to the ease of understanding provided by these models. In addition the linear models can be developed relatively easy and
also provide acceptable results when the plant is operated in the neighborhood of the operating point. Most Linear MPC algorithms use one of the following models to predict the dynamics of the process depending on the context.

**Finite Impulse Response model**

In FIR model, the output at a discrete time step \( k \) is expressed as the following function of input states (Eqn.5.1). The model is illustrated in Figure 5.3. This model has certain advantages from a practical implementation viewpoint as it eliminates the need to specify the time delays and therefore even complex dynamics can be represented with equal ease. However the use of this model is limited to only stable process

\[
y(k) = \sum_{i=1}^{N} h_i u(k - i)
\]

**State Space Model**

State space model is the common technique of model representation. The system to be controlled is described by a linear discrete time model. The state-space models have several advantages including easy generalization to multi-variable systems, ease of analysis of closed loop properties, and on-line computation. The state space models are expressed as

\[
x(k) = A \ x(k-1) + B \ u(k-1)
\]

\[
y(k) = C \ x(k)
\]

**Step-Response Model**

The step-response model is used in DMC algorithm originally proposed by Cutler and Ramaker, 1980. A Step Response model is usually expressed as

\[
Y(k) = \sum_{i=1}^{N} a_i \Delta u(k - i) + a_{ss} \ u(k - N - 1)
\]

Where \( a_i \) is the step-response coefficient and the last term represents the steady state bias. The model horizon \( N \) defines the memory of the model where \( \Delta u(k) = u(k) - u(k-1) \). The values of
a_i at different intervals are obtained by using the unit step response for the process at sampling periods \( \Delta t \). \( a_i = 0 \) for \( i < 0 \) and \( N \Delta t \) is the settling time of the process. The model is illustrated in Figure 5.4.

![Figure 5.3 The Finite Impulse Response model](image1)

Assumptions:
- \( H_0 = 0 \): no immediate effect
- The response settles back in \( n \) steps s.t. \( H_{n-1} = H_{n-2} = \ldots = 0 \) “Finite Impulse Response” (reasonable for stable processes).

### Figure 5.3 The Finite Impulse Response model

![Figure 5.4 The Step Response Model](image2)

Assumptions:
- \( S_0 = 0 \): no immediate effect
- The response settles in \( n \) steps s.t. \( S_n = S_{n-1} = \ldots = S_0 \) the same as the finite impulse response assumption
- Relationship with the impulse response coefficients:
  \[
  S_k = \sum_{i=1}^{k} H_i \\
  H_k = S_k - S_{k-1}
  \]

### Figure 5.4 The Step Response Model

#### 5.4 Limitations

However, there are some practical limitations related with MPC in terms of stability and robustness. The need for an optimal control solution to improve performance in multiple dimensions involves a higher level of mathematical and computational complexity in derivation of control law. The MPC are highly dependent on the model and therefore the performance of
these controllers is directly related to the accuracy of the model. Any inconsistencies between the actual process and the model used for prediction will affect the control performance severely. The Lundstrom et al., 1994 reported a few limitations of DMC including it may perform poorly for multivariable plants with strong interaction. The other drawbacks related to operation, high maintenance cost, lack of flexibility of MPC are argued in several papers (Hugo, 2000).

5.5 Role of Simulation in MPC Identification

Traditionally, MPC implementation is a tedious job that involves extensive operator interference. Industrial experience has shown that the most difficult and time-consuming effort in an MPC project is model identification. The model identification is done by a series of lengthy step tests. Each step test requires the operator to make a step move and allow the process to settle to reach a new steady state. The response data is then analyzed and is used to develop the model. However, the quality of collected data depends on the technical competence and experience of the control engineer and the operator as well. This procedure is repeated for every manipulated variable. Because such deliberate step tests are quite expensive, disruptive, invasive and time consuming (may extend to several months in case of a large unit), a significant incentive exists to minimize the step tests, if not eliminate them entirely (Hokanson, D.A et al, 1992). This approach has other drawbacks such as it is often required to perform aggressive testing to determine a signal to noise ratio for process model identification and also certain external disturbances cannot be included in the model.

Recently, there is a growing demand for more efficient model identification methods and some APC vendors started to respond on this demand. Some effort has been made in model identification by several MPC vendors to utilize modeling and simulation tools. The actual process is simulated using the state of the art simulation tools and the step tests are performed in the simulation environment. The use of this approach based on steady and dynamic state simulations to develop the necessary models avoid disruptive and costly step testing to the extent feasible (Umesh et al, 2008)
5.6 Building the MPC Controller

HYSYS is capable of performing advanced control strategies such as the Model Predictive Control (MPC). The following is the summary of steps to install and run the MPC controller in HYSYS. The proper dynamic model of the process should be available before building the MPC controller. The model should run with no errors and instabilities.

1. The foremost step is to determine the number of inputs and outputs there are in the control problem. In most problems the number of inputs will be equal to the number of outputs, i.e., a square system.

2. Once the number of inputs and outputs are known some basic modeling is required. A step response data can be used to represent the models between the inputs and the outputs. A multivariable open loop test can be performed to obtain the step response data for the selected controlled and the manipulated variables. A step change of 5% is introduced in each of the MV and the CV’s are monitored.

3. Add the MPC controller and input the required information to configure the controller using the model data obtained in the previous steps. In addition to the control interval, the other configuration parameters can also be defined. The following are the control parameters that can be adjusted in the HYSYS

A. *Step response length:* This is the length of the step response that will be used in the controller calculation. The default is 50 and the maximum is 100.

B. *Prediction horizon:* This value determines how far into the future the predictions are made when calculating the controller output. It is bounded by the length of the step response.

C. *Control horizon:* This value represents the number of controller moves into the future
that will be made to achieve the final set point. The value is bounded by the prediction horizon.

D. *Gamm_U and Gamma_Y:* These are weighting functions associated with the optimization problem that is solved to produce the controller output every control interval.

E. *Reference Trajectory:* On set point changes this value represents the time constant of a filter that acts on the set point, i.e., a filtered set point can be used for the control. When the value is small the controller essentially sees a pure step as the set point is changed.

### 5.7 Application to the Packed Distillation Column

Referring to the packed distillation unit modeled, the column’s top and bottom temperature are chosen as the controlled (dependent) variable. The reflux flow and reboiler hot stream flow are chosen as manipulated (independent) variables. The main objective of the process is to obtain the required purity or composition in both the distillate and the bottoms of column. However since there are no online composition analyzers to measure composition of the streams, the tray temperatures are used to infer the composition. Per the method of Moore, the top tray temperature was used to represent the top product composition and bottom tray temperature was used to represent the bottom product composition. Since we have a 2x2 multivariable process, there will be four process models to be determined. A multivariable open loop test is performed to obtain the step response data for the selected controlled and the manipulated variables. A step change of 5% is introduced in each of the MV and the CV’s are monitored. Using the step response data obtained the model transfer functions are developed by exporting to control station software. These models are based on percent changes in input PVs and percent
changes in the corresponding Ops. Table 5.1 summarizes the transfer function matrix while

Figure 5.5 gives an overview of the MPC controller developed for the process.

Table 5.1 Transfer Function Matrix of the process

<table>
<thead>
<tr>
<th>MV/CV</th>
<th>MV1-Reflex flow</th>
<th>MV2 – Reboiler duty</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV1 - Top tray temp.</td>
<td>[-0.288, 2.2, 0.0]</td>
<td>[0.112, 14.5, 0.33]</td>
</tr>
<tr>
<td>CV2 – Bottom tray temp</td>
<td>[-0.2340, 32.0, 0.0]</td>
<td>[0.278, 45.0, 1.0]</td>
</tr>
</tbody>
</table>

* Transfer Function is expressed as: [gain, time constant (min), delay (min)]

Figure 5.5 Overview of the MPC controller developed

Once the model information is defined in the controller, the control parameters are adjusted. Table 5.2 gives the summary of control parameters used in developing the MPC controller.

Table 5.2 MPC Controller parameters used in the simulation

<table>
<thead>
<tr>
<th>Control Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step response length</td>
<td>50</td>
</tr>
<tr>
<td>Prediction horizon</td>
<td>25</td>
</tr>
<tr>
<td>Control horizon</td>
<td>2.0</td>
</tr>
<tr>
<td>Gamm_U and Gamma_Y</td>
<td>1.0</td>
</tr>
<tr>
<td>Reference Trajectory</td>
<td>1.0</td>
</tr>
</tbody>
</table>
It should be noted that, in the proposed methodology, the results from the steady state optimizer are exported to MPC controller. Hence, the optimal conditions achieved from the optimizer can be validated for the operability and controllability. The MPC controller then provides the set points to the basic PID controllers installed in the column environment. The controller is evaluated by installing the strip chart for the selected variables. The response plot for a set point change in the top temperature is shown Figure 5.6.

![Response plot for a setpoint change in top temperature](image)

**Figure 5.6 Response plot for a setpoint change in top temperature**
CHAPTER 6
TRAINING SIMULATOR

6.1 Introduction

Training simulators have been widely accepted as the most effective method for training in the many industries especially nuclear, aerospace and military industries. Besides the governmental regulations, an important factor in using simulated training programs is the ability to train the inexperienced operator on abnormal and emergency scenarios that are seldom encountered in real life. The high capital investment and lack of sophisticated modeling techniques have limited the scope of these simulators in process industries. The training simulators use process models to produce a real time dynamic representation of the plant. The analysis of unsteady conditions performed by tools based on dynamic models can be dated back to the 1990s, with the industrial case studies analyzed by Bretelle and Macchietto, 1993; Bretelle et al., 1994 and Pantelides and Oh, 1996. They were mainly used for accident prevention and were limited to a single unit operation or a small section of the plant.

