

**A FRAMEWORK FOR INTEGRATED REACTIVE SCHEDULING
OF PLANT OPERATIONS AND MAINTENANCE**

**A FRAMEWORK FOR INTEGRATED REACTIVE SCHEDULING
OF PLANT OPERATIONS AND MAINTENANCE**

By

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A Thesis

Submitted to the School of Graduate Studies

in Partial Fulfillment of the Requirements

for the Degree

Master of Applied Science

McMaster University

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MASTER OF APPLIED SCIENCE (2009)

(Chemical Engineering)

McMaster University

Hamilton, Ontario, Canada

TITLE: A Framework for Integrated Reactive Scheduling of Plant Operations and Maintenance

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SUPERVISOR: Dr. T.E. Marlin

NUMBER OF PAGES: xiv, 218

Abstract

This thesis addresses a reactive (closed-loop) scheduling framework for integrated scheduling of process operation and maintenance. Ethylene plant furnace scheduling is chosen as the process example because it is concerned with optimally scheduling the furnace operations and its periodic maintenance shutdowns. The main reason for choosing this example is that it addresses a special class of scheduling problems where the operations and maintenance have strong interactions and so integrated decision making becomes necessary.

The major goal of this research was to select an appropriate closed-loop framework and develop a reactive scheduling system. With the rolling horizon approach being the most suitable method for closed-loop schedule implementation, a Model Predictive Control (MPC) framework is chosen in this thesis. The presence of integer variables in the scheduling model made the reactive scheduling systems resemble a hybrid MPC problem.

The research was performed in two phases. In the first phase, an open-loop scheduling model was formulated as a Mixed Integer Linear programming problem (MILP) using discrete time representation. To ensure the tractability of the model, tailored formulation methods (disjunctive reactor modelling, constraint reformulation and tightening constraints) and efficient solution heuristics (two-stage temporal decomposition heuristic) were developed in this thesis. In the second phase, the open-loop scheduling model was applied in the prototype closed-loop framework to develop a reactive scheduling system to assist engineers make appropriate decisions in a timely manner.

The automated scheduling system developed in this thesis was tested for several scenarios and proved to have significant benefits over manual scheduling procedures, confirmed that the scheduling model is tractable and achieved feasible solutions for all the scenarios considered, including large problems with multiple feeds, multiple reactors and a long (90-day) scheduling horizon. We conclude that the technology is appropriate for further improvement and eventual application in the industry.

Acknowledgements

I thank my supervisor Dr. T.E. Marlin for his continuous support, patience and invaluable guidance during the period of my study. Without his help, it would not have been possible to finish the thesis.

Thanks to my friends at MACC who were very helpful during the initial phases of my research. I appreciate Zhiwen Chong for assisting me in different phases of my research with his computer expertise.

Special thanks to my beloved wife (Madhuri) who has been so cooperative during my thesis writing. I appreciate her patience on a number of occasions, especially those weekends when I had to spend time on thesis instead of being with her.

Lastly, I thank my parents (Ramulu & Ramadevi) for motivating me to pursue higher education and my brothers (Chaitanya & Kartik) for their friendly support. My father's moral support during difficult times can never be forgotten.

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Chapter 1. Introduction

Process scheduling has recently gained prominence because of the competitive pressures in the process industry to improve productivity and reduce operational costs. Scheduling integrates the production objectives with the process operations and could be very effective in increasing the expected plant profits. It mainly defines the timing and values of activities to be performed in a plant over a period of time. Broadly, the key decision variables are the start time of an operation, the unit it will run on, its duration, process conditions and the amount of material processed. Scheduling decisions are made over a defined finite horizon in such a way that the maintenance requirements are fulfilled, customer demands are met and the inventory levels are kept as low as possible while the overall profit is maximized. The time horizon for scheduling depends on the typical run length of an operation in a unit and could range from few days to 2-3 months (Mendez et al., 2006 and Kallrath, 2002).

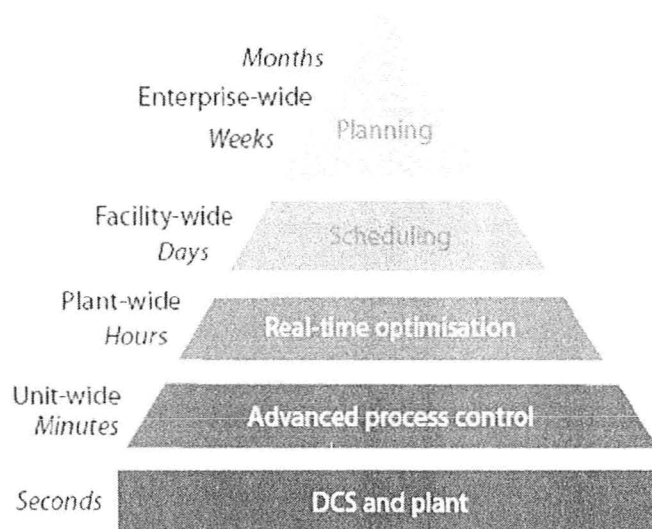


Figure 1-1: Hierarchy of plant automation

In the hierarchy of plant automation shown in Figure 1-1, scheduling lies between planning and real-time process optimisation (RTO). Planning layer deals with long term decisions such as feedstock purchase, production levels and product inventories for given marketing forecasts and demands, which are forwarded to the scheduling layer. Subsequently, the scheduling decisions are made by considering the planning decisions. These decisions are then sent to the RTO layer, which communicates with the lower levels of automation. At present, the RTO technology is well developed for plants that operate at steady state (Yip and Marlin, 2004, Beautyman, 2004, Marlin and Hrymak, 1997). It uses a rigorous steady state plant model to obtain optimal operating conditions. Consequently, simple and approximate plant models can be used for scheduling continuous processes due to the cascade structure in the hierarchy of plant automation.

Process scheduling methods adopted in industry currently optimize the open-loop behaviour of the system model. The open-loop scheduling models are solved by an engineer in a batch manner using simulation or optimization tools to obtain feasible schedules. He/she then picks the most profitable schedule and implements it and periodically updates the model using feedback information. However, with few experienced human schedulers available for the entire production facility, it becomes extremely difficult to generate consistent schedules. This could have a great effect on the expected plant profit.

The existing manual procedures for plant scheduling can be improved by automating the scheduling system so that the on-line scheduler generates good feasible schedules consistently with little involvement of human expertise. Our goals in this thesis are to (a) formulate an open-loop scheduling model that can be solved in reasonable computing time and (b) to apply this model in a prototype closed-loop scheduling system that can assist engineers to make appropriate decisions in a timely manner.

1.1 Thesis Objectives

The main overall objective of this research work is to develop a reactive (closed-loop) scheduling system that automatically generates the schedule and implements it into the plant in real time. Typically, closed-loop schedule implementation is done once every day.

In this thesis, the scheduling system is developed as a stand alone system and not integrated with the RTO or any other layers of automation. The system can be considered as a closed-loop Model Predictive Controller (MPC), which has a Mixed Integer optimization problem (MIP) at each iteration (hybrid MPC problem). The schematic of a typical reactive scheduling framework (Bose and Pekny, 2000, Perea et al., 2003) is shown in Figure 1-2. This framework provides feedback information to update the plant model in order to compensate for model errors and disturbances entering the plant.

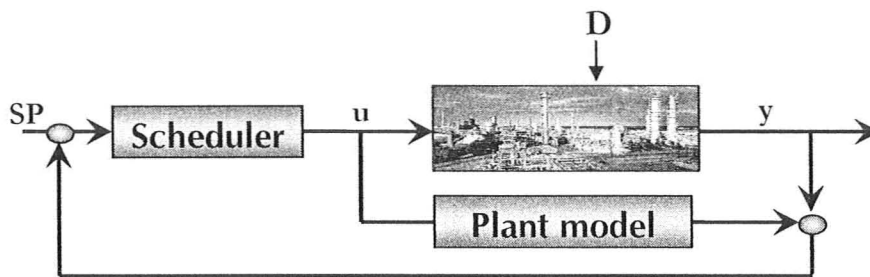


Figure 1-2: Reactive (closed-loop) scheduling framework

In order to achieve this objective, the work was planned to be carried out in two phases.

- In the first phase, an open-loop scheduler is developed. The open-loop scheduler is a multi-period optimization problem that is formulated as a Mixed Integer programming problem (MIP). The aim of this open-loop scheduler is to determine a feasible schedule that maximizes the plant profit and leaves the plant in an

operable state at the end of horizon. The product developed in this phase can be used as an optimization tool to assist the engineers for offline schedule generation and manual implementation.

- In the second phase, a closed-loop framework is selected to implement the online scheduling system. Necessary modifications to the open-loop scheduling model should be accounted for to make it compatible for closed-loop application, specifically to reduce the changes in plant operation between optimisation solutions. Therefore, proper care should be taken during implementation phase to make the closed-loop scheduler suitable for real time application.

1.2 Scope of work

Mixed Integer Linear Programming (MILP) has become one of the most widely explored methods for process scheduling because of its rigorousness, flexible, extensive modelling capability and the availability of state-of-the-art solvers (Floudas and Lin, 2002). Also, the main advantage with MILP's is that they are well understood and the techniques to solve them are well developed. For this reason, we intend to formulate the scheduling model in this thesis as a MILP.

To avoid the non-linear sub-problems (relaxations), the nonlinearity in the scheduling models are modelled as linear constraints using approximation and reformulation techniques in this thesis. In general, MILP's embed a combinatorial aspect. When this is combined with the large size of optimization problems, it makes the optimization exceptionally difficult to solve in a reasonable amount of time. Thus, the main scope of this work is to develop a tailored formulation and an efficient solution strategy to reduce the computational time of the scheduling model and make it feasible for real time application.

This thesis is mainly concerned with deterministic scheduling; therefore, uncertainty is not explicitly addressed. Constant model parameters, product demands and

prices are assumed. Feedback information available in the closed-loop system compensates for model errors and disturbances entering the system.

1.3 Research Emphasis

In many processes, operations and maintenance often (not always) have interactions. The main emphasis of this research is on a particular class of processes where the operations and maintenance have strong interactions and so integrated decision making is necessary. Let us consider a chemical reactor with a catalyst as an example. If the temperature in the reactor increases, the catalyst decays quickly. As a result, the reactor should be shutdown to replace the catalyst. Therefore, reactor operation (temperature) interacts with its maintenance (shutdown). Other similar examples include processes where process flow affects the adsorption run length (water treating system), process flow can cause pump wear, reactor severity can cause coking in cracking coils (ethylene plants), etc.

In order to capture the interactions between the process operation and maintenance, integrated decision making is required.

1.4 Case study: Ethylene furnace scheduling

Ethylene plant furnace scheduling is chosen as the process example in this thesis. This problem is concerned with optimally scheduling the furnace operations and its shutdown (maintenance) simultaneously (Schulz et al., 2006 and Lim et al., 2006). The interaction between reactor operation (severity and steam to hydrocarbon ratio) and furnace maintenance is clearly evident in this example. Furnace scheduling lies at the heart of every production and maintenance scheduling activity for a petrochemical complex. Ethylene plant is the key source of intermediates for all downstream production units and its operation directly affects downstream production quantities and qualities.

There is a huge cash flow in these plants (millions of dollars per day); therefore, any small improvement in such a facility will produce significant economic benefits.