However with the advances in the field of information technology, there are now fewer limitations for developing detailed, high-fidelity training models which are capable of being utilized for engineering applications prior to training. The advent of advanced modeling environments has significantly increased the role of simulation in the plant operations, planning and supply chain domains and in other engineering areas. The training models can also be used to validate process designs, verify control configurations and perform operability studies. Therefore the training simulators justified for simply “training” are now paying for themselves in other engineering benefits prior to operator training. The accurate and realistic simulations allow engineers/students to broaden the limits of a plant’s capability and identify operational and
physical constraints in a safe and theoretical environment. The training simulators are now considered as the state of art for training and plant trouble shooting. The use of simulated environment for training facilitates understanding fundamental plant operations and improves their ability to optimize plant performance with the same simulation tool. Such practice enables operators to exercise best practice methods for safe and efficient plant operation. In recent years, the cost of these training models has reduced considerably mainly because there has been a significant improvement in the computing cost/performance ratio.

6.2 System Architecture

The various components present in the training simulator are the process model, the control system and the visual interface (HMI). The control system can be either the actual controller module or an “emulated” controller that represent the control system. The information is exchanged between the process model and the control system through the use of standard Object Linking and Embedding for Process Control (OPC) technology. The overall architecture of the training simulator is shown in Figure 6.1

Figure 6.1 System Architecture of the Training Simulator
6.2.1 The Process Model

The process model is a crucial part of the simulator. Through the use of appropriate process modeling tools, unit operations are parameterized to match the exact features of the plant to produce a real-time dynamic representation of the unit. The overall fidelity of the model should ensure that operators can be trained to observe and respond correctly to a variety of operating conditions. The model should be accurate enough to reproduce not only plant responses due to disturbances around the normal operating conditions, but also the dynamic behavior for non-design operations including process upsets and emergency conditions. The detailed description of the dynamic simulation is provided in Chapter 2. For a typical plant, many major units can be modeled. These include such compressors, pumps, fired furnaces, heat exchangers, reactors etc.

6.2.2 The Control System

These systems normally include a Distributed Control System (DCS), Programmable Logic Controllers (PLCs), and Emergency Shutdown Systems (ESDs). The control system can be either the actual controller or the simulated controller software which emulate the plant's actual control strategies into modules that can be used within the training simulator without the need to buy an additional DCS. The use of high-fidelity simulated operator stations can considerably reduce the capital investment on training simulators.

**Distributed Control System:** It refers to the type of automated industrial control system and is extensively used in process-based industries like oil & gas, refining and petrochemical, pharmaceutical, food & beverage, pulp & paper, etc... The main function of a DCS is to monitor and control the various field devices that are distributed across the network. The DCS was first introduced in 1975. Honeywell’s TDC 2000® and Yokogawa’s CENTUM® DCS were released independently during the mid-1970s. US-based Bristol also introduced their UCS 3000 universal controller in 1975. The market for DCS has been steadily growing and currently there
are about 35 DCS manufactures available in the market. The most prominent are Honeywell, ABB, Yokogowa, and Invensys.

A typical industrial plant can have thousands of input/output points (analog and digital), multiple control loops, several safety interlocks and program sequences. The control functions are distributed among different control processors often configured in redundant pairs. DCS use decentralized elements or subsystems to control distributed processes or complete manufacturing systems. They employ proprietary networking and communication protocols to communicate between the various components. Today’s controllers have extensive computational capabilities and can generally perform logic and sequential control in addition to proportional, integral, and derivative (PID) control. A server and/or applications processor may be included in the system for extra computational, data collection, and reporting capability. The general architecture of the DCS is shown in Figure 6.2

![Figure 6.2 A Typical Distributed Control System (DCS) Architecture](image-url)
The DCS reads the input from the transmitter or a sensor stores the information in a database and performs the control logic. The output/command from the controller is sent to actuators (e.g. valves) on the plant. The DCS also forms the interface between the plant and the operating personnel. Typically, the operators are provided with graphical representation of the processes along with the real time information of the operating parameters. DCS performs various tasks such as data collection, trending and alarming which are useful for monitoring and to control the plant in a safe and efficient manner.

Typical components within the control environment are the control modules and the input/output (I/O) modules. The control module is the component where the control strategies are executed. It communicates with the I/O modules using a communication protocol. Control functions are often supplied through a library of the templates called function blocks and the control strategies are built using the graphical engineering tools called control builders. I/O modules provide the terminal and processing power to accept input signals from the transmitters, thermocouples and send output signals to final control elements such as control valves.

6.2.3 The HMI Model

The Human Machine interface (HMI) is the only component which has direct contact with the student/operator. It is the front end of the training simulator. The HMI system usually presents the process information to the operator, in the graphical form. The visual displays consist of line graphics and schematic symbols with proper animation to represent the condition or state of different process elements like the pump, controller. It provides all the necessary process information like the temperatures, pressures, flow rates, alarms on the screen and thereby enable the operator to act accordingly. The operating personnel can visualize the schematic representation of the plant being controlled. An HMI is linked to the control system and software programs, to provide trending and history of process data, management information such as
maintenance procedures, emergency control actions, logistic information and detailed displays. Training simulators can either use the actual DCS console connected to the training simulator or an emulation of the operator's console.

### 6.3 OPC Connectivity

Once the process model and control system components are configured, they have to be linked. The simulation variable in the process model is to be linked to the corresponding I/O point in the control system representation or the actual controller. The controller reads the information from the simulated variable and performs the necessary calculations accordingly and returns the output again to the simulated variable. The flow of information between the model and the controller is described in Figure 6.3.

The exchange of data and commands is based on Object Linking and Embedding for process control (OPC) technology. OPC consists of a series of standards that define interoperability among different automation and control applications, field systems, other business and office applications. OPC defines a standard interface for allowing applications to access data from a variety of process control devices. OPC is fast and can handle the very large data transfer rates required for this application. There are mainly two components involved, OPC server and OPC client. OPC server provides the standardized interface for OPC client to query data and OPC client provides an interface to request and write data to an OPC server. Therefore it provides data from a server and communicates the information to any client application in a standard way, thereby eliminating the need to have extensive knowledge about the data source, such as its internal configuration and communications protocols.

It is also expected that the server will consolidate and optimize data accesses requested by the various clients to promote efficient communications with the physical device. For inputs (Reads), data returned by the device is buffered for asynchronous distribution or synchronous
collection by various OPC clients. For outputs (writes), the OPC Server updates the physical device data on behalf of OPC Clients.

![Diagram of OPC Architecture]

**Figure 6.3 OPC Architecture**

### 6.4 Case Study of the Packed Distillation Unit

The above methodology is implemented on the packed distillation unit example discussed in the previous chapter and the results of each step are discussed below.

#### The Process Model

The dynamic state model developed in HYSYS is used to represent the plant dynamics. The controllers implemented are removed as they are controlled using the Honeywell’s C200 controller. The simulation time is adjusted to the real time basis to synchronize the real controller and the simulation.

#### The Control System

In this work, Honeywell’s Experion® Process Knowledge System (PKS) is used as the control system. Multiple controller modules are available with Experion® to provide the ultimate flexibility: the C200 Process Controller, the C300 Process Controller, the Application Control Environment (ACE), the C200 Simulation Environment (SIM-C200) and the C300 Simulation Environment (SIM-C300). The current system is configured for C200 controllers.
with modules supporting LSU’s existing system, a Field bus Interface Module, and HART input and output modules. Other key features include OPC interfacing, Microsoft Excel Data Exchange, and e-Server. C200 process controller is a compact and cost-effective solution with direct I/O connections, making it ideal for integrated regulatory, fast logic, sequential, and batch control applications.

The C200 controller along with any other controller modules in Experion ® uses the Control Execution Environment (CEE) software that provides an execution and scheduling environment where control strategies are configured from a rich set of standard and optional function blocks using a single builder tool, Control Builder. It provides the comprehensive handling of the I/O and covers continuous, logic, sequential and advanced control functions through a library of function blocks. Each function block has a specific function and is inbuilt in the Honeywell software. The function blocks are interconnected via “soft wires” to develop the control strategies. Figure 6.4 is an example of the actual PID controller used to control the feed temperature in the packed distillation unit. The definitions of the function blocks used are as follows

**AICHANNEL:** Analog Input Channel block provides a standard analog interface to control function blocks. It is used to fetch PV data from an associated IOMODULE block and to provide an appropriate PV parameter status.

**DACA:** Data acquisition block with the primary functions of filtering, fixing PV values, and limiting maximum and minimum alarm values.

**PIDA:** Regulatory control function blocks with the primary feature of setting the PID loops for this particular control scheme

**AOCHANNEL:** Analog Output Channel block provides a standard analog output signal for operating final control elements and then performing the necessary control actions on the
physical plant devices.

Figure 6.4 FBs used to develop a PID control loop for the feed temperature

The AICHANNEL and AOCHANNEL used in the control strategy are the standard analog interface to control data to/from the physical plant devices such as the transmitters and control valves. However, in our case study the actual plant is being replaced with the process simulation and there are no physical devices such as the transmitter or a control valve. Therefore these function blocks cannot be used and have to be replaced with the Numeric Function block as shown in the Figure 6.5. This block provides storage for a floating-point value which is accessible through the PV configuration parameter. It also supports a configurable access lock which determines who can write a value to the block (such as operator, engineer, other function block). The NUMERIC_IN block is used to receive the input data from HYSYS model and NUMERIC_OUT block is used to send the output back to the HYSYS model.
Figure 6.5 FBs used to develop a simulated PID controller for feed temperature

The HMI Model

Experion® PKS uses patented HMIWeb technology, a web-based architecture supporting integration of human machine interfaces (HMI), application, and business data. This advanced interface solution combines consistent and secure access, robustness, and performance with state-of-the-art web graphics capabilities. HMIWeb technology offers the benefit of fully integrated data delivery using standard Internet technologies such as HTML and XML. The overview of the graphic display used to control the process and the controller face plate are shown in Figure 6.6.

OPC Connectivity

The OPC defines a standard interface for allowing applications to access data from a variety of process control devices. The OPC Data Access Automation Interface Standard Version 2.02 is used to develop the application. This specification is an interface for developers of OPC
Figure 6.6 Overview of the HMI display used for the control clients and OPC Data Access Servers. The application is programmed in Visual Basic Application. The front end for the application is Microsoft Excel. The overview of the spreadsheet interface developed is shown in Figure 6.7. The process parameters are recorded in the history and are trended using the standard Honeywell features. Figure 6.8 is the response plot for the simulated feed flow controller in DCS. Table 6.1 summarizes the controllers implemented in the DCS.

Table 6.1 List of controllers developed in the model

<table>
<thead>
<tr>
<th>Controller Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIC300</td>
<td>Feed Flow Rate Control</td>
</tr>
<tr>
<td>TIC350</td>
<td>Feed Preheater Control</td>
</tr>
<tr>
<td>TIC305</td>
<td>Distillate Composition Control</td>
</tr>
<tr>
<td>TIC340</td>
<td>Bottoms Composition Control</td>
</tr>
<tr>
<td>LIC310</td>
<td>Reflux Drum Level Control</td>
</tr>
<tr>
<td>LIC330</td>
<td>Bottoms Level Control</td>
</tr>
</tbody>
</table>
Figure 6.7 Overview of the spreadsheet interface for OPC communication

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>FT390</td>
<td>Feed Flow Rate Control</td>
<td>48.631</td>
<td>GPH</td>
<td>Open: Allows to open the HYSYS file and connect to OPC</td>
</tr>
<tr>
<td>6</td>
<td>TC390</td>
<td>Feed Preheater Control</td>
<td>43.652</td>
<td>Deg</td>
<td>Exit: Ends the communication but still connects to OPC HYSYS Integrator will be paused</td>
</tr>
<tr>
<td>7</td>
<td>TC330</td>
<td>Distillate Composition Control</td>
<td>56.6192</td>
<td>Deg F</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>TC340</td>
<td>Bottoms Composition Control</td>
<td>56.2154</td>
<td>Deg F</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>UC310</td>
<td>Reflux Drum Level Control 48.6491</td>
<td>Percent</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>UC330</td>
<td>Bottoms Level Control</td>
<td>56.6853</td>
<td>Percent</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>UC390</td>
<td>Bottoms Temperature</td>
<td>37.5802</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>TC350</td>
<td>Feed Preheater Control</td>
<td>143.0000</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>TC355</td>
<td>Distillate Composition Control</td>
<td>163.000</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>TC345</td>
<td>Bottoms Composition Control</td>
<td>172.000</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>UC310</td>
<td>Reflux Drum Level Control</td>
<td>51.8415</td>
<td>Percent</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>UC330</td>
<td>Bottoms Level Control</td>
<td>54.7005</td>
<td>Percent</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>UC390</td>
<td>Bottoms Temperature</td>
<td>1.3053</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>FT310</td>
<td>Feed Flow Rate Control</td>
<td>1.0892</td>
<td>GPH</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>F319</td>
<td>Distillate to Storage</td>
<td>1.3553</td>
<td>GPH</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>FT330</td>
<td>Bottoms to Storage</td>
<td>1.3534</td>
<td>GPH</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>FT390</td>
<td>Cold Feed to Preheater</td>
<td>96.0000</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>TT360</td>
<td>Bottoms to Reboiler</td>
<td>174.7005</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>TT390</td>
<td>Bottoms to Reboiler</td>
<td>172.0004</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>TT311</td>
<td>Bottoms to Reboiler</td>
<td>98.0000</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>TT220</td>
<td>Cooled Distillate Product</td>
<td>86.0000</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>TT330</td>
<td>Cooled Bottoms Product</td>
<td>86.0000</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>TT341</td>
<td>Hot Oil to Preheater</td>
<td>240.0003</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>TT350</td>
<td>Hot Oil to Preheater</td>
<td>164.3888</td>
<td>Deg</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>TT360</td>
<td>Distillate from Condenser</td>
<td>99.9987</td>
<td>Deg</td>
<td></td>
</tr>
</tbody>
</table>

Figure 6.8 Response plot in DCS for a set point change in the feed flow controller
CHAPTER 7

CASE STUDY OF THE CRUDE DISTILLATION UNIT

7.1 Introduction

The petroleum refining processes are highly complex and integrated. The crude oil distillation (CDU) is the most important process for petrochemical industries because it produces a wide range of products, such as gasoline, naphtha, kerosene, diesel, etc. It is also one of the most complicated operations in any refinery as they have unique characteristics that set them apart from other chemical processes, including:

- Process feedstocks, which consist of complex and wide-boiling mixtures of hydrocarbons, whose exact compositions are unknown
- Highly-coupled and heat-integrated fractionation units, used to separate feedstocks into a variety of products with different specifications
- Product specifications given in terms of stream properties such as distillation temperatures, flash point, pour point, sulfur content, and octane number

The dynamic and multivariable nature of the process coupled with stringent quality and environmental constraints make it difficult to operate the process units steadily and safely. It provides opportunities for implementation of advanced control strategies to achieve optimal process operation. The crude oil distillation unit discussed in this work covers the preheat trains (where the feed exchanges heat with the pumparounds and column products) and three main distillation columns: preflash, atmospheric crude distillation unit (ADU), and vacuum distillation unit (VDU). In this chapter, the modeled CDU process will be described in detail together with the simulation environment for both steady and dynamic state. Thereafter, the proposed framework is implemented on the case study as described in Chapter 2 to Chapter 5 and the results are discussed.
7.2 Process Description

The crude/vacuum distillation is the foremost step in the petroleum refining process. The crude from storage tanks is preheated by exchanging with the atmospheric/vacuum column products before entering the desalter, where the salts present in the crude are removed in the water phase. The crude is preheated to around 135°C to 140°C, by exchanging heat with hot streams from ADU viz. Diesel, Heavy Naphtha Circulating Reflux, Kerosene-1 product and Kerosene Circulating Reflux.

The desalted crude is then pumped through another preheat train where it is heated with the Diesel product and pump around stream and is routed to prefractionator column. The lighter fraction, Naphtha (IBP -110°C) is recovered in the prefractionator column as the overhead product. The removal of the lighter fraction decreases the vapor load on the main atmospheric distillation unit. The pre-topped crude from the column bottom is routed through a third preheat train. The hot streams from vacuum distillation unit, HVGO circulating reflux and VR are used to heat pre-topped crude. The feed is then heated in the furnace to a temperature of around 650°F (varies with crude) and is being fed to the main atmospheric distillation unit. The heated crude oil enters the column flash zone where it comes in contact with the stripping vapors from the bottom stripping section and the liquid reflux (overflash) from the tray above. The overflash is controlled at around 3.0 - 5.0 volume percent of the crude oil. The flash zone liquid flows into the stripping section, where some of the lighter components get steam stripped.

The crude distillation column is a typical fractionation column with an overhead condenser and side strippers. It consists of several trays and packing for vapor liquid contact. The cold reflux for condensing the products is provided by the overhead reflux and the pump arounds at different sections. The heat from the pump around and the product streams is recovered in the crude preheat trains. The unstabilized overhead liquid product from the
condenser is routed to the stabilizer section for further treatment. The un-condensed gas (if any) is routed to the refinery fuel gas system or fired in the crude heater. The distillate products are drawn from the trays above the flash zone according to their boiling range. The products are steam stripped in the side strippers with the stripped vapors being routed to the main column.

The topped crude from the column bottom is routed to the vacuum unit furnace. The transfer line temperature at the furnace outlet is maintained at around 750°F (varies with crude properties) to avoid excessive cracking. The hot oil from the furnace is transferred to the flash zone of the vacuum distillation column maintained below atmospheric pressure by the steam ejectors. The purpose of this unit is to make feed of required quality to be processed in Fluid catalytic cracking unit (FCCU). The topped crude is distilled under vacuum into four different cuts namely Vacuum Diesel Oil (VDO), Light Vacuum Gas Oil (LVGO), Heavy Vacuum Gas Oil (HVGO) and Slop distillate (SD). The flash zone liquid, called Vacuum Residue (VR), is routed to storage as LSHS/FO or to a Bitumen unit. The process flow diagram of the crude distillation unit is shown in the Figure 7.1.