A wide variety of petrochemical products are produced in ethylene plants by thermal cracking of feedstocks in the cracking furnaces. Continuous operation of the furnaces leads to coke formation on the inner surface of the cracking coils. Coke hinders heat transfer through the coil wall and thus decreases the productivity of the furnace. To maintain the productivity, input energy must be continuously increased, and this raises the tube skin temperature (coil surface temperature). Furthermore, excessive coke deposition plugs the coil. Therefore, in order to maintain production efficiency and plant safety, the furnace has to be periodically shutdown for cleaning the coke. This cleaning process is called decoking. Typically, this is done when the tube skin temperature or the pressure drop of the coil reaches its maximum limit. Therefore, optimization of the decoking schedule is highly desirable to maximize the overall profit of the furnace system.

On the other hand, the type of cracking feedstock (Ethane, Propane, Naphtha etc.) and the operating conditions in the furnace (Severity, S/HC) directly effect coking in the cracking coils and thus the decoking time periods. This signifies the interaction between furnace operation and its maintenance shutdown. Therefore, an optimal schedule for this problem would determine both the daily plant operations and the required maintenance actions. More specifically the key optimization decisions of this furnace scheduling problem are,

- i) Selection of appropriate furnace feed selection (integer decision),
- ii) Selection of optimal furnace operating conditions (Flow rates, Severity, Steam to Hydrocarbon ratio (S/HC)) for the reactors (continuous decisions), and
- iii) Determination of furnace shutdown time periods (integer decision).

The details of this scheduling problem and the challenges associated with it are discussed in Chapter 3.

1.5 Thesis Outline

The thesis is laid out as six chapters. Figure 1-2 shows the schematic of thesis outline. Brief details of each chapter are as follows.

Chapter 2 reviews the concepts of open-loop optimization and closed-loop optimization for ethylene furnace scheduling. An overview of optimal scheduling is provided with emphasis on time representation and model formulation in order to develop a tractable open-loop optimization model. Challenges posed by the furnace scheduling problem are discussed through a review of open-loop furnace scheduling literature. Several reactive (closed-loop) frameworks available in the literature are presented and the advantages and disadvantages of each are discussed in this chapter.

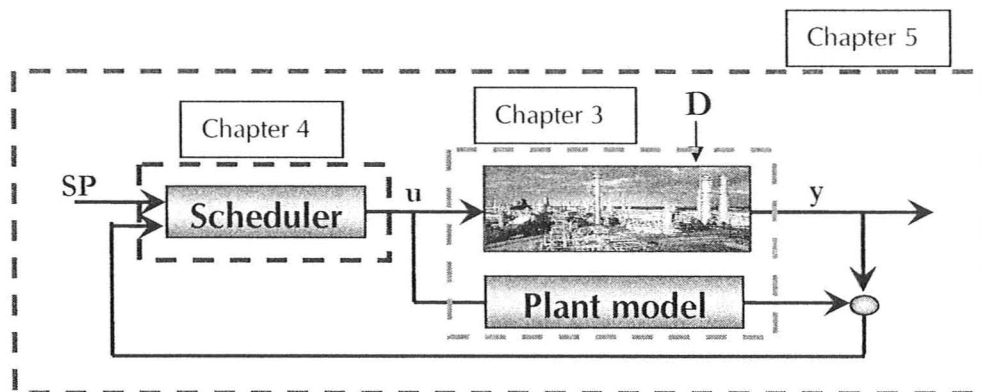


Figure 1-3: Schematic of the thesis outline

Chapter 3 provides an overview of the chemical engineering principles of olefin production process. First, a detailed description of the chemical processes and general operating procedures in Ethylene plants are presented. The details of furnace scheduling problem are discussed next, and the objectives and scope of the optimization problem are clearly defined in this chapter.

Chapter 4 emphasises the mathematical formulation of the open-loop scheduling model. Although, the yield and coking data in an ethylene plant are nonlinear, a linear

scheduling model (MILP) was developed based on the modelling principles such as discrete time formulation and disjunctive modelling. Challenges posed by this optimization problem and the techniques (reformulated constraints, tightening constraints and solutions heuristics) used to overcome them are elaborated. Extensive open-loop case studies are considered, and the results are discussed in detail to assess the performance of the open loop scheduling model.

Chapter 5 discusses the framework for reactive (closed-loop) scheduling and some important implementation issues associated with it. The modifications necessary to the open-loop scheduling model to make it applicable for closed-loop scheduling are also discussed in this chapter. Several closed-loop case studies are considered to study the performance of the reactive scheduling system.

Chapter 6 draws the conclusions of this thesis. The main contributions of the work are elaborated, and the issues that are outstanding in the research work are pointed out for future work.

Chapter 2. Literature review

This chapter reviews the concepts of open loop optimization and closed loop optimization for ethylene furnace scheduling, which are the two main topics that form the basis for this thesis. The discussion emphasises different methods and procedures available in the literature to formulate an open loop scheduling optimization problem and to develop a closed loop scheduling system for real time implementation.

2.1 Open loop optimization

Open loop optimization discusses mathematical formulations which can be evaluated for offline scheduling. The following sections provide an overview of optimal scheduling with more emphasis on mathematical formulation and solution procedures.

2.1.1 Overview of optimal scheduling

Optimal scheduling problems mainly involve sequential decision-making with continuous and discrete decisions. Decisions are made over a finite horizon in such a way that the production requirements are met and the customer demands are satisfied with the optimal utilization of the process equipment and raw materials. Typically, these problems are solved using a plant model, and the scheduling decisions are made over a multiple time periods in the defined horizon; thus, these problems are often referred as multi-period model based optimization problems. Due to the presence of continuous and discrete decisions, scheduling problems are formulated as mixed integer programs (MIP). It is important to know that these optimization problems are highly combinatorial in nature and the typical nature of these types of problems is that in a worst case, the computational time increases exponentially with the problem size (Kallrath, 2002, Grossmann, 2005 and Mendez et al., 2006).

For the past two decades, there has been a significant contribution to the field of optimal scheduling. The key focus has been on these topics, (i) Time representation, (ii) Model formulation, and (iii) Solution heuristics.

2.1.1.1 Time representation

Time representation is important while formulating multi-period optimization problems. Based on the available literature, the techniques developed so far are grouped into two categories (i) Discrete time representation (Kondili et al., 1993 and Shah et.al., 1993), and (ii) Continuous time representation (Ierapetritou & Floudas, 1998, Floudas & Lin, 2004, Maravelies & Grossmann, 2003 and Mokus & Reklaitis, 1999).

In discrete-time models, the time horizon is divided into a finite number of uniform or non-uniform time intervals of predefined durations and the scheduling tasks are performed only at the boundaries of each time interval. In this way, time is just modelled as a reference grid and is defined as a parameter in the optimization problem. The advantage with discrete models is the concept of reference time grid, which is useful to formulate difficult scheduling constraints easily while maintaining linearity in the model. The disadvantage with these models is that they may lead to a large number of time intervals in the problem. The number of binary variables in these models scales proportionally with the time intervals in the scheduling horizon, thus making the models computationally expensive. However, a modified formulation and tailored heuristics can eliminate this difficulty in some cases, making the discrete time models acceptable for large scale scheduling problems.

In contrast, continuous-time models are proposed to reduce the number of time intervals and hence solve the problem of large binary variables in the model. These models are based on the concept of variable time intervals. Here, the time horizon is divided into 'n' time intervals, where the number of time intervals 'n' and the length of each interval are unknown. They are defined as variables in the optimization problem, thus the final solution would find the optimal number of time intervals and their lengths.

In these models, time is therefore, modelled as a variable which in many cases leads to nonlinear constraints in the scheduling model.

2.1.1.2 Model formulation and solution procedure

Model formulation is critical to the development of a scheduling optimization problem. Tractable formulation is very important and also since the scheduling models are mixed integer optimization problems, additional care should be taken while formulating the constraints as they have a direct effect on the computational time. For example, in the case of big-M type constraints (Wolsey, 1998), improper specification of 'M' value can effect the search space and in turn the computational time.

As discussed earlier, time representation influences the formulation of the scheduling model. In general, continuous time formulation leads to nonlinear constraints in the model; thus, the resulting optimization problem would be a Mixed Integer Nonlinear Programming problem (MINLP). Discrete time formulation, on the other hand, is advantageous as it does not add any additional nonlinear constraints to the model because of the reference grid for time. This way, discrete time models preserve the linearity of the formulation.

The plant model is equally important while developing a scheduling model. For example, if the plant model is linear, the scheduling model can be formulated as a Mixed Integer Linear Programming problem (MILP) using discrete time representation. However, if the plant model is nonlinear, the resulting scheduling model would be a MINLP for either discrete time or continuous time formulation.

Mixed integer optimization problems are combinatorial optimization problems which can have a finite but usually very large number of feasible solutions. The branch and bound (B&B) technique is the most widely used algorithm to search for an optimal solution from the search space. B&B algorithm searches the complete space of solutions for a given problem for the best solution. However, explicit enumeration is normally

impossible due to the exponentially increasing number of potential solutions. Therefore, the use of bounding and pruning techniques enables the algorithm to search only part of the solution space to find the best solution. The algorithm operates by relaxing selected integer variables to be continuous between their bounds and fixing the remaining integer variables. The bounding is achieved by maintaining rigorous upper and lower bounds on the objective function in a fashion that the best solution is never lost (Wolsey, 1998, CPLEX, 2006). The procedures for B&B algorithm can remain the same for MILP and MINLP optimization problems. The only difference is that in the case of MILP, at every node of the branch a Linear programming problem (LP) is solved, whereas a Nonlinear Programming problem (NLP) is solved for MINLP problems.

The state-of-the-art MILP solvers commercially available at present and widely used are CPLEX (ILOG CPLEX, 2008) and XPRESS-MP (Dash Optimization, 2008). Both these solvers embed a B&B algorithm to solve MILP problems. They have an additional feature to add a variety of cuts at every node of the tree search in order to restrict non-integer solutions that would otherwise be solutions of the continuous relaxation. Cuts are constraints which usually reduce the number of branches needed to solve a problem so that it can be solved quickly.

At present, the most widely used MINLP solvers are BARON (Tawarmalani and Sahinidis, 2002), MINOPT (Floudas, 1995) and DICOPT (Quesada and Grossmann, 1992, Sahinidis and Grossmann, 1991). These solvers were successfully used to solve a few MINLP scheduling problems; however, the problem size and the convexity of the optimization problem are always a main concern with these solvers.

2.1.1.3 *Solution heuristics*

Scheduling problems are usually large scale mixed integer optimization problems. Sometimes these problems are difficult to solve with stand alone optimization solvers. In such circumstances, solution heuristics are useful to solve those problems with less

difficulty (Honkomp et al., 2000 and Kelly, 2005, Heejin Lim et al, 2006 and Grossmann, 2006).

A commonly used heuristic to solve MINLP scheduling problems (Heejin Lim et al, 2006 and Kelly, 2005) is to decompose the optimization problem into two sub-problems (MILP & NLP) and solve in two stages. In the first stage, a MILP is obtained by fixing some of the model variables that cause nonlinearity in the model (e.g. flow rates) and solved using a MILP solver. In the second stage the integers decisions are fixed and the variables which were fixed earlier are relaxed, so that the resulting problem is a NLP which is solved using a NLP solver to obtain a better solution. This way a difficult MINLP can be solved using the available state-of-the-art MILP and NLP solvers. Although, these decomposition heuristics do not guarantee optimality, they yield a feasible solution and provide a good alternative to solve difficult scheduling problems.