### 7.3 Steady State Simulation

The refinery process simulation is developed using Aspen HYSYS. The simulation of petroleum processes is unique and challenging due to the complex and dynamic nature of these processes such as the complex feed stocks, highly coupled and integrated processes and stringent product specifications and environmental regulations. For this study a crude oil blend 75 wt% -Masila & 25 wt% - Dubai crude is selected. The blending of different stocks is normally done to obtain the required product yields and also to meet the process constraints. The crude assay data is presented in Table 7.1. The following are the important steps used in the development of the steady state model. The detailed information about refinery process modeling is provided in Gerald. L, 2000 and Aspen HYSYS user guide.
7.3.1 Defining the Simulation Basis

The foremost step is the selection of lighter components and the appropriate thermodynamic method. The thermodynamic fluid package selected is Peng Robinson, equation of state which is recommended for the petroleum components. Since the exact composition of the crude is unknown and is defined in terms of distillation temperatures the feed developed is a combination of pure library components (lighter components) and pseudo components. The lighter components, methane, propane, i-butane, n- butane, i-pentane, n-pentane and hexane are added to the pure component library.

7.3.2 Developing Crude Oil Feed or Oil Characterization

The data from the crude assay is used to define the petroleum pseudo-components. The pseudo components are the theoretical components that are not readily available in the component library and have to be defined. The data from the pure component library are used to represent the defined light components in the crude oil. It is required to input the laboratory
distillation curve (TBP or ASTM data) and any bulk property such as Molecular Weight, Density, or Watson K Factor. It should be noted that the more the information is provided to the simulation, the accuracy of the property prediction is improved. In this study, the light end composition, TBP distillation curve, density, viscosity @ 10 & 50 deg are used in characterizing the oil. Each crude type is characterized separately and finally the required crude oil blend is defined and installed into the flow sheet. The calculated TBP data by HYSYS for the given crude is compared to the input data to identify any inaccuracies.

7.3.3 Installing the Preheat Train Exchangers

It is more efficient to solve the crude and vacuum columns independently from the preheat train. This is possible since the inlet temperatures to each of these columns are defined by the furnace. In HYSYS, the pumparound streams are considered to be the flowsheet recycle streams. It is necessary to provide estimates for these streams, so the crude stream may be carried through the heat exchanger. The estimates will be replaced when the crude/vacuum calculations have been completed and the streams become available. So the heat exchangers are first modeled using the fictitious pump around streams to preheat the crude. These streams will be then replaced and linked with the actual product streams from the column. This approach is more realistic but adds instability to the calculations since it removes the pumparound coolers from the column sub model. If the crude and vacuum columns are simulated independently prior to the heat exchangers then since the product streams are calculated, these stream conditions can be used as initial estimate for the fictitious pumparound streams. If the columns are not simulated, the crude oil stream composition and the appropriate conditions are used to define the stream.

The Weighted Exchanger Design model is selected for the Heat Exchanger Model. In addition to defining the pressure drop across both the tube and shell side, the UA of the exchanger is specified to meet the degrees of freedom. The UA specification is the product of the
Table 7.1 Assay data for Dubai and Masila crude

<table>
<thead>
<tr>
<th>Properties</th>
<th>Masila Crude</th>
<th>Light End Analysis</th>
<th>TBP distillation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density at 15 °C, kg/m³</td>
<td>874</td>
<td>Component</td>
<td>°C</td>
</tr>
<tr>
<td>° API</td>
<td>30</td>
<td>Ethane</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Propane</td>
<td>15</td>
</tr>
<tr>
<td>Viscosity, cSt at 10°C</td>
<td>20</td>
<td>iso-butane</td>
<td>149</td>
</tr>
<tr>
<td>Viscosity, cSt at 50°C</td>
<td>5.9</td>
<td>n-Butane</td>
<td>232</td>
</tr>
<tr>
<td>Pour Point, °C</td>
<td>-30</td>
<td></td>
<td>342</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>362</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>509</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>550</td>
</tr>
<tr>
<td>Dubai Crude</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density at 15 °C, kg/m³</td>
<td>868</td>
<td>Component</td>
<td>°C</td>
</tr>
<tr>
<td>° API</td>
<td>31</td>
<td>Ethane</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Propane</td>
<td>15</td>
</tr>
<tr>
<td>Viscosity, cSt at 10°C</td>
<td>22</td>
<td>iso-Butane</td>
<td>32</td>
</tr>
<tr>
<td>Viscosity, cSt at 50°C</td>
<td>7.3</td>
<td>n-Butane</td>
<td>93</td>
</tr>
<tr>
<td>Pour Point, °C</td>
<td>-9</td>
<td></td>
<td>149</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>182</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>260</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>371</td>
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<td></td>
<td></td>
<td></td>
<td>427</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>482</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>538</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>550</td>
</tr>
</tbody>
</table>

Overall Heat Transfer Coefficient and the Total Area available for heat transfer. The use of UA specifications instead of end point calculations greatly increases the calculation time for the exchangers, since the solution path involves a triple trial and error procedure.
7.3.4 Installing the 3-Phase Separator (Desalter)

In this case a 3-phase separator is used to simulate the Desalter. A 3-phase separator in general is used to separate the feed into vapor light liquid and heavy liquid (aqueous phase). The water phase is considered as the pure phase and thereby we neglect any effects of salt in both water and oil phase. A calculation block can be used to set the proper flow of another water stream based on the desired residual water content of the treated crude oil. It can also be simulated using a component splitter.

7.3.5 Installing the Prefractionator

The prefractionator column simulation configuration is shown in Figure 7.2. The refluxed absorber with a 3-phase condenser is used to simulate the column. The stripping steam is fed to the column bottom to strip the light fractions from the topped crude. The prefractionator column is simulated using 30 actual trays using the efficiencies defined in Gerald.L, 2000, with feed entering the 12th tray from bottom. Table 7.2 summarizes the performance specifications used to define the columns.

7.3.6 Installing the Atmospheric Distillation Unit

The crude column simulation configuration is shown in Figure 7.3. The atmospheric crude column is simulated as a Refluxed Absorber first and then the side equipments such as pumparounds, side strippers are added. The material streams are created to represent the stripping steam used in the column and the side strippers. The flow rate of each steam varies with the product drawn. The actual column comprises of both trays and packing. Therefore the packing section is converted to the equivalent number of theoretical trays using the HETP approach with the available packing correlation. By default HYSYS uses theoretical stages, as the stage efficiency is set to one. Since the trays are the actual trays in this case the efficiencies have to be adjusted. The condenser is considered as a separate stage and is not included in the
number of stages. The sub-cooling effect of the condenser is taken into consideration by defining the reflux stream to the desired temperature and the vapor coming from the condenser to zero. In addition to defining the pressure across the column, distillate and the over head vapor are specified to run the column.

Adding the side operations to the column

Side Strippers are added to the column in order to improve the quality of the four products (Kerosene-I & II, Diesel, and AGO). The steam is specified to enter at the bottom of the side stripper and the vapor from the top of the stripper is fed to the column again. The side stripper is simulated using the prebuilt side operations available in the simulation. For each stripper, the product flow is specified to meet the degrees of freedom. In some cases the column also consists of side rectifiers. In addition three pumparounds are defined by adding the pump around coolers each for the Heavy Naptha, kerosene-I and Diesel. Pumparounds help to improve
Figure 7.3 Overview of atmospheric distillation column

the column’s efficiency. They operate by drawing a liquid stream from one stage cooling it, and pumping it into a higher stage. In effect, this process adds to the reflux between these two stages. The pumparound coolers are used in first place to run the column. Each pumparound cooler has two degrees of freedom which are defined by specifying the flow rate and the pumparound duty. The pumparound streams are used to exchange heat with the crude oil feed stream. The fictitious pumparound streams defined in installing the preheat trains are replaced with the actual pumparound streams and the products from the column. The outlet streams from the exchangers are linked to the distillation unit. However this approach of putting the column sub-models within recycle loops greatly increases the number of calculations for any given case.

7.3.7 Installing the Vacuum Distillation Column

The vacuum column simulation configuration is shown in Figure 7.4. The vacuum column consists of different types of packing to account for the lower pressure drop across the
column. The actual packing from the PFD can be translated to the theoretical trays using the HETP approach. A theoretical tray is used to represent the column flash zone. This allows the use of a feed trim heater to adjust the feed temperature as needed for the initial calculation attempts. The pump arounds are handled within the column sub model. In this approach the pump arounds are considered in the column mathematics and not as recycle operation. The bottom product is used to exchange heat with the incoming crude to ADU in the third preheat train. In the actual column, all the HVGO is withdrawn from the collector tray, with a small stream (wash oil) pumped back over the bottom packing. In this model, the wash oil and bottom recycle are taken care by setting up a recycle unit operation. The solving of vacuum column is often difficult because of the conflicting performance specifications. The feed tray “trim” heater is useful in establishing an initial solution. If the trim heater duty is large, the furnace operating data or the composition of the topped crude are inaccurate and need to be reconciled.

7.3.8 Complete Flow Sheet Solution

Once the vacuum column is defined the HVGO pumparound and the VR product is used to replace the fictitious pumparound streams used in the third preheat train and the flowsheet is solved. The complete flow sheet solution is shown in figure 7.5.