There are several other aggregation and decomposition heuristics proposed in the literature (Honkomp et al., 2000 and Kelly, 2005) to overcome the computational burden of MIP's and solve them in a reasonable amount of time. Aggregation techniques rely on the idea of aggregating the time periods within the specified horizon in order to reduce the dimensionality of the problem. This way the number of binary variables are reduced and the optimization problem can be solved quickly to provide an approximate solution of the scheduling problem. Decomposition techniques, on the other hand, rely on the idea of decomposing a large problem into several small problems and solving them sequentially until the entire model is solved.

In a temporal decomposition heuristic (Kelly, 2005), the time horizon is first spliced into a number of small horizons and the decisions are made sequentially by solving the smaller problems arising in each sub horizon. Here, the decisions in the succeeding horizons are made while fixing the decision in the earlier horizons. In this way, decisions can be obtained for the entire time horizon. The main advantage here comes in the form of lesser computational burden because only smaller problems are solved without any computational problems. However, the main disadvantage is that it

cannot guarantee optimality and also by splicing the time horizon to solve smaller problems, this heuristic doesn't look far into the future. It just looks locally and obtains a feasible solution. However, one should realize that in most scheduling problems, process changes, product demands and disturbances etc. can occur over a long period of time, so that it becomes necessary to employ an appropriate heuristic that looks into the future over a longer period of time. Details on the tailor- made solution heuristic used in this research are discussed in Chapter 4.

2.1.2 Ethylene furnace scheduling literature

This section reviews the literature particularly dealing with Ethylene furnace scheduling problems. The main emphasis of the discussion will be on model formulation and solution technology used by various researchers. The challenges posed by this problem and the methods used to overcome those challenges are presented here.

Schulz and co-workers (2006) developed a furnace scheduling model to optimally schedule the production and furnace decokes in an Ethane cracker. A discrete time formulation was used to develop the model. Due to nonlinearity in the plant model, the optimization problem was formulated as a MINLP, which was very difficult to solve. The nonlinearity in the mixed integer program is always difficult to compute because of no good solver and no optimality guarantee due to non-convexity in the model. As a solution heuristic the authors reduced the dimensionality of the problem by aggregating the time periods (each time period was equal to 1 week) and solved the MINLP using DICOPT (Quesada and Grossmann, 1992). Although, several scenarios were solved, the coarse formulation is unrealistic because it assumes that during any decoke, a reactor would be offline for 1 week, which is much too long.

A similar furnace scheduling model was developed by Lim and co-workers (2006) for naphtha crackers based on a discrete time representation. This model was also formulated as a MINLP due to the nonlinearities present in the Ethylene plant model. They found it difficult to solve the resulting large scale MINLP. Therefore, they adopted

a decomposition heuristic to decompose the MINLP into MILP and NLP and solved it in two stages. Specifically, in the first stage, feed flow rates, severity and S/HC ratio were fixed and the resulting MILP was solved using CPELX solver. In the second stage, the restriction on the flow rates was relaxed and the resulting NLP was solved using CONOPT solver. Besides using this heuristic, the model also assumed fixed chemical reactor operating conditions (severity and S/HC ratio) to make the problem easily computable. It is important to know that, feed flowrates, severity, S/HC ratio and decoking periods are the main degrees of freedom for the furnace scheduling problem and fixing the major variables doesn't make the model complete for real-life application.

Kelly (2005) also proposed a furnace scheduling model for multi-feed crackers based on discrete time representation. The model was formulated as a MINLP and solved using the decomposition heuristic in two stages. In the first stage, feed flow rates were fixed and the resulting MILP was solved using the solver XpressMP and the NLP in the second stage was solved using SLP. Furthermore, the sequential temporal decomposition heuristic discussed in section (2.1.1.3) was used to solve the MILP in the first stage. This was done because the MILP was large and difficult to compute in its current state. The heuristics could not guarantee optimality; however, a feasible solution was obtained. Note that this approach would not be successful if the production rate changed during the horizon and decokes should be performed to prepare for the higher demand. This is because the temporal decomposition heuristic doesn't look far into the future due to the splicing of the time horizon.

Grossmann et al. (1998) formulated a furnace scheduling model for multi-feedstock crackers based on continuous time representation. The model was formulated as a MINLP and solved using the software developed in their group that employed the branch and bound algorithm. Although, the model has all the features that existed in a true plant, it lacks a true coking model. The scheduling model assumes an exponential decay in the reactor performance with time independent of operating conditions. In addition, the flow rates were assumed to be constant while solving the model in order to

exploit special properties of the model. The main disadvantage with the model was that the continuous time formulated led to bilinear constraints which are non-convex.

From this review, it is clear that all the scheduling model formulations are large scale MINLP's. The nonlinearity in the formulation is mainly due to nonlinear yield and coking patterns in the Ethylene plant model. Therefore, nonlinearity is inherent to the furnace scheduling model. Due to the difficulties posed by the MINLP's (often non convex and difficult to solve) and lack of an efficient MINLP solver, it is always a challenge to solve the furnace scheduling model.

One alternative to overcome this difficulty is to reformulate the scheduling model as a MILP. However proper care should be taken during the formulation so that the nonlinearity in the Ethylene plant model is appropriately captured without losing any information. There are few nonlinear approximation techniques available in the literature such as separable programming and disjunctive programming (Williams, 1985, Grossmann, 2002), which can be used to re-formulate the nonlinear constraints into linear constraints; it is however accomplished by introducing new integer variables.

2.2 Closed loop optimization

Closed loop scheduling is also called as Reactive scheduling. Closed loop scheduling frameworks are known for their ability to periodically update and modify the optimal decisions to compensate for disturbances and modelling errors based on new information. This reactive nature is very elegant and provides an ideal framework to develop a closed loop scheduling system for online implementation. Some of the reactive frameworks available in the literature are discussed here.

2.2.1 MPC framework

Model predictive control (MPC) has been widely accepted by the process industries as a tool to effectively control multivariate systems with input and output constraints (Qin and Badwell, 2003, Marlin, 2000). MPC uses a plant model for prediction and solves an optimization problem to optimize the future process behaviour to obtain optimal control moves. These control moves are then implemented in the plant in a rolling horizon fashion. The plant model used in MPC is periodically updated using the feedback information at each controller execution. This particular framework has found wide application that extends beyond the field of process control.

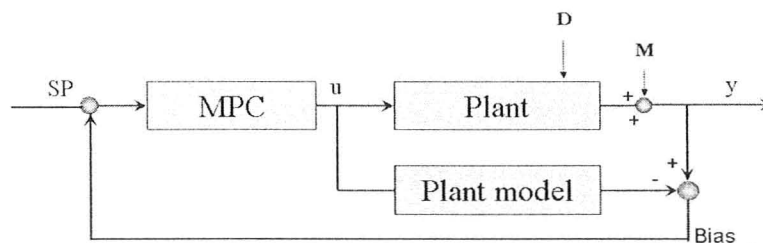


Figure 2-1: MPC framework

2.2.1.1 Nominal MPC

In the nominal MPC framework, no explicit model of uncertainty is used for the plant model parameters or the exogenous variables (measured and unmeasured disturbances) (Qin and Badwell, 2003, Marlin, 2000). Instead, the parameters are tuned to obtain closed loop stability, good dynamic performance and robust constraint handling. Appropriate safety margins are provided to deal with potential constraint violations. Since, feedback information is available at every execution time, the controller can quickly react to disturbances and modeling errors, and the control moves are recalculated accordingly.

The mathematical formulation of scheduling optimization and supply chain optimization problems are similar and both of them involve continuous and discrete variables. Recently, (Bose and Pekny, 2000, Mestan et al. (2006) and Perea-Lopez et al. (2003) proposed nominal MPC frameworks to address the supply chain optimization problems. The supply chain model consisting of suppliers, production facilities, distribution network, retailers and customers was formulated as a MILP with an objective of maximizing the profit. At every MPC execution the states of the system (inventories, accumulated orders) were updated, and the resulting MILP problem was solved to obtain optimal control decisions (production schedule in the plant, orders placed between the nodes and shipment amounts among the nodes). Fixed demand patterns, processing times and transportation costs were used within the supply chain model. Therefore, any disturbances entering the system and any model errors are compensated via feedback.

2.2.1.2 Robust MPC

In robust MPC, explicit models of uncertainty are defined in order to maintain a particular closed-loop behavior in the presence of model mismatch and disturbances. Three main issues that are commonly addressed in robust analysis are robust stability (Bemporad and Morari, 1999), robust performance and robust constraint handling (or robust feasibility) (Warren, 2004, Van Hessem and Bosgra, 2006). Different formulations have been proposed to address each of these issues..

Most of the robust controller formulations result in convex optimization problems, e.g. robust feasibility, is addressed by reformulating the linear constraints into second order conic constraints while robust stability is achieved by semi-definite programming. These are computationally tractable formulations, which guarantee global optimality in a reasonable amount of time when the controller model includes only continuous variables. With the presence of discrete variables (as in scheduling models), robust MPC framework leads to a problem formulation that is presently intractable. Also, the robust

formulation of a MILP ends up being non-linear resulting in a MINLP (Lin et al., 2004 and Janak et al., 2007).

2.2.2 Stochastic programming with recourse

In this framework, the decisions are made sequentially in stages. Mainly the decisions are separated into proactive and reactive decisions. The proactive decisions are made before the actual realization of the uncertain parameter, and the reactive decisions are made after the realization of uncertainty, generally with the assumption that the uncertainty in the parameters is eliminated through measurement. These reactive decisions are usually interpreted as corrective measures or recourse actions to improve the solution when the uncertainty no longer exists. Thus, recourse provides feedback of a special type. A recent review on stochastic programming and its application in the process systems area can be found in Sahinidis (2004).

The most common recourse problem is the two-stage program in which the decisions are made in two stages leading to an underlying assumption that uncertainty is propagated only over two stages. Its application for robust process scheduling has been considered recently (Sand and Engell, 2004). However, two stage programs cannot model the closed loop uncertainty in multi-period optimization problems accurately because the uncertainty propagates over time and not only over two stages. Thus, multistage stochastic programs are appropriate for such problems in that the uncertainty is propagated over all the stages considered in the problem. The number of stages depends on the size of the time horizon considered in the optimization problem. Computationally, small-scale stochastic programs with continuous variables are found to be tractable that can be solved using exact algorithms or using some approximation schemes (Birge, 1997). They tend to become intractable with the introduction of integer variables in the formulation and hence several approximation solution procedures and decomposition schemes have been reported in the literature (Birge, 1997, Balasubramanian et al., 2004).

2.2.3 Simulation based re-optimization

Jung et al. (2004) have recently proposed a simulation-based optimization framework for supply chain optimization problems involving both continuous and integer decisions. This is slightly different from the nominal MPC framework in that, a deterministic optimization problem is solved at each execution time and subsequently the feasibility of the solution is verified before being implemented. This is carried out by using two simulation models (a deterministic model and a stochastic model), which can verify the robustness of the solution for a sample of realizations of uncertainty. If in any case, the solution is found to be infeasible or below the specified tolerance limits over the finite horizon (i.e. prediction horizon), re-optimization is triggered and the robustness check is performed again. Once the solution is verified for its robustness and performance, the current time period decisions are implemented and the whole process continued.

The main advantage here is computational efficiency because only a deterministic optimization problem is solved. However, no clear strategy is available to correct the optimization results when infeasibilities occur; Jung et al. (2004) allow only the current and future decisions in the horizon to be adjusted, with all decisions prior to the infeasibility in the horizon fixed at the result from the deterministic solution values. This is a very limiting strategy and may not be able to lead to a feasible, let alone optimal, result. In addition, if many re-optimizations are triggered before the implementation of each control move, there can be a serious computational difficulty as opposed to solving a single robust optimization problem.

2.3 Summary

The main concepts of open loop scheduling and the frameworks for closed loop scheduling are discussed in this chapter. First, a review of open loop furnace scheduling models developed in the past has revealed that all the models were formulated as large

scale MINLP's. The nonlinearity is inherent to the ethylene furnace scheduling model because of the nonlinear yields and coking rates in the ethylene plant model. It was a great challenge to solve the MINLP's and as a result several solution heuristics were proposed by the authors.

One alternative to overcome the difficulties posed by nonlinear scheduling models is to formulate them as linear models (MILP's). While doing so, proper care should be taken to capture the nonlinear information in the plant. Nonlinear approximation techniques such as Separable programming and Disjunctive programming could be used for this purpose. The main advantage with MILP's is that they are well understood and the techniques to solve them are well developed. Irrespective of the linearity or nonlinearity of the model, it is always important to develop a tractable formulation to preserve the fidelity of the scheduling model so that it guarantees that the model could be solved efficiently with the available solvers. Therefore, every attempt should be made to develop a tractable formulation.

Open loop optimization provides an optimal schedule that needs to be implemented manually in the plant. A closed loop system would automatically implement the schedules into the plant in real time. Furthermore, it uses feedback information to update the plant model in order to compensate for model errors and disturbances entering the plant. Several reactive frameworks were reviewed and the advantages and disadvantages of the frameworks were discussed in this chapter. Reactive approaches provide a framework for reactively updating the decision upon the realization of uncertain parameters. Nominal MPC framework provides an elegant way to update the decisions using the feedback information. Other reactive frameworks such as simulation based optimization techniques and stochastic programming could be computationally expensive when it comes to solving scheduling problems, which are often large optimization problems.

Chapter 3. Ethylene plant process technology and furnace scheduling challenges

The emphasis of this chapter is on the chemical engineering element of the olefins-producing process, which is the process example considered throughout the thesis. First, detailed descriptions of the processes in ethylene plants are provided and some general operating procedures are discussed. Ethylene plant furnace scheduling problem is presented next and the scope and objectives of the scheduling are clearly mentioned. The assumptions made to develop the scheduling model are briefly discussed, and the plant capacity details used as a basis for the case studies are also elaborated.

3.1 Introduction

Ethylene is the lightest olefinic hydrocarbon that is not available freely in nature. It is produced in ethylene plants by thermal cracking of hydrocarbon feedstocks. Olefins such as propylene, butylene and other side products are also produced in these plants. Ethylene is an intermediate petroleum product primarily used in the production of other chemicals such as polyethylene, the world's most widely used plastic, polyvinyl chloride, ethylene oxide and ethyl benzene (Albright et al., 1983, Ethylene, 1992).

An ethylene plant forms a core facility of a fully integrated petrochemical complex producing a variety of products. The capacity of most plants designed since the year 2000 ranges between 800,000 and 1,300,000 MTA ethylene with typically 4 to 6 cracking heaters (reactors) in a plant. In today's design, a single cracking heater is built with a capacity of 200,000 to 300,000 MTA ethylene (Meyers, 2005).

Some ethylene plants are designed to crack only gas feeds and some to crack liquid feeds. However, due to increased profitability when a plant is able to respond to price fluctuations, new facilities are designed with the flexibility to handle a combination of feeds ranging from gas to liquid hydrocarbons.

3.2 Process description

Thermal cracking is also commonly known as steam cracking or pyrolysis. Cracking is highly endothermic and involves a large number of chemical reactions following a free-radical mechanism. A simplified process flow diagram of an ethylene plant is shown in Figure 3-1. Each section of the plant is briefly discussed here.

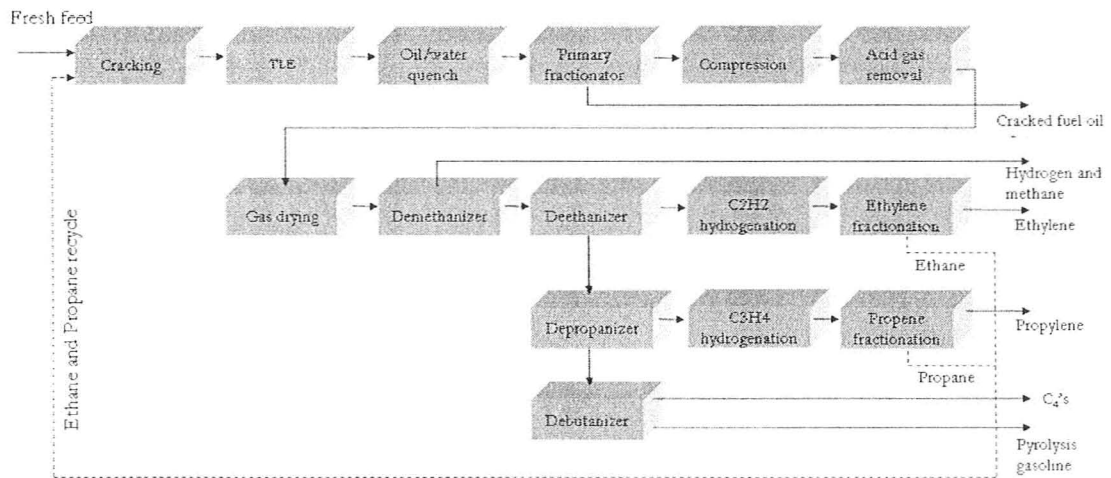


Figure 3-1: Simplified process flow diagram of an Ethylene plant

Feedstocks

The most common feedstocks cracked in ethylene plants are ethane, propane, ethane/propane mixture, butane, naphtha and gas oil [3]. The choice of feedstock mainly

depends on the cracker design, availability of the particular feed, its current market price, and the desired end-products.

Ethane is usually cracked at a conversion level of between 60-65% per pass, with a single pass ethylene yield of approximately 51 wt% at 65% conversion and ultimate yield of 81 wt% at 60% conversion (Albright et al., 1983, Froment et al., 1976 and Sundaram et al., 1981). Very small amount of by-products are produced from an ethane cracker. Usually, when there is large demand for ethylene and by products are less important, ethane feed is an ideal choice.

Propane is normally cracked at a conversion level of 65-93% per pass, depending on the desired ratio of propylene to ethylene. At a conversion level of 93% per pass, the ultimate yield of ethylene is approximately 47 wt% (Albright et al., 1983, Vandamme et al., 1975, Sundaram et al., 1979). When there is large demand for propylene and the economics for propane are favourable, propane is the preferred feedstock.

Naphtha is widely used for the production of olefins and aromatics all over the world. One of the advantages naphtha feedstock has over gaseous feedstocks is the wide spectrum of possible co-products. Butadiene and BTX (Benzene, Toulene and Xylene) are the most important ones. By varying the cracking severity, propylene to ethylene ratio on a once through basis may be changed from about 0.40 at high severity to about 0.75 at low severity (Plehiers et al., 1987, Kumar et al., 1985).

The prices of the feedstocks and end products are shown in Table 1. They reflect the prices from an oil refinery in the US gulf cost (Oil and gas journal, 1992), and they are the prices used throughout this thesis.

Table 3-1: Prices of feedstock and end products

Feedstock	Price (US\$/Kg)	Product	Price (US\$/Kg)
Ethane	0.240	Hydrogen (H ₂)	0.881
Propane	0.260	Methane (CH ₄)	0.220
n-Butane	0.300	Ethylene (C ₂ H ₄)	0.650
Light Naphtha	0.361	Propylene (C ₃ H ₆)	0.511
Gas oil	0.297	Butadiene (C ₄ H ₆)	0.852
		Butylene (C ₄ H ₈)	0.811
		Pentanes plus (C ₅ +)	0.401

Cracking section

The schematic of a typical pyrolysis furnace is shown in Figure 3-2. It consists of a convection section and radiation section. In the convection section, feedstocks are mixed with dilution steam and preheated to the cross over temperature. The objective is to heat the feed to a temperature just below the point at which cracking is initiated. The crossover temperature ranges from 550 to 700⁰ C depending on the feedstock.

Feedstocks are cracked in the radiation section of the coil. Energy required for the endothermic cracking is provided by the furnace. The cracked products leave the radiant coils at a temperature of 750 to 900⁰ C, depending on feedstock, cracking severity, and selectivity (Steam to Hydrocarbon ratio).

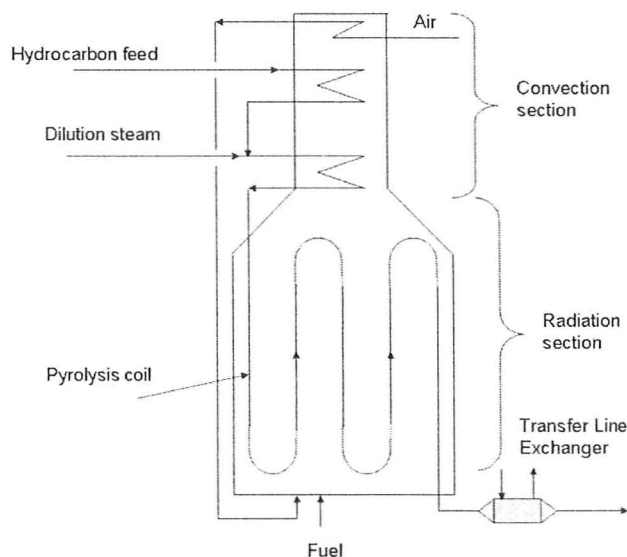


Figure 3-2: Diagram of a typical pyrolysis furnace

Transfer Line Exchangers and Quench coolers

In order to maintain the overall process efficiency, it is required to efficiently recover the heat in the cracked effluents. This heat is recovered mainly in the convection section of the furnace and in the Transfer Line Exchangers (TLE's). The effluents from the cracking section are immediately cooled in TLE's to temperatures around 350 to 600⁰ C depending on the feedstocks. This cooling ensures that the olefins are not further cracked to less valuable products. Energy is recovered in the TLE's during this cooling process and used to generate medium pressure and high pressure steam that is used to boil dilution steam and elsewhere in the plant.

For gas feedstocks, cracked gas is further cooled to nearly 200⁰ C in secondary TLE's and water quench towers. For liquid feed crackers, this cooling is achieved by direct quenching in oil quench towers and later the heavier products (C₅+ components) are separated from the product mixture in primary fractionators. During this quenching process, dilution steam which was mixed with the feed in the convection section is also condensed and recycled.

Compression

The cracked gases leaving the quench tower are then compressed to 32–38 bars for further processing. Compression is carried out in a four to six stage centrifugal compressor. The number of stages depends primarily on the cracked gas composition and the highest temperature allowed for inter-stage discharge. Condensed water and hydrocarbons are separated from cracked gas between the stages. Water is returned to the quench water system and hydrocarbons are sent to other sections for further processing.