7.4 Process Optimization

Modern refining industries have become an extremely competitive business. The deteriorating quality of the crude oil and the increasing product specifications together with the stringent environmental regulations are forcing the refiners to become more efficient to survive financially. The complex heat integration schemes and the interactive nature of the process due to the presence of pump around and side-strippers make it difficult to operate at the optimal conditions. The huge capital expenditure involved in the refining operations creates good opportunities for optimization.
Figure 7.4 Overview of the vacuum distillation column

Figure 7.5 Overview of the main flowsheet
Table 7.2 Performance specifications for prefractionator, ADU and VDU

<table>
<thead>
<tr>
<th>Prefractionator</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapor flow rate, m³/hr</td>
<td>3.23</td>
</tr>
<tr>
<td>Light Naptha ASTM 95% cut, deg C</td>
<td>95</td>
</tr>
<tr>
<td>Bottom steam rate, Kg/hr</td>
<td>6000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Atmospheric distillation column</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapor rate, m³/hr</td>
<td>0</td>
</tr>
<tr>
<td>LN rate, m³/hr</td>
<td>12.0525</td>
</tr>
<tr>
<td>HN rate, m³/hr</td>
<td>27.5086</td>
</tr>
<tr>
<td>Kerosene-1 rate, m³/hr</td>
<td>98.5738</td>
</tr>
<tr>
<td>Kerosene-2 rate, m³/hr</td>
<td>46.1232</td>
</tr>
<tr>
<td>Diesel rate, m³/hr</td>
<td>106.031</td>
</tr>
<tr>
<td>HN P/A rate, m³/hr</td>
<td>330.303</td>
</tr>
<tr>
<td>Kerosene P/A rate, m³/hr</td>
<td>390</td>
</tr>
<tr>
<td>Diesel P/A rate, m³/hr</td>
<td>394.367</td>
</tr>
<tr>
<td>HN steam rate, kg/hr</td>
<td>654.662</td>
</tr>
<tr>
<td>Kerosene-I steam rate, kg/hr</td>
<td>3229.3</td>
</tr>
<tr>
<td>Kerosene-2 steam rate, Kg/hr</td>
<td>997.872</td>
</tr>
<tr>
<td>Diesel steam rate, Kg/hr</td>
<td>2194.79</td>
</tr>
<tr>
<td>Bottom steam rate, Kg/hr</td>
<td>6022.41</td>
</tr>
<tr>
<td>ADU feed temperature, deg C</td>
<td>372</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Vacuum distillation column</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>VDU feed Temperature deg C</td>
<td>398</td>
</tr>
<tr>
<td>Vapor to ejector, m³/hr</td>
<td>5.22402</td>
</tr>
<tr>
<td>VDO rate, m³/hr</td>
<td>20.6416</td>
</tr>
<tr>
<td>LVGO rate, m³/hr</td>
<td>16.6767</td>
</tr>
<tr>
<td>HVG0 rate, m³/hr</td>
<td>110.776</td>
</tr>
<tr>
<td>SD rate, m³/hr</td>
<td>21.1926</td>
</tr>
<tr>
<td>VDO P/A rate, m³/hr</td>
<td>171.57</td>
</tr>
<tr>
<td>LVGO P/A rate, m³/hr</td>
<td>61.2264</td>
</tr>
<tr>
<td>HVG0 P/A rate, m³/hr</td>
<td>177.602</td>
</tr>
<tr>
<td>Bottom steam rate, Kg/hr</td>
<td>3000</td>
</tr>
</tbody>
</table>
It is estimated that crude oil cost account for about 85-90% of the total operating cost and therefore a wide variety of crude blends are processed depending on the cost and demand of the various products. This change in feed composition often results in inferior crude unit performance and reduces the unit’s run length. Therefore the optimal conditions vary depending on the crude selected and optimizing the operation of the crude unit is essential to maximize a refiner’s economics. In addition, recent crude oil price fluctuations and increased economic pressure further emphasize the importance of optimizing crude unit performance.

The following section describes the formulation of the optimization problem and the results of each step in the methodology. The process modeling step included in the framework is the developing the steady state model of the plant which is discussed in the previous section.

7.4.1 Information Transfer

The information transfer between the simulation model and the environmental analysis is made using a spreadsheet as interface (Fig 7.6). The bridge code is written in Visual Basic Application (VBA). It allows the user to import and export any selected variables between the model built in HYSYS and Excel worksheet. The process parameters including the decision variables, the constraints and the energy and utility consumption used in the environmental analysis are imported to the spreadsheet.

7.4.2 Environmental Analysis

Considering that the plant requires electricity and steam, the production of which consumes natural resources and generates releases to the environment. The main sources of emissions in this process are the process heaters and utility boilers. The foremost step in the environmental analysis is the inventory calculations mainly the energy and steam consumption of the process. The total heat duty of the process which is the sum of the crude and vacuum furnaces is calculated and the total steam consumption is calculated by summing the stripping
steam used in the product side strippers and the bottom stripping steam used in the columns i.e. prefractionator, ADU and VDU.

Figure 7.6 Optimization interface in Excel

The total energy and steam consumed in the process are then converted to the net equivalent electricity to estimate the emissions released. Heat to power ratio of 1.25 and an efficiency of 70% for the cogeneration plant is assumed in the computation of the net equivalent electricity. The heat duty of the stripping steam @ 245°C is calculated using an enthalpy of 13.5 MMKJ per ton of steam. The net equivalent electricity consumed is calculated in Giga Watt Hr (GWH). Then the quantity of each environmental load is estimated using the available correlation in Table 7.3. In this study, sulfur dioxide (SO2), carbon dioxide (CO2), and nitrogen oxides (NOx) are chosen as Environmental Load (EL). It is assumed that a portion of the net energy required is obtained by using the overhead gas of the prefractionator as the fuel in the furnace and the balance is met from fuel oil.
Table 7.3 Environmental loads for electricity generation from different sources

<table>
<thead>
<tr>
<th>Environmental Loads</th>
<th>Fuel oil</th>
<th>Fuel gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO2, Ton/GWH</td>
<td>657</td>
<td>439</td>
</tr>
<tr>
<td>SO2, Kg/GWH</td>
<td>1030</td>
<td>1</td>
</tr>
<tr>
<td>NOX, Kg/GWH</td>
<td>988</td>
<td>1400</td>
</tr>
</tbody>
</table>

*special report of World Energy Council, July 04

From the above data it is evident that the use of fuel gas in the furnace reduces the emissions to a greater extent but at the same time aiming at more fuel gas i.e. the vapor from the prefractionator has a negative impact on the column economics as it reduces the quantity of the Light Naptha.

7.4.3 Optimization Model

The optimization model is performed within Excel® using the information transferred from HYSYS based on the operating profit. For this case study, the optimization model is simplified by assuming a constant throughput. The environmental cost is estimated as a fraction of the feed cost and hence is ignored in the optimization model. It is also assumed that there are no processes utilizing the emissions in the plant i.e. there is no sustainable credits associated with the process. Therefore, only the sustainable debit for the process is used in the optimization model which is computed using the Eq. 7.1 while Table 7.4 shows the price for different environmental loads used in the calculation of sustainable debit.

Sustainable debit = Σ Environmental load, Ton * Cost, $/Ton  \hspace{1cm} (7.1)

Table 7.4 Price for different environmental loads

<table>
<thead>
<tr>
<th>Environmental Load</th>
<th>$/Ton</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO2</td>
<td>3.25</td>
</tr>
<tr>
<td>SO2</td>
<td>192</td>
</tr>
<tr>
<td>NOX</td>
<td>1030</td>
</tr>
</tbody>
</table>
The decision or the manipulated variables in the optimization problem are mainly the flow rate of the products, pumparounds, stripping steam flow rates and the feed temperature to the ADU and VDU. This formulation is performed based on the calculation shown in Eq. 7.2 while Table 7.5 summarizes the product and utility used in the optimization model.

Objective Function = Product revenues – Utilities cost – Sustainable debit

\[ (7.2) \]

In addition to the constraints on the decision variables, the optimization problem is subjected to process and environmental constraints such as those on quality, heating and cooling duty specifications. It should be noted that the decision variables used in the optimization should be specified as active specifications in the steady state simulation case in order for the optimizer to manipulate the variables. The Table 7.6 summarizes the results as well as the decision variables and the constraint imposed in the optimization problem.

<table>
<thead>
<tr>
<th>Product</th>
<th>Price ($/m3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LN</td>
<td>300</td>
</tr>
<tr>
<td>CN</td>
<td>225</td>
</tr>
<tr>
<td>HN</td>
<td>240</td>
</tr>
<tr>
<td>kerosene-1</td>
<td>265</td>
</tr>
<tr>
<td>Kerosene-2</td>
<td>285</td>
</tr>
<tr>
<td>Diesel</td>
<td>250</td>
</tr>
<tr>
<td>VDO</td>
<td>250</td>
</tr>
<tr>
<td>LVGO</td>
<td>200</td>
</tr>
<tr>
<td>HVGO</td>
<td>200</td>
</tr>
<tr>
<td>SD</td>
<td>165</td>
</tr>
<tr>
<td>VR</td>
<td>165</td>
</tr>
<tr>
<td><strong>Duty</strong></td>
<td><strong>Price ($/MMKJ)</strong></td>
</tr>
<tr>
<td>Condenser duty</td>
<td>4</td>
</tr>
<tr>
<td>Furnace duty</td>
<td>75</td>
</tr>
</tbody>
</table>
Table 7.6 Summary of the optimization variables