Following compression, acid gases such as carbon dioxide and hydrogen disulfide are removed from the cracked effluent and water is (nearly) completely removed via gas dryers in preparation for cryogenic separation, where water would freeze in the equipment if not removed.

Hydrocarbon fractionation

There are several hydrocarbon fractionation sequences commonly being employed in ethylene plants (Ethylene, 1992 and Meyers, 2005). The front end demethanizer process is the most commonly used sequence which is shown in Figure 3-1 and described here.

The fractionation sequence begins by removal of hydrogen and methane as overhead products in the demethanizer. The bottom product is directed into deethanizer column where acetylene, ethane and ethylene are removed as overhead product and C₃ and heavier components as bottom product. The overhead products are separated in ethylene fractionation column, while the bottom products are routed to a depropanizer. Propadiene, propane and propylene are taken as overhead products and the heavier bottom components are next processed in debutanizer column and so on. More details about the processes are available (Ethylene, 1992).

The major products obtained after eventual separation are ethylene and propylene; however, many side products are also obtained. Ethane obtained in the products stream is recycled back to the cracking section for further cracking.

Ethylene obtained as a result of fractionation is usually stored as a liquid in pressurized vessels and is transported as a gas via pipelines to various production sites. Sometimes, it is transported by cargo tanks or tank cars to its destination.

Economic considerations and operating procedures

The economics of an ethylene plant are not simple. It is important to know that because of the current energy situation and since an ethylene plant is severely energy intensive, the pyrolysis section of the plant has the greatest impact on economics (Albright et al., 1983 and Meyers, 2005). Therefore, some description of the general operating policies of an ethylene furnace is provided here.

There are four main operating variables for an ethylene steam cracker, and the optimization of these variables determines the end products produced and the efficiency of the unit and hence the profitability of the facility. The variables are:

- Feedstock and its composition
- Residence time (flowrates or hydrocarbon and steam)
- Temperature of the feed in cracking coil (Severity)
- Steam to hydrocarbon ratio (Selectivity)

By operating the furnace at a particular combination of the variables the engineer attempts to achieve the desired yields of various end products. The common procedure is to first select a particular feedstock based on the product demand and then to operate the reactors at an optimum severity and selectivity levels. Once this is done, he/she then adjusts the throughput by setting average flow rates again based on the expected product demand. These variables can be adjusted accordingly at any time to meet the demands and to respond to unexpected events. For example, if there is a sudden demand for the products, the processing rates or the severity can be increased depending on the magnitude of spike in the demand. The proper choice of variables to adjust depends on the yields and other effects (such as coking which will be discussed shortly); therefore,

standard operating rules will be able to achieve desired production rates, but not at maximum profit.

In this thesis, a systematic method is developed for optimal scheduling that assists the engineers to make appropriate decisions in a timely manner that will maximize profit.

3.3 Ethylene plant furnace scheduling

This section introduces the concept of furnace scheduling in ethylene plants. A schematic of an ethylene plant with multiple feeds, several furnaces and a separation system is shown in Figure 3-3. As discussed earlier, the feeds are processed into the reactors where they are cracked. From the cracked products, the heavier ones (C_5+) are removed first and the remaining gases are processed further into the separation system for their eventual separation. The ethane product stream is recycled back to cracking furnaces for further processing. In reality, there are no feed tanks for ethane and propane; they flow directly from pipelines to reactors; they flow directly from pipelines to reactors.

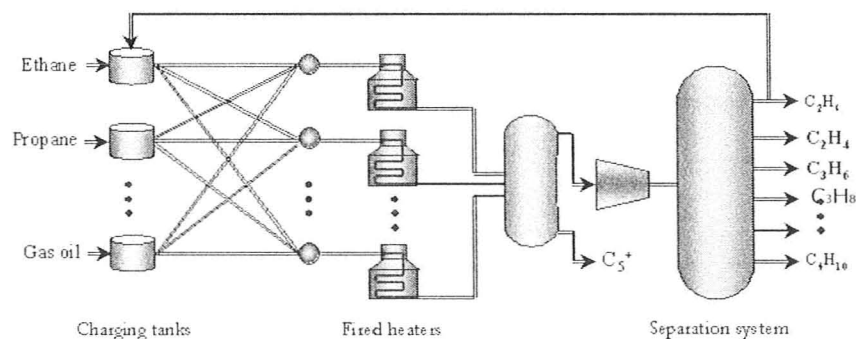


Figure 3-3: Schematic of an Ethylene plant

Cracking furnaces are generally operated at very high temperatures, around $825^{\circ}C$. During this energy intensive operation, coke deposits on the inner surface of the

reactors due to several catalytic and non-catalytic mechanisms. Deposition of coke inside the reactors is known to degrade the reactor performance.

First, coke acts as insulation and hampers heat transfer from furnace to the gaseous mixture in the reactor. Due to this heat loss, severity in the reactors reduces and as a result olefin yield decreases. Therefore, to maintain a constant severity, furnaces should supply additional energy to the reactors. Providing additional energy in turn heats up the external wall of the reactors, thus increasing the reactor's external skin temperature. Due to material limitations, a maximum value for the reactor coil cannot be exceeded, or the metal will fail catastrophically.

Second, coke deposition decreases the cross sectional area of the tubular reactor causing the pressure drop across the tube to increase. Therefore, in order to maintain the nominal feed flow, pressure in the inlet side of the reactor has to be increased. Higher pressures lead to reduction in olefin yields and causes additional safety concerns. For both these reasons, furnaces have to be periodically shut down for coke cleanup.

In general, when the tube walls reach their maximum allowable temperature set by tube metallurgical limits, shutdown of the furnace is necessary for cleanup. This cleanup operation is known as decoking, which is accomplished by removing the coil from service and using a steam-air mixture to burn the carbon out of the coil. The steam air mixture is heated to 900-1000⁰ C and is slowly reacted with the carbon to produce hydrogen and carbon monoxide. Typical run lengths (furnace operation time between decokes) for naphtha feedstock is 20-30 days (Plehiers et al., 1975), propane is 20-50 days (Vandamme et al., 1975) and ethane is 20-60 days (Froment et al., 1976).

Furnace scheduling is mainly concerned with optimally (1) selecting feedstocks, (2) selecting operating conditions, and (3) scheduling the maintenance shutdowns of furnaces for periodic decoking. An appropriate time for decoking is strongly affected by cracking feed and reactor operation. Typically, heavy hydrocarbons yield more coke than the lighter ones. Reactor operation at higher severity produces better yields, but leads to

faster coke accumulation, thus shorter run lengths and frequent decokes. Also, a decoking operation leads to a downtime (production loss) of approximately 8-10 hrs. Therefore there appears to be a trade-off between choosing heavy feed, operating at higher severity and decoking frequently versus choosing a light feed, operating at lower severity and decoking less frequently. This is ultimately an economics based decision.

Therefore, we define the ethylene plant furnace scheduling problem as a source to automatically consider the trade-off and make optimal decisions on appropriate feed selection, reactor operation and its maintenance that maximises the plant economics. With the main objective to obtain appropriate feed, optimal reactor operating conditions and shutdown policies over a defined time horizon, we model furnace scheduling as a Mixed Integer optimization problem (MIP). The problem overview is described as follows for any given scenario description.

Maximize the Plant profit for a selected time period

Decision variables

- The optimal feed to be cracked in the furnaces (integer decisions),
- The optimal operating conditions (flowrates, severity, S/HC) for the reactors (continuous variable decisions),
- Furnace maintenance decoking, which furnace and when (integer decisions), and
- The number of furnaces in production service at any time (integer decisions)

The problem above must be defined for a specific set of conditions, which we will term a scenario. A scenario is usually defined by the initial process conditions, equipment capacity limits, product demands, economics, and any other requirements that need to be satisfied by the model. A scenario can be described by the following parameters, which are the constants necessary to define the problem.

- Initial process conditions
 - Number of Furnaces available and their capacities,
 - Feedstocks available and their capacities
 - Accumulated coke in the reactors
 - Operating conditions (Severity, S/HC, Flow rates etc. needed for move suppression in closed-loop cases)
- Production requirements (Product demands and sales limits)
- Requirements on end conditions (end of finite horizon)
- Limitations on process equipment performance, e.g., capacity
- Time horizon of interest
- Economics

A detailed mathematical formulation of this scheduling model is provided in Chapter 4. The basic structure is provided here as shown below.

Maximize:	Plant profit
Subject to:	<ul style="list-style-type: none"> - Feedstock allocation constraints (<i>feeds and amounts available</i>) - Normal plant operation constraints (<i>flows, material balances</i>) - Severity and selectivity bounds (<i>conversion, S/HC</i>) - Coking model constraints (<i>coke accumulation</i>) - Decoking constraints (<i>cleanup</i>) - Equipment capacity limits - Integrated product demand and sales limits - Bounds on all the variables - Initial conditions - Data for all the parameters {<i>Continuous and binary variables</i>}

3.4 Major challenges

Ethylene furnace scheduling problem has some important characteristics which pose significant modelling and computational challenges. They are discussed here.

3.4.1 Interaction

As discussed earlier, there is a strong interaction between ethylene plant furnace maintenance and operation. Therefore, while scheduling ethylene furnaces, proper care should be taken to consider the tradeoff between these two factors. This problem is interesting because we cannot make the maintenance or furnace operation decisions separately; both have to be made simultaneously in an integrated approach.

Earlier there were instances where authors understood the difficulty of solving this problem and proposed some heuristics (Bizet et al., 2005). They tried to solve the problem in two stages. In the first stage they would fix the furnace operating conditions and obtained the maintenance schedule. Once they had the maintenance schedule, it was fixed and the furnace operating conditions were adjusted to meet the demands and operate the plant profitably. Although this type of heuristic yields a feasible schedule, it usually ends up in sub-optimal schedules.

If we want to obtain an optimal solution or at least a good feasible solution for this problem, it should be solved in a single stage without fixing any of the key decision variables. This means that decisions on the maintenance and furnace operation should be made together. Dealing with such a condition is challenging for large scale mixed integer optimization problems.

3.4.2 Non-Linearity

In ethylene plants, we encounter significant nonlinearities in product yields and coking rates. Plant data (product yields and coking rates as a function of furnace operating conditions) for various feeds are provided in Appendix A. This data has been obtained from pilot plant studies conducted by Foment and coworkers [4, 5].

Typical product yield profiles for a propane feedstock over a range of furnace operating conditions are shown in Figure 3-4. Clearly, propylene and pentanes (C_5+) yields are strongly nonlinear, while the other products exhibit slight nonlinearity. Similar

nonlinearities also exist for naphtha, butane and gas oil feeds. This leads to nonlinear yield models.

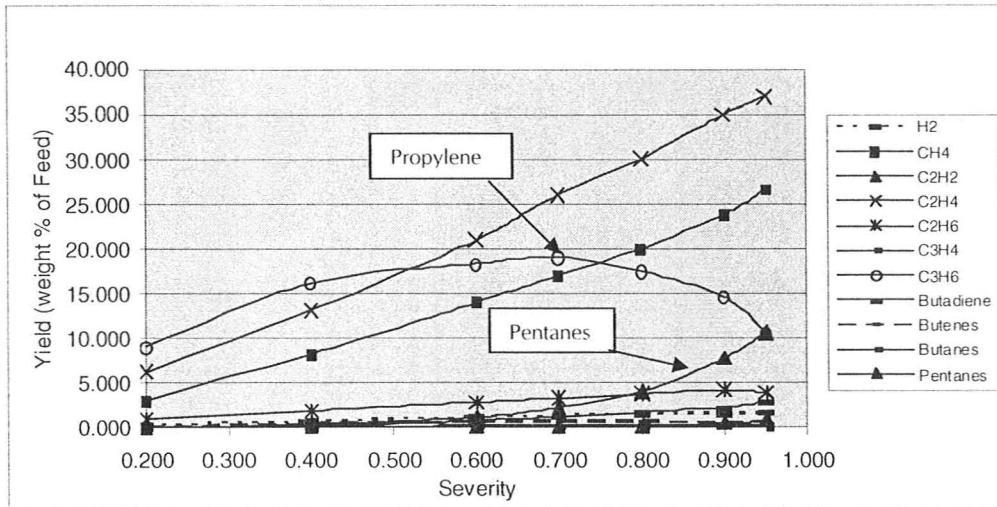


Figure 3-4: Propane feedstock yield profiles

A linear approximation of the yield models could be reasonable within a narrow range of operating conditions. However this approximation becomes inexact when used over a broad range of operating conditions. A direct implementation of nonlinear yield models in the furnace scheduling problem would result in a Mixed Integer Nonlinear Programming problem (MINLP), which poses significant computational difficulties.

3.4.3 Computational burden

The resulting furnace scheduling problem leads to a large scale Mixed Integer optimization problem (MIP). Typical problem size for a case study involving 3 different feeds and 5 reactors over a 90 day horizon is 3100 binary variables, 297794 continuous variables and 308629 constraints. Even if all the constraints are linear, solving this problem becomes difficult for any standalone commercial solver such as CPLEX, XPRESS etc. In a worst case, any mixed integer solver will have to search 2^{3100} nodes to obtain an optimal solution. Even if it takes 1 sec to solve the problem at each node, it takes centuries to search through the entire nodes.

The main concerns for this scheduling problem are (i) the presence of large number of binary variables, and (ii) type of constraints (linear or non-linear). MIP's are combinatorial in nature where the number of binary variables is directly related to the computational complexity. On top of that, nonlinearity in the model could make it exceptionally difficult to solve.

This is a major challenge for solving large scale scheduling problems. It is therefore, necessary to understand the structure of the optimization problem and exploit the structure through several ways.

3.5 Modelling assumptions

The model for scheduling major decisions in the ethylene plant requires a tailored model. If the model were too complex, it would not be computationally tractable; if it were too simple, the important interactions among decokes, feed materials, and operating conditions cannot be included. Therefore, the general goal is to include all important decisions and model features that determine the integer decisions (feed selection, number of reactors in operation and decoking). To do this, the operating conditions of the reactors must be optimized; however, the operating conditions could be fine-tuned by a real-time, steady-state optimization (RTO) of the plant that would be executed several times a day (Marlin and Hrymak, 1997). The RTO typically uses a much more complex and accurate model, but it does not optimize the integer decision variables.

The model assumptions are briefly introduced here, and the detailed model equations are presented in the next chapter.

- Model accuracy – The model structure and parameters are known exactly. Therefore, uncertainty is not considered explicitly in the optimization. However, feedback based on measurements will be considered in the reactive scheduling work in Chapter 5.

- Furnace operation
 - No change to the properties of feed material
 - Feed flow rate doesn't affect the severity in the reactors
 - Feed conversion is used as a measure of severity (reactor temperature) in the reactors. It is assumed that each reactor effluent is measured and controlled by adjusting the temperature. This is standard practice in industry using transfer line analyzers. In this thesis, the terms severity and conversion are used interchangeably.
 - Flow rates do not affect the rate of coking in the reactors
 - Coke deposited in the reactors doesn't affect the product yields
 - Recycle streams are assumed to be pure, which is a result of the perfect separation assumption.
 - Cracked gas processing through the separation equipments is not modelled in detail. Perfect separations are assumed. Constraints in the equipment could be included based on the material flow rates.
- Refrigeration and separation energy costs are not included in the model.
- Efficiency for compression is considered to be 100 % .
- Product inventory is not modelled. The products are assumed to be directly delivered to the clients via pipelines without storage.
- Integrated demand is considered which needs to be satisfied appropriately. Therefore, some deviation from instantaneous demand is allowed without penalty.
- All prices are assumed to be constant during all time periods in the schedule.
- Product yields and coking rates do not change over the time horizon.

- The model assumes that only one reactor exists in a furnace (fired heater). Therefore, the terms like reactor or furnace are used interchangeably; in reality, several reactors exist in a furnace, and their operating conditions can be slightly different.
- Most dynamics within an ethylene plant units are not considered and therefore, quasi steady-state models are used in each time period of the schedule. Note, that the key variables that “link” time periods are the dynamics of coke in the reactors.

Clearly, the greatest emphasis is placed on the reactor models that are needed for optimal scheduling. Detailed optimisation of the separations plant is not addressed in this research.

3.6 Plant capacity details

In order to make the case studies in this thesis more realistic, data corresponding to commercial sized ethylene plant were used in the model. The capacity of the plant is considered to be around 800,000 – 1,000,000 MTA ethylene. It can crack three feedstocks ethane, propane and naphtha. A single ethane cracker has a capacity of 200,000 MTA ethylene whereas propane and naphtha has 175,000 MTA and 150,000 MTA respectively. An overview of the process structure and a few additional capacities are depicted in Figure 3-5 and provided in Table 3-2.

Table 3-2: Plant capacity details

Feedstock	Reactor processing rates		Capacity	
	Pmin (Kg/hr)	Pmax (Kg/hr)	Single cracker (MTA C=C)	Plant (5 crackers) (MTA C=C)
Ethane	32620	46600	200,000	1,000,0000
Propane	40000	57140	175,000	875,000
Naphtha	46106	65865	150,000	750,000

PLANT CAPACITY

0.8 - 1 Million MTA, C₂H₄

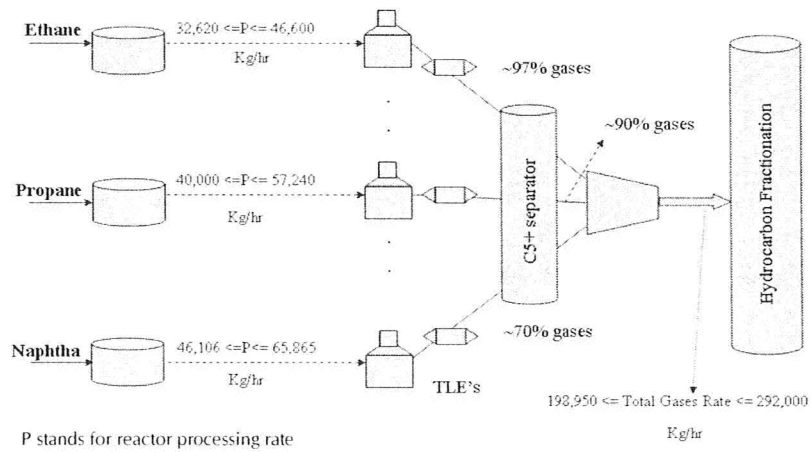


Figure 3-5: Plant capacity details

3.7 Typical scheduling simulation result

Let us look at a scenario with two furnaces cracking naphtha feed. Based on the initial conditions on the coke state, there is already 250 kg of coke deposited in both the reactors. The maximum limit for tube metal temperature is 1050⁰ C, which corresponds to 300 kg of coke deposited in the furnace. Demand for ethylene over a period of 90 days is a maximum of 49,500,000 kg, and demand for propylene is unlimited.

In simulation based scheduling, it is important to know that the main decisions variables that affect the plant economics (e.g. conversion, steam to hydrocarbon, feed flowrates) have to be determined by the engineer. For unlimited propylene sales, guidelines would generally select low severity and low steam to hydrocarbon ratio because this operation will be close to the propylene yield peak. Therefore, for this scenario, we have fixed the severity to a conversion of 82% and steam to hydrocarbon to 0.5. The processing rates in the reactors are then selected appropriately to meet the product demands. Finally, decokes will be performed when the coke limit is reached.

Based on these conditions, the maintenance schedule obtained by simulation is shown in Figure 3-6. The production rates of the key products – ethylene and propylene – are plotted versus time, but all products are modeled and included when calculating the economic performance. The furnace (reactor) status – either processing feed or decoking – is also plotted versus time. Finally, the coke accumulation in each reactor is plotted versus time. The schedule predicts the plant behaviour for 90 days.

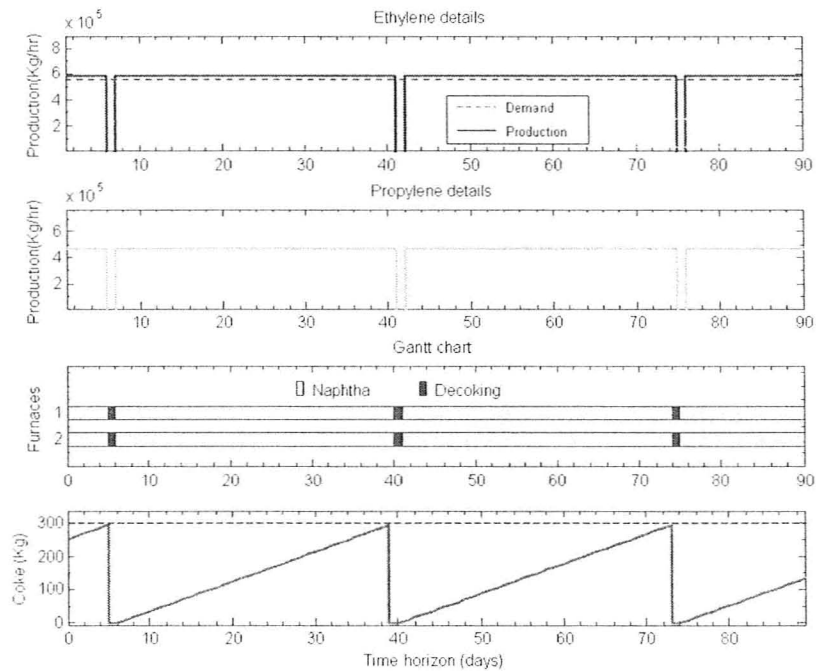


Figure 3-6: Direct simulation results

From the results, it is clear that both the reactors have to be decoked on the same day leaving no option for production in the plant during that day. This is because the same severity in both the reactors leads to equal accumulation of coke and since both of them had same initial coke condition, the day for decoking turned out to be the same. This can be seen from the coke accumulation part of the graph where the coking contours for both reactors are identical and appear to be a single line.

These results are unacceptable, because the entire plant would have to shutdown for the decoking time. The time and cost for restarting the plant are very high, so high that the optimizer will not allow such a schedule, and full plant start-up costs are not included in the model.

Simulation case studies require the engineer have the intelligence to overcome this infeasibility condition (no production condition), as well as economically optimize

the variables. The person has to make appropriate changes to the schedule to make it feasible for implementation. He/she can choose an early decoke for furnace 1 and the result of such a change on the overall schedule can be seen in Figure 3-7.