<table>
<thead>
<tr>
<th>Decision Variables</th>
<th>Optimal value</th>
<th>Constraints (Max)</th>
<th>Constraints (Min)</th>
<th>Initial Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vapor flow rate, m3/hr</td>
<td>3.23</td>
<td>3.00</td>
<td>4.00</td>
<td>3.23</td>
</tr>
<tr>
<td>Pre flash btm. steam rate, Kg/hr</td>
<td>6053.14</td>
<td>4500.00</td>
<td>8000.00</td>
<td>6009.02</td>
</tr>
<tr>
<td>LN rate, m3/hr</td>
<td>12.05</td>
<td>10.00</td>
<td>14.00</td>
<td>12.00</td>
</tr>
<tr>
<td>HN rate, m3/hr</td>
<td>27.51</td>
<td>26.00</td>
<td>30.00</td>
<td>27.30</td>
</tr>
<tr>
<td>Kerosene-1 rate, m3/hr</td>
<td>98.57</td>
<td>95.00</td>
<td>99.00</td>
<td>96.70</td>
</tr>
<tr>
<td>Kerosene-2 rate, m3/hr</td>
<td>46.12</td>
<td>44.00</td>
<td>49.00</td>
<td>45.60</td>
</tr>
<tr>
<td>Diesel rate, m3/hr</td>
<td>106.03</td>
<td>102.00</td>
<td>107.00</td>
<td>104.00</td>
</tr>
<tr>
<td>HN P/A rate, m3/hr</td>
<td>330.30</td>
<td>325.00</td>
<td>335.00</td>
<td>329.00</td>
</tr>
<tr>
<td>Kerosene P/A rate, m3/hr</td>
<td>390.00</td>
<td>385.00</td>
<td>390.00</td>
<td>387.99</td>
</tr>
<tr>
<td>Diesel P/A rate, m3/hr</td>
<td>394.37</td>
<td>390.00</td>
<td>395.00</td>
<td>393.01</td>
</tr>
<tr>
<td>ADU feed temperature, deg C</td>
<td>372.00</td>
<td>372.00</td>
<td>385.00</td>
<td>378.00</td>
</tr>
<tr>
<td>HN steam rate, Kg/hr</td>
<td>654.66</td>
<td>300.00</td>
<td>1000.00</td>
<td>652.19</td>
</tr>
<tr>
<td>Kerosene-I steam rate, Kg/hr</td>
<td>3229.30</td>
<td>2000.00</td>
<td>5000.00</td>
<td>3217.04</td>
</tr>
<tr>
<td>Kerosene-2 steam rate, Kg/hr</td>
<td>997.87</td>
<td>500.00</td>
<td>2000.00</td>
<td>993.13</td>
</tr>
<tr>
<td>Diesel steam rate, Kg/hr</td>
<td>2194.79</td>
<td>1000.00</td>
<td>4000.00</td>
<td>2183.54</td>
</tr>
<tr>
<td>Bottom steam rate, Kg/hr</td>
<td>6022.41</td>
<td>4000.00</td>
<td>8000.00</td>
<td>5987.41</td>
</tr>
<tr>
<td>VDU feed Temperature deg C</td>
<td>398.00</td>
<td>398.00</td>
<td>410.00</td>
<td>405.00</td>
</tr>
<tr>
<td>Vapor to ejector, m3/hr</td>
<td>5.22</td>
<td>4.50</td>
<td>6.00</td>
<td>5.19</td>
</tr>
<tr>
<td>VDO rate, m3/hr</td>
<td>20.64</td>
<td>18.00</td>
<td>23.00</td>
<td>20.50</td>
</tr>
<tr>
<td>LVGO rate, m3/hr</td>
<td>16.68</td>
<td>15.00</td>
<td>18.00</td>
<td>16.60</td>
</tr>
<tr>
<td>HVGO rate, m3/hr</td>
<td>110.78</td>
<td>105.00</td>
<td>112.00</td>
<td>109.00</td>
</tr>
<tr>
<td>SD rate, m3/hr</td>
<td>21.19</td>
<td>19.00</td>
<td>24.00</td>
<td>21.10</td>
</tr>
<tr>
<td>VDO P/A rate, m3/hr</td>
<td>171.57</td>
<td>168.00</td>
<td>174.00</td>
<td>171.00</td>
</tr>
<tr>
<td>LVGO P/A rate, m3/hr</td>
<td>61.23</td>
<td>58.00</td>
<td>63.00</td>
<td>61.00</td>
</tr>
<tr>
<td>HVGO P/A rate, m3/hr</td>
<td>177.60</td>
<td>175.00</td>
<td>180.00</td>
<td>177.00</td>
</tr>
</tbody>
</table>
7.5 Dynamic Modeling and Plant Wide Control

As mentioned earlier, the petroleum refining processes are highly complex and integrated in nature, where a large number of variables are required to be controlled. It is well known that integrated processes involving energy integration and recycle loops greatly impact the performance of the individual units and consequently the whole plant. These processes are significantly interactive and often provide unique challenges to the plant personnel. It is also very difficult to understand the behavior of these processes. In addition to the interactive nature the control of these processes is a difficult task due to the excessive settling time. The use of the large number of trays in the column and large hold up volumes, the settling time following a process change or disturbance spans several shifts. The design features also include the process recycles, minimum holdup, and safety valves which further add to the complexity. The last stage of the proposed framework is developing the overall plant-wide control strategy and its validation based on the entire plant’s dynamic behavior. The development of the plant-wide control system is performed into two main stages as follow:

- First, the basic regulatory control layer is implemented. This layer includes the PID controllers and forms the Level I in the multi layer control architecture. The dynamic model of the plant is developed and the controllers are installed. This stage is performed and evaluated, according to its dynamic performance, as a first step to make sure that the basic designed process is controllable.

- Then, the advanced control strategy, Model Predictive control layer is implemented above the basic layer. This allows operation of the process closer to plant constraints including product specifications, resulting in increased throughput, improved product yield pattern, reduced energy consumption etc.

As discussed, two layer control strategy has been implemented in HYSYS. The advanced
process control, MPC is configured above the basic regulatory controls which include the PID controllers. The MPC receives the set point from the steady state optimizer and manipulates the set point of the PID controllers installed in either the main or column sub flowsheet in order to achieve the objectives. Moreover, a rigorous dynamic model was used to implement and validate the developed plant-wide control structure and to test the overall dynamic performances of the plant. MPC improves control of critical variables of processes, which are interactive in nature.

7.5.1 Basic Regulatory Control Layer

The steady state model developed is modified and transitioned into dynamic state by specifying the additional engineering details, including pressure/flow relationships and geometry. A dynamic model can either be developed from the steady state model or directly in the dynamic mode with no prior steady state model. The control objectives of the process are identified and valves are added to the flow sheet to achieve basic regulatory control. Each control objective represents a degree of freedom for control. The equipment dimensions including the column details such as tray parameters are specified. The tray sizing utility is used to estimate the missing sizing parameters.

The pressure flow specifications are added across the flowsheet. In general, one pressure-flow specification is required per flowsheet boundary stream. It should be noted that the pressure drop across the flowsheet is user specified in the steady state but in the dynamic mode it is calculated using dynamic hydraulic calculations. Therefore complications arise in the transition from steady state to dynamics if the steady state pressure profile across the flowsheet is very different from that calculated by the dynamic pressure-flow solver. First the basic control schemes are configured using the pre-built suite of function blocks for the PID controller. Once all the unit operations are added and the dynamic performance specifications are specified, the integrator is run for few minutes so that all the values can propagate through the column
flowsheet. The desired face plates and strip charts are added to evaluate and tune the performance of the controllers. Figure 7.7 is the overview of the main flowsheet of the dynamic model developed for the basic regulatory control. Table 7.7 summarizes the basic PID controllers configured with the control and manipulated variables.

**Controllability Study**

To study the plant controllability and to understand the dynamic behavior of the process let us consider the prefractionator section of the unit which is less complicated than the Atmospheric and Vacuum distillation columns. The prefractionator column is the upstream unit of the ADU. The pairing of the controlled and the manipulated variables for the prefractionator controllers are shown in Table 7.7. This column itself is interactive in nature and a set point change in one of the controller will affect the other controllers.

![Figure 7.7 Main flowsheet of the plant model](image)
# Table 7.7 Pairing of controlled and manipulated variables