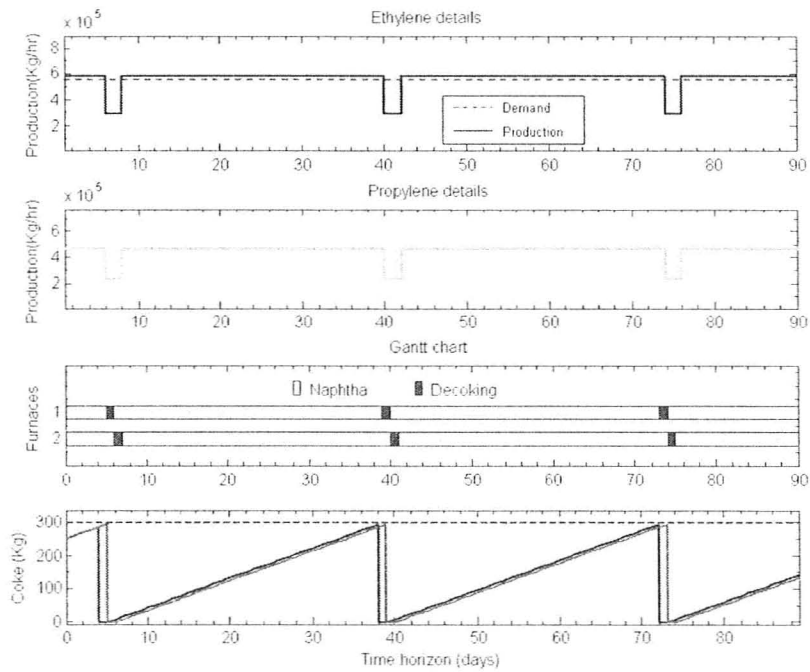


Figure 3-7: Schedule after operators changes

Clearly this is a feasible schedule suitable for implementation. However, we cannot say if this is the most profitable schedule. We need to try various combinations of flowrates, severity and selectivity values to find a profitable solution. Arguably, this is a tedious process.

An optimal scheduling model such as the one introduced in the next chapter would have the intelligence of looking for feasibility and optimality. It would react to any condition in the following ways.

To maintain feasibility, it can

- Adjust reactor operation, and
- Decoke early

To maximize Plant profit, it can

- Adjust reactor operation (change the severity or S/HC),
- Decoke optimally,
- Choose feed appropriately, and
- Choose the number of reactors in service.

This scenario is also considered in the case studies (Section 4.5.1.4) of Chapter 4, where optimal results are discussed and compared with these simulation results.

3.8 Summary

The challenges posed by ethylene plant furnace scheduling are clearly identified in this chapter. An integrated scheduling approach is deemed necessary to capture the interaction between furnace operation and maintenance. While developing a scheduling model, tailored formulation schemes should be used to preserve the linearity of the scheduling model without losing nonlinear information in the yield and coking models. Unfortunately, a well developed scheduling model inevitably ends up in a large scale MILP, posing computational difficulties. Therefore, appropriate solution heuristics may be needed to reduce the computational time. More details on the mathematical model development and solution strategies are discussed in the next chapter.

Chapter 4. Open-loop Scheduler formulation

The main emphasis of this chapter is on the mathematical modelling of the open-loop scheduler and testing its performance through various case studies. First, an overview of the scheduling model is presented in this chapter with discussion on the importance of preserving linearity and on the techniques used for that purpose. Details of the scheduler are presented next followed by detailed mathematical formulation of the optimization model. Tailored constraint formulation and solution heuristics proposed to help improve the computational time are also discussed in this chapter. Finally, several open loop case studies are considered, and the results discussed in detail for single feed and multiple feed scenarios.

4.1 Model overview

As discussed in Chapter 3, the open-loop scheduling model leads to a mixed integer optimization problem with continuous variables to model reactor operating conditions and integer variables to model feed allocation, furnace operation and decoking. We have also seen that there are significant nonlinearities in the yield and coking model relating to reactor conditions. These nonlinearities in the scheduling model could lead to a Mixed Integer Nonlinear Programming problem (MINLP), which is a difficult problem to solve for the size of the our scheduling problem.

Therefore, our main objective here is to preserve the model linearity, so that the resulting scheduling model can be formulated as a Mixed Integer Linear Programming problem (MILP). Model linearity is preserved for several reasons, such as (1) Linear relaxations are convex problems, (2) State-of-the-art MILP solvers are available (CPLEX, XPRESS etc).

In order to preserve model linearity, we used discrete time representation for model formulation and adopted disjunctive modelling technique to handle the nonlinearity in the yield profiles. The concepts behind the linear formulation are discussed in the next sub-sections and then, details of the formulation are given in Section 4.2.

4.1.1 Discrete time formulation

Discrete time formulation is based on the concept of dividing the time horizon into a finite number of uniform or non-uniform time intervals of predefined durations and modelling the scheduling tasks only at the boundaries of each time interval.

The most notable feature of this formulation is that time is modelled as a reference grid and is defined as a parameter in the optimization problem. Therefore, we avoid nonlinear constraints due to time representation in scheduling models. With this reference grid, we can formulate difficult scheduling constraints easily. The only disadvantage with these models is that they lead to a large number of binary variables. The number of binary variables in these models scales proportionally with the time intervals in the scheduling horizon, thus making the models computationally expensive. However, a better formulation with tailored heuristics can eliminate this difficulty, making the discrete time models best suitable for large scale scheduling applications (Schulz et al., 2006, Kelly, 2005 and Lim et al., 2006).

4.1.2 Disjunctive modelling

In an attempt to capture the nonlinearity, in the yields and coking rates, using linear constraints without compromising on losing the nonlinear information, the concept of disjunctive programming (Williams, 1985) was employed. The main idea of disjunctive programming is to first formulate several alternative linear disjunctive models for a system. These alternatives could be different process technologies or as in this case,

different operating conditions for an existing process. The typical disjunctive modelling approach selects one disjunctive model using binary variables. In this research, the disjunctive models approximate the nonlinear reactor yields with a set of linear yields at specific reactor operating conditions. Therefore, selecting one disjunctive model is equivalent to selecting one from several operating conditions, although the operating conditions are continuous in the real plant and in the underlying nonlinear model.

As an example, let us recollect the nonlinearities in the yield profiles of propane feedstock, which is shown in Figure 3-4. To approximately capture the nonlinearities in those yields, eight disjunctive models were formulated as shown in Table 4-1. Each disjunctive model corresponds to a particular conversion and S/HC ratio, which represents one operating condition for a reactor. Therefore, selecting a disjunctive model is equal to choosing a particular furnace operation. This selection can be accomplished by using binary variables in the scheduling model.

Table 4-1: Disjunctive models for Propane feed

Disjunctive models	S/HC (ratio)	Conversion (%)	COT ($^{\circ}$ C)	Coking rate (Kg/day)
Propane1	0.4	70	814.31	7.56
Propane2	0.4	80	825.85	9.63
Propane3	0.4	90	840.42	11.62
Propane4	0.4	95	851.37	12.61
Propane5	1	70	832.57	6.85
Propane6	1	80	844.50	8.51
Propane7	1	90	859.57	10.07
Propane8	1	95	870.91	10.86

Although disjunctive programming captures the nonlinear relationship using linear constraints, the main disadvantage with this technique is that it requires binary variables to make the selection of a single disjunctive model. As discussed earlier, binary variables are very critical to any optimization problem as they are directly related to the computational burden of the optimization problem.

Initial computational experience validated our expectation that adding many thousands of binary variables to select the reactor operations for many reactors, feed types and time steps yielded intractable optimization problems. While a very small problem might be solved within reasonable computing times, large problems required more than one day of computing time. A few cases studies are described in Appendix B.

Therefore, we evaluated a simplified alternative formulation in which all disjunctive reactor models could be selected, i.e., have non-zero feed rates. This approach is formulated by removing the integer variables that require only one disjunctive model to be selected for a specific feed material to a reactor in a time period. This formulation has dramatically fewer integer variables and could be implemented in the real plant under two situations. First, if the optimal solution had non-zero feed flows in only one of the disjunctive models, the result can be directly implemented. Secondly, if the solution contains non-zero feed flows to “adjacent” operating conditions, an interpolated set of operating conditions could be implemented in the plant. By adjacent, we mean two conditions having the same conversion and different steam-to-hydrocarbon or different conversions and the same steam-to-hydrocarbon, with “different” referring to only one entry different in Table 4-1. If one of these situations does not occur, the optimal solution could not be implemented in the real plant. Further details on the valid combinations are elaborated in Appendix B.

Extensive computational experience with this problem has shown that the optimum operating condition corresponds to a single disjunctive model, i.e., that only one disjunctive model (at most) has a non-zero feed flow rate. Therefore, using the integer variables to restrict the selection of disjunctive models are not required to obtain the global optimum of the problem. If more than one “non-adjacent” model were selected, some integer variables would have had to be added and the problem resolved; to reiterate, this did not occur in this research.

4.2 Scheduler details

Using the discrete time representation and disjunctive modeling techniques, the scheduler is formulated as a deterministic MILP model. The inputs and outputs of the scheduling optimizer (scheduler) are shown in Figure 4-1. Outputs are the decision variables of the optimization model, and inputs are the initial conditions (furnace coke conditions), model parameters and other parameters necessary to define the problem scenario (sales demands, economics, furnace availability, and so forth).

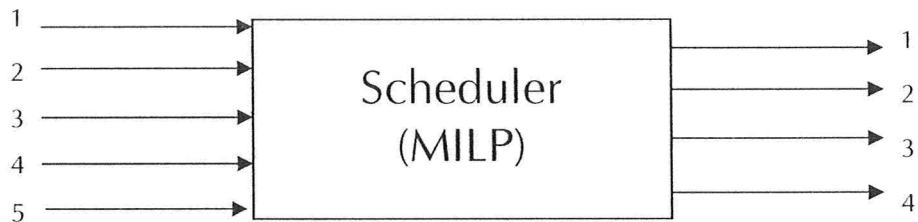


Figure 4-1: Inputs and outputs of the Scheduler

Inputs (parameters)		Outputs (optimization variables)	
1	Initial process conditions (Coke, severity, S/HC, available feeds and number of furnaces)	1	Feedstock to each reactor
2	All constraint values, e.g., Product demand and sales limits	2	Feed flow rates
3	End conditions	3	Reactor severities
4	Time horizon	4	Reactor selectivities (S/HC)
5	Economics		

4.3 Mathematical formulation

4.3.1 Basic formulation

In this formulation, continuous variables are used to represent the quantity of material flow, coke accumulation, and the operating conditions (Severity, S/HC) in the reactors. Binary variables are used to select appropriate feedstock for cracking, to decide the optimal number of furnaces in service and to initiate a furnace shutdown for deocking. Variables and parameters declared in the model are defined as follows:

Indices

i	Feedstock, $i = 1, \dots, NF$
j	Reactor, $j = 1, \dots, NR$
k	Disjunctive model, $k = 1, \dots, ND_i$
c	Product component, $c = 1, \dots, NP$
t	Time period, $t = 1, \dots, NT$

Where the set dimensions are,

NF	Number of feeds
NR	Number of reactors
ND_i	Number of disjunctive models for cracking feed i
NP	Number of products
NT	Number of discrete time intervals within the specified time horizon ($NT = Thorz/\Delta t$)
Thorz	Time horizon (hrs)