<table>
<thead>
<tr>
<th>No</th>
<th>Controlled variable</th>
<th>Manipulated Variable</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Crude-I flow</td>
<td>Crude-I flow</td>
<td>FC</td>
</tr>
<tr>
<td>2</td>
<td>Crude-II flow</td>
<td>Crude-II flow</td>
<td>FC</td>
</tr>
<tr>
<td>3</td>
<td>Desalter abnormal pressure</td>
<td>Desalter vent flow</td>
<td>PC</td>
</tr>
<tr>
<td>4</td>
<td>Desalter pressure</td>
<td>Desalted crude flowrate</td>
<td>PC</td>
</tr>
<tr>
<td>5</td>
<td>Preflash column top temperature</td>
<td>Preflash reflux flow</td>
<td>TC</td>
</tr>
<tr>
<td>6</td>
<td>Preflash column pressure</td>
<td>Preflash vent flow</td>
<td>PC</td>
</tr>
<tr>
<td>7</td>
<td>Preflash reflux drum level</td>
<td>Preflash drum flow</td>
<td>LC</td>
</tr>
<tr>
<td>8</td>
<td>Preflash bottom level</td>
<td>Preflash bottom flow</td>
<td>LC</td>
</tr>
<tr>
<td>9</td>
<td>Atm. column feed temperature</td>
<td>Atm. heater duty</td>
<td>TC</td>
</tr>
<tr>
<td>10</td>
<td>Atm. top temperature</td>
<td>Atm. Reflux flow</td>
<td>TC</td>
</tr>
<tr>
<td>11</td>
<td>Atm. column pressure</td>
<td>Reflux drum vent flow</td>
<td>PC</td>
</tr>
<tr>
<td>12</td>
<td>Atm. Reflux drum level</td>
<td>Reflux drum product flow</td>
<td>LC</td>
</tr>
<tr>
<td>13</td>
<td>HN product flow</td>
<td>HN product flow</td>
<td>FC</td>
</tr>
<tr>
<td>14</td>
<td>Kerosene-1 flow</td>
<td>Kerosene-1 flow</td>
<td>FC</td>
</tr>
<tr>
<td>15</td>
<td>Kerosene-2 flow</td>
<td>Kerosene-2 flow</td>
<td>FC</td>
</tr>
<tr>
<td>16</td>
<td>Diesel flow</td>
<td>Diesel flow</td>
<td>FC</td>
</tr>
<tr>
<td>17</td>
<td>HN PA flow</td>
<td>HN PA flow</td>
<td>FC</td>
</tr>
<tr>
<td>18</td>
<td>Kerosene-I PA flow</td>
<td>Kerosene-I PA flow</td>
<td>FC</td>
</tr>
<tr>
<td>19</td>
<td>Diesel PA flow</td>
<td>Diesel PA flow</td>
<td>FC</td>
</tr>
<tr>
<td>20</td>
<td>Atm. Bottom level</td>
<td>Atm. Bottom flow</td>
<td>LC</td>
</tr>
<tr>
<td>21</td>
<td>Vacuum column feed temp.</td>
<td>Vacuum heater duty</td>
<td>TC</td>
</tr>
<tr>
<td>22</td>
<td>VDO flow</td>
<td>VDO flow</td>
<td>FC</td>
</tr>
<tr>
<td>23</td>
<td>LVGO flow</td>
<td>LVGO flow</td>
<td>FC</td>
</tr>
<tr>
<td>24</td>
<td>HVGO flow</td>
<td>HVGO flow</td>
<td>FC</td>
</tr>
<tr>
<td>25</td>
<td>SD flow</td>
<td>SD flow</td>
<td>FC</td>
</tr>
<tr>
<td>26</td>
<td>VR flow</td>
<td>VR flow</td>
<td>FC</td>
</tr>
<tr>
<td>27</td>
<td>VDO PA flow</td>
<td>VDO PA flow</td>
<td>FC</td>
</tr>
<tr>
<td>28</td>
<td>LVGO PA flow</td>
<td>LVGO PA flow</td>
<td>FC</td>
</tr>
<tr>
<td>29</td>
<td>HVGO PA flow</td>
<td>HVGO PA flow</td>
<td>FC</td>
</tr>
<tr>
<td>30</td>
<td>Wash oil flow</td>
<td>wash oil flow</td>
<td>FC</td>
</tr>
<tr>
<td>31</td>
<td>VR bottom level</td>
<td>VR flow</td>
<td>LC</td>
</tr>
<tr>
<td>32</td>
<td>VR recycle flow</td>
<td>VR recycle flow</td>
<td>FC</td>
</tr>
</tbody>
</table>
To demonstrate the dynamic behavior of the plant a set-point change is introduced in the top temperature controller of the prefractionator unit. As mentioned previously the prefractionator is used to reduce the vapor load in the atmospheric distillation unit and to separate the Light Naptha from the crude. The downstream of the prefractionator is the third preheat train followed by the ADU. Figure 7.8 is the step response of the top temperature controller. As discussed earlier these processes are highly integrated and interactive in nature. To analyze the process behavior, the responses of the other variables are plotted in the Figure 7.9. Because of the plant size, there are a large number of possible variables to be plotted, however only the response of the key affected variables are shown here. Similarly, this disturbance propagates toward the Atmospheric and Vacuum distillation column and the pressure and temperature controllers adjust their corresponding process variables as shown in the Figure. 7.10

![Figure 7.8 Step response plot of the Preflash top temperature](image)

Furthermore, the disturbance will spread over the entire plant through the heat exchanger network. It should be noted that the disturbances across the column is spread over a time i.e. is the effect of the disturbance on the variables associated with VDU will be slower than compared to the ADU variables indicating the presence of the high settling time due to the high liquid holdups or residence time.
Figure 7.9 Response plots of the Preflash bottom level and Reflux drum Level

This dynamic analysis could go on for many pages demonstrating many interesting behaviors in this complex and integrated plant. However and through these dynamic simulations, the key message is to show that the process under the proposed plant-wide control structure is operable and controllable as it holds the system at the desired optimal operating conditions (set points) and shows good disturbance rejection capabilities.

From the above discussion, the effects of the disturbances on the integrated processes and how it is amplified and propagated over the entire plant is demonstrated. Therefore, it shows the importance of a satisfactory and integrated plant-wide control structure to keep the designed processes within the required operability region. From the above discussion it is clear that the control of such systems is often difficult and needs more advanced control strategies to achieve a satisfactory control performance.

7.5.2 Model Predictive Control Layer

The primary objective of the controller is to maximize the high valued products and to maintain all the controlled variables within the limits. The control variables include mainly the tray temperatures which correspond to the product qualities. These advanced strategies also provide stable unit operations in the wake of disturbances. The MPC controllers developed are
Figure 7.10 Response plots of the key variables in ADU and VDU
simplified and the effects of disturbance variables are neglected. The controlled and the manipulated variables are identified for each controller. The controlled variables are mainly the draw temperatures which represent the ASTM distillation temperatures of the products. The manipulated variables are the product and the pumparound flow rates. Step tests are conducted in the unit and process data collected during the testing period is used for modelling. The simulated model, in HYSYS, is linked with spreadsheets in Excel which is used as a data historian of each individual controlled variable response for a step change of each process input, manipulated variable. These responses are then used to identify the relationships between the process inputs and outputs through process identification tools. The transfer function matrix of each evaluated unit is developed using the Loop-Pro®, model identification software.

Two independent MPC controllers are developed one for the ADU including the pre flash and the distillation column and the other for vacuum column operation. The MPC controller for the ADU has 6 controlled and 9 manipulated variables. Table 7.8 and 7.9 summarizes the transfer function matrix of the ADU MPC controller. The implementation of MPC involves generation of a dynamic model of the process and configuration of the controller. Therefore a reliable dynamic model of the process should be available to install the MPC controller.

Table 7.8 Transfer function matrix of the ADU and Preflash MPC controller

<table>
<thead>
<tr>
<th>MV/CV</th>
<th>MV1-Pre temp.</th>
<th>flash temp.</th>
<th>MV2-Atm.column top temp.</th>
<th>MV3-Diesel flow</th>
<th>PA flow</th>
<th>MV4-Kerosene flow</th>
<th>PA flow</th>
<th>-1</th>
<th>MV5-HN PA flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV1-Preflash top</td>
<td>1.8,11.0</td>
<td>0.434,17.35</td>
<td>0.11.1</td>
<td>-0.001,0.45</td>
<td>24.85</td>
<td>0.005,44.28</td>
<td>28.00</td>
<td>0.0</td>
<td>0.020,132.32</td>
</tr>
<tr>
<td>CV2 -column top</td>
<td>-1.11,10.7</td>
<td>1.35,4.0</td>
<td>-0.032,38.00</td>
<td>-0.056,25.0</td>
<td>0.0</td>
<td>-0.092,18.06</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CV3-HN draw temp.</td>
<td>-0.955,7.25</td>
<td>1.25,40.5</td>
<td>-0.040,28.50</td>
<td>-0.058,22.92</td>
<td>0.0</td>
<td>-0.097,19.70</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CV4-Kerosene-1</td>
<td>-0.388,0.66</td>
<td>0.976,0.5</td>
<td>-0.020,18.26</td>
<td>-0.047,2.46</td>
<td>1.93</td>
<td>-0.071,20.83</td>
<td>0.15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CV5-Kerosene-2</td>
<td>-0.23,0.36</td>
<td>0.995,1.83</td>
<td>-0.02,21.615</td>
<td>-0.051,2.73</td>
<td>1.62</td>
<td>-0.059,2.26</td>
<td>0.86</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CV6-Diesel draw</td>
<td>-0.21,1.53</td>
<td>0.778,1.5</td>
<td>-0.017,2.37</td>
<td>-0.027,1.76</td>
<td>4.55</td>
<td>-0.064,3.25</td>
<td>2.13</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 7.9 Transfer function matrix of the ADU and Preflash MPC controller

<table>
<thead>
<tr>
<th>MV/CV</th>
<th>MV6-HN flow</th>
<th>MV7-Kerosene-I flow</th>
<th>MV8-Kerosene-II flow</th>
<th>MV9-Diesel flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV1-Preflash top temp.</td>
<td>0.303,76.5,7.12</td>
<td>0.179,29.6,0</td>
<td>0.29,88,12.7</td>
<td>0.063,25.5,5.5</td>
</tr>
<tr>
<td>CV2-column top temp.</td>
<td>-0.073,4,19.8</td>
<td>-0.354,41,17.3</td>
<td>-0.08,5,16</td>
<td>-0.117,36.7,12.45</td>
</tr>
<tr>
<td>CV3-HN draw temp.</td>
<td>0.841,100,61.5</td>
<td>-0.341,34,8,18.35</td>
<td>-0.096,4,7,13.2</td>
<td>-0.108,31,1,14.1</td>
</tr>
<tr>
<td>CV4-Kerosene-1 draw temp.</td>
<td>0.582,27.7,0</td>
<td>-0.044,0,9.30,67</td>
<td>0.172,41,8,49.7</td>
<td>-0.077,4,36,19.6</td>
</tr>
<tr>
<td>CV5-Kerosene-2 draw temp.</td>
<td>0.644,29.9,0</td>
<td>0.376,6,26,0,16</td>
<td>0.575,54,18,0</td>
<td>-0.055,5,56,20,35</td>
</tr>
<tr>
<td>CV6-Diesel draw temp.</td>
<td>0.507,26,55,0</td>
<td>0.4,11,6,0,33</td>
<td>0.673,35,08,0</td>
<td>0.139,14,1,0,0</td>
</tr>
</tbody>
</table>

The MPC controller for the Vacuum Distillation Unit has 4 controlled and 7 manipulated variables. Table 7.10 and 7.11 summarizes the transfer function matrix of the VDU MPC controller.