Δt Duration of each time interval (hrs)

Continuous Variables

F_{it}	Flow rate of fresh feed i at time t (Kg/hr)
$FRcy_{it}$	Flow rate of the recycled feed i at time t , for cracking (Kg/hr)
$frcy_{it}$	Flow rate of feed i at time t , recycled to the storage tank (Kg/hr)
Rcy_Inv_{it}	Inventory of feed i at time t , in the recycle storage tank
P_{ijt}	Processing rate of feed i in reactor j at time t (Kg/hr)
PD_{ijkt}	Processing rate of feed i in disjunctive model k corresponding to reactor j at time t (Kg/hr)
X_{ijkt}^d	Fraction of flow through each disjunctive model w.r.t. the maximum processing rate
σ_{ijkt}^{disj}	Adjusted fraction of flow through each disjunctive model
S_{ijkt}^d	Slack variable used in the disjunctive model constraint
$PRate_{ijkct}$	Production rate of product c , while cracking feed i in disjunctive model k corresponding to reactor j at time t (Kg/hr)
$Prod_c$	Amount of product c produced from all the reactors during the defined time horizon (Kg)
$E_t^{compressor}$	Energy required for a compressor in a single train compression system at time t (KJ/hr)

E_{jt}^{furnace}	Energy required for cracking in furnace j at time t (KJ/hr)
F_{ijt}^{HPsteam}	Flow rate of high-pressure steam generated while cracking feed i in reactor j at time t (Kg/hr)
F_{ijt}^{MPsteam}	Flow rate of medium-pressure steam generated while cracking feed i in reactor j at time t (Kg/hr)
Coke_{jt}	Coke deposited in reactor j at time t (Kg)
ΔCoke_{ijkt}	Coke deposited in the disjunctive model k corresponding to reactor j while cracking feed i in time Δt (where, Δt is the time period) (Kg)
ΔDecoke_{jt}	A large decoke variable used to erase the total coke in the reactor j at time t when de-coke is active. (Kg)
Tw_{jt}	Tube wall temperature of reactor j at time t ($^{\circ}\text{C}$)
s_{ijt}^c	Slack variable used in the decoking model
Inv_{ct}	Inventory of product c at time t (Kg)
Sales_{ct}	Sales of product c at time t (Kg/hr)
$\text{Penalty}^{\text{coke}}$	Penalty term for coke accumulated at the end of time horizon (\$/Kg)
$\text{Penalty}^{\text{Rcy_Inv}}$	Penalty term to minimize the cost associated with recycle feed inventory in the model (\$/Kg)

Binary variables

Variables to model Feedstock allocation

$$W_{ijt} = \begin{cases} 0 & \text{When feed } i \text{ is not allocated to reactor } j \text{ at time } t \text{ for} \\ & \text{cracking} \\ 1 & \text{When feed } i \text{ is allocated to reactor } j \text{ at time } t \text{ for cracking} \end{cases}$$

Variables to model furnace decoking

$$\delta_{jt}^{\text{decoke}} = \begin{cases} 0 & \text{Normal operation of reactor } j \text{ at time } t \\ 1 & \text{Decoking of reactor } j \text{ at time } t \end{cases}$$

Variables to model the number of furnaces in service

$$\delta_{jt}^{\text{shutdown}} = \begin{cases} 0 & \text{Reactor } j \text{ in operation at time } t \\ 1 & \text{Reactor } j \text{ shutdown at time } t \end{cases}$$

Parameters

P_{ij}^{\min}	Minimum processing rate of feed i in reactor j (Kg/hr)
P_{ij}^{\max}	Maximum processing rate of feed i in reactor j (Kg/hr)
X_{ijkc}	Weight fraction of product component c , in disjunctive model k corresponding to reactor j while cracking feed i
E_{ijk}	Energy required in disjunctive model k corresponding to reactor j while cracking feed i (KJ/Kg)

$RCoke_{ik}$	Coking rate corresponding to disjunctive model k while cracking feed i (Kg coke/hr)
$\rho_{ik}^{S/HC}$	Steam to hydrocarbon ratio for feed i corresponding to disjunctive model k
$\rho_{ik}^{Severity}$	Severity for feed i corresponding to disjunctive model k
MW_c	Molecular weight of component c
$Cost_c^{product}$	Cost of product c (\$/Kg)
$Cost_i^{feed}$	Cost of feed i (\$/Kg)
$Cost_{steam}^{dilution}$	Cost of dilution steam (\$/Kg)
$Cost_{energy}^{furnace}$	Cost of furnace energy (\$/KJ)
$Cost_{energy}^{compressor}$	Cost of compressor energy (\$/KJ)
$Cost_{steam}^{HP}$	Cost of high-pressure (HP) steam (\$/Kg)
$Cost_{steam}^{MP}$	Cost of medium pressure (MP) steam (\$/Kg)
$Cost_{changeover}^{furnace}$	Cost of furnace changeover/maintenance (\$)
Δt^{decoke}	Duration of a decoke operation (hrs)
c_p	Heat capacity of steam (1.937 KJ/Kg.K)
$T_2^{HPsteam}$	Temperature of the generated high-pressure steam (586.6 ⁰ K)
$T_2^{MPsteam}$	Temperature of the generated medium-pressure steam (514.9 ⁰ K)
T_1	Feed water temperature used to generate high-pressure and medium-pressure steam (323.150 ⁰ K)
$G^{HPsteam}$	Constant used for the calculation of flow-rate of high-pressure

	steam, $\frac{1612.572}{c_p(T_2^{\text{HPsteam}} - T_1)}$ (Kg steam/Kg reactor effluent)
G^{MPsteam}	Constant used for the calculation of flow-rate of medium-pressure steam, $\frac{602.721}{c_p(T_2^{\text{MPsteam}} - T_1)}$ (Kg steam/Kg reactor effluent)
$\text{Coke}_j^{\text{max}}$	Maximum limit on deposited coke for reactor j (Kg)
M	Constant (Big-M type) used in the decoking model to erase coke (300 Kg)
T_j^{max}	Maximum limit on tube wall temperature for reactor j ($^{\circ}\text{C}$)
$\text{Coke}^{\text{initial}}$	The amount of coke in the reactor at time 0 (Kg)
$\text{Demand}_c^{\text{min}}$	Minimum demand for component c (Kg/time horizon)
$\text{Demand}_c^{\text{max}}$	Maximum demand for component c (Kg/time horizon)
$\text{Inv}_c^{\text{min}}$	Minimum inventory for component c (Kg)
$\text{Inv}_c^{\text{max}}$	Maximum inventory for component c (Kg)
τ	Number of reactors allowed to decoke in a coarse time grid
η	Minimum number of days a reactor should operate before decoke, taken from operators experience.
β	Maximum number of decokes possible in a defined time horizon, from operators experience
γ	Number of days before which decoking is not possible (days)
α	Days at the beginning of horizon when a decoking is compulsory (days)

$\text{Coke}_{\text{allowed}}^{\text{decoke}}$	The amount of coke allowed to accumulate (to avoid premature decokes) before each possible decoke (Kg)
$\text{Coke}_{\text{endcondition}}^{\text{decoke}}$	The amount of coke that cannot be exceeded at the end of the time horizon (Kg)
λ	Penalty coefficient for Inventory of recycled ethane (0.001 \$/Kg)
T_w^{const}	Parameter used in the Tube wall temperature model ($0.37 \text{ }^0\text{K/Kg}$)

Constraints

A list of conditions that are modeled as constraints in the scheduling model are summarized first.

- Only one feed can be cracked in a furnace at any time;
- Feedstock cannot be switched during normal operation;
- Account for mass flow rates of all the components leaving a reactor;
- Model the non-linear relationships (yields and coking) using linear disjunctive constraints;
- Account for recycled ethane during cracking;
- Account for energy required in furnace and compressor;
- Model coking in the reactors and the corresponding tube metal temperatures;
- While decoking, consider complete cleanup of the reactors (i.e. coke =0 after cleaning);
- No more than one reactor can be decoked at any time;
- Consider the end point conditions on the coke accumulated in the reactors;
- Integrated demand over the time horizon should be met.

The associated constraints in the mathematical formulation are discussed as follows.

Feedstock allocation

The condition that no more than one feedstock can be cracked in a particular reactor at any time is modeled using a binary allocation variable, as shown in equation (4.1). Also, the condition that feedstock switching is not allowed between decokes is modeled as equation (4.2). The constraint ensures that there is no feedstock switching during the normal plant operation. It can occur only after the reactor is decoked.

$$\sum_i W_{ijt} \leq 1 \quad \forall j, t \quad (4.1)$$

$$W_{ijt-1} - W_{ijt} \leq \delta_{jt}^{\text{decokc}} \quad \forall i, j, t = 2..NT \quad (4.2)$$

Equations (4.3) specifies the bounds on the reactor processing feed rates. It models the condition that the processing rate for a feed i is zero when it is not allocated to a reactor j at time t .

$$P_{ij}^{\min} \cdot W_{ijt} \leq P_{ijt} \leq P_{ij}^{\max} \cdot W_{ijt} \quad \forall i, j, t \quad (4.3)$$

Reactor operation

Feed balance constraints

The total amount of feed processed into the reactors is equal to the amount of fresh feed plus the recycled feed, given as equation (4.4). Only ethane in the products is recycled back for subsequent cracking. One of the reactors is allocated exclusively to crack recycled ethane. Whenever, the dedicated ethane cracker is scheduled for maintenance, the recycled ethane has to be stored for subsequent cracking. This recycle storage is modeled using equations (4.4 to 4.6). The amount recycled to the storage ($frcy_{it}$) is given by equation (4.5). The inventory in the recycle storage is then modeled as equation (4.6), which is penalized in the objective function to minimize the cost

associated with inventory. This ensures that inventory is always zero except during decoke. It was found that the penalty does not affect the total fresh ethane feed purchase, operating conditions, or end conditions for the recycle inventory; however, it reduces the ethane recycle inventory to its minimum at every time throughout the horizon which smoothes variation in fresh and recycle flow rates. A schematic of recycle stream and inventory is shown in Figure 4-2

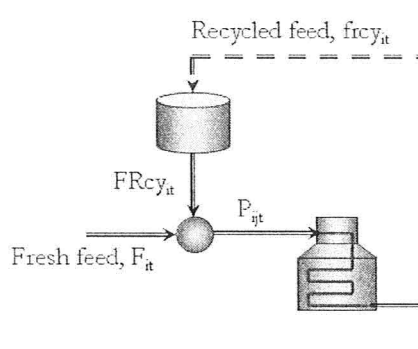


Figure 4-2: Recycle stream and inventory

$$F_{it} + FRcy_{it} = \sum_j P_{ijt} \quad \forall i, t \quad (4.4)$$

$$frcy_{it} = \sum_j \sum_k PD_{ijkt} \cdot X_{ijkc} \quad c = \text{ethane}, \forall t \quad (4.5)$$

$$Rcy_Inv_{it} = Rcy_Inv_{it-1} + frcy_{it} - FRcy_{it} \quad i = \text{ethane}, \forall t \quad (4.6)$$

Disjunctive reactor model constraints

As discussed earlier, these constraints model the nonlinear patterns in yields and coking using a set of linear algebraic