Table 7.10 Transfer function matrix of the VDU MPC controller

<table>
<thead>
<tr>
<th>MV/CV</th>
<th>MV1-VDO draw flow</th>
<th>MV2-LVGO draw flow</th>
<th>MV3-HVGO draw flow</th>
<th>MV4-SD draw flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV1-column top temp.</td>
<td>-1.75,6,6,5,3</td>
<td>-0.25,5,45,6,89</td>
<td>0.05,0,03,0,33</td>
<td>0.05,0,03,0,33</td>
</tr>
<tr>
<td>CV2-VDO draw temp.</td>
<td>-0.553,6,0,8,0</td>
<td>-0.15,5,32,7,42</td>
<td>0.01,0,03,0,33</td>
<td>-0.05,0,03,0,33</td>
</tr>
<tr>
<td>CV3-LVGO draw temp.</td>
<td>1.09,6,72,0</td>
<td>0.14,5,87,0</td>
<td>0.05,0,5,0,64</td>
<td>-0.01,0,03,0,33</td>
</tr>
<tr>
<td>CV4-HVGO draw temp.</td>
<td>1.04,3,28,0,12</td>
<td>0.41,3,42,0</td>
<td>0.27,3,15,0,0</td>
<td>0.007,1,9,0,0</td>
</tr>
</tbody>
</table>

Table 7.11 Transfer function matrix of the VDU MPC controller

<table>
<thead>
<tr>
<th>MV/CV</th>
<th>MV5-VDO PA flow</th>
<th>MV6-LVGO flow</th>
<th>MV7-HVGO PA flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>CV1-column top temp.</td>
<td>-0.98,0,11,0,26</td>
<td>-0.49,2,55,0,20</td>
<td>-0.42,5,33,0,0</td>
</tr>
<tr>
<td>CV2-VDO draw temp.</td>
<td>-0.54,0,88,0,0</td>
<td>-0.32,3,6,0,2</td>
<td>-0.26,5,98,0,0</td>
</tr>
<tr>
<td>CV3-LVGO draw temp.</td>
<td>-0.08,0,33,0,98</td>
<td>-0.14,1,98,0,05</td>
<td>-0.08,2,28,0,27</td>
</tr>
<tr>
<td>CV4-HVGO draw temp.</td>
<td>-0.05,0,03,0,33</td>
<td>-0.06,1,48,0,48</td>
<td>-0.12,2,45,0,08</td>
</tr>
</tbody>
</table>
Controllability Study

To demonstrate the performance of the MPC controller and to study the process behavior the controller (ADU) is subjected to the following disturbances

1. A set-point change in the diesel draw temperature (SP_6)

2. A perturbation on the feed temperature to the Atmospheric column.

Following each disturbance, the response plots of the key variables which include the other controlled variables in the MPC controller are recorded. Figure 7.11 shows the response plots of the key parameters and the controller output for a set point change in Diesel draw temperature.

![Response plots of the controlled variables for a setpoint change (Diesel draw temperature, SP_6)](image-url)
It should be noted that the MPC controller manipulates the basic controllers in an orderly fashion and reaches the new set point while maintaining the other controlled variables at their respective set points with minimal variations.

To demonstrate the controller performance for any disturbance, a step change is introduced in feed temperature to Atmospheric column and the response behavior is recorded (Figure 7.12). It shows the ability of the MPC controller to reject the disturbances.
Figure 7.12 Response plots of the controlled variables for a disturbance (SP change in feed temperature to Atmospheric column)
7.5.3 Optimal Transition

As discussed the MPC controller receives the set points from the optimizer developed earlier using the steady state model. The optimization layer forms the Level III of the Multi layer architecture proposed in the Thesis. The controlled variables used in the MPC controller are actually the calculated variables in the optimized steady state model. The MPC layer developed will allow the smooth transition to the optimal conditions with minimal deviations from the desired set points. Figure 7.13 shows the response plots during the transition to the optimal conditions.

7.6 Conclusions

In this chapter, the proposed framework is implemented and demonstrated on an industrial case study of primary unit of the crude oil refinery which includes the preflash, ADU and VDU. The case study, and through the integrated framework, shows the multi layer control architecture along with the benefits in a transparent way. It was noticed that improved energy efficiency generally increases plant complexity and may have significant impacts on the process operability and/or controllability. Moreover, a rigorous dynamic model was used to implement
and validate the developed plant-wide control structure and to test the overall dynamic performances of the plant.

Figure 7.13 Response plots during the transition to the optimal conditions
CHAPTER 8
CONCLUSIONS AND FUTURE WORK

8.1 Conclusions

The area of optimization and controllability of the manufacturing plants is still an open and challenging research field in the process systems engineering. The main objective of this thesis was to develop an overall framework that assist the process engineers to evaluate and/or retrofit their designed or operating processes respectively allowing all relevant considerations to be formulated and accounted. In this thesis, an integrated methodology has been developed and implemented, that incorporates economical, environmental, and operational considerations within an improved optimization framework. Another important problem addressed in this work is the formulation and implementation of multi-layer (hierarchical) operational architecture which includes a model predictive control strategy (MPC) that can handle constraints and presents good robustness features against model mismatch and perturbations.

The developed integrated framework was validated through its application to a large-scale industrial complex case study. The process considered is the primary section of the crude distillation unit which include mainly the preflash, atmospheric and vacuum distillation column along with the preheat train. This case study features many unit operations, complex dynamics, heat integration, recycle streams and opportunities for implementation of the advanced control strategies. The selected case study provides the necessary challenges to highlight the potential benefits the framework can provide to the plant personnel.

The study explains the various aspects of the methodology and the importance of each step in a transparent way. Modeling and simulation forms the core of the methodology. The optimization framework takes into account the sustainable cost to repair damages done to society,
cost to comply with regulations. The incorporation of environmental considerations converts the single economic optimization problem into a multi-objective optimization problem with conflicting objectives. The developed framework utilizes the capabilities of existing commercial software (Aspen HYSYS and Microsoft Excel) to presents a clear view to the decision maker for the interactions between the designed processes and the environment and the trade-offs between the economic and environmental objectives.

Dynamic evaluation and plant-wide control were integrated within the framework to assess the operability and controllability of the plant. Complex plants are highly integrated, through mainly recycled streams, even without heat integration. Plant-wide process control forms the final stage of the process synthesis, design and operation assessments. A rigorous dynamic model is used to implement and validate overall dynamic performances of the plant. A two layer control strategy has been developed. The advanced model predictive control strategy forms the superior layer above the basic regulatory control layer. Nevertheless, the simulation models both steady state and dynamic state models can be used for further economical, environmental and operational evaluations. Finally, the methodology is extended to develop the training simulators which are ideal to train students and operating personnel with the industrial control systems.

8.2 Future Recommendation

Despite the great deal of effort and the significant advances that have been achieved in this thesis, it is clear that there are still a number of potential areas that could be addressed and considered for further investigations. The proposed integrated framework was developed as a generic open-ended assessment methodology where a number of issues could be readily incorporated to extend the scope of the work reported in this thesis. Some of the future potential areas to be addressed are outlined below:
1. The majority of chemical engineering problems involve multiple objectives which are required to be considered simultaneously. As a consequence, the use of multi-objective optimization has been increasing exponentially in recent years. In this study, generalized reduced gradient method was selected as solver strategy; however, further studies on alternatives approaches such as Generic or evolutionary Algorithms (GA) could prove extremely useful to obtain the global optimal solution. These approaches are potentially attractive and are expected to become even more accepted in the future due to some of their comparative advantages.

2. In the optimization, the key parameters are only partially known where there is significant uncertainty regarding their future values. Furthermore, there are inherently uncertainties associated with both the plant model as well as the environmental model. The optimization of chemical processes under uncertainty has received considerable attention in recent years. A natural extension in the formulation proposed in this thesis is the incorporation of uncertainty in the formulation of the optimization problem. This, however, would naturally increase the computational complexity (Bhari et al., 1996)

3. There have been several advances in the design and planning under uncertainty that allow top level management to study the impact and to take appropriate decisions (Barbaro and Bagajewicz, 2002). This thesis can be extended further to develop and implement decision support system for enterprise-wide optimization problem which would consider the medium to long term strategies which is necessary to thrive the business in this competitive world. The long term strategic layer consists of problems such as retrofit/capacity expansion of facilities while the medium term layer includes problems such as production scheduling and logistics planning. This layer actually forms the uppermost layer in the control hierarchy as discussed in Chapter 4.
4. Finally, as the proposed integrated framework was developed to be a generic assessment methodology, further case studies could be investigated and considered in future studies. The methodology can be extended to other refining processes such as the fluid catalytic cracking unit or reformer to derive a complete refinery modeling.
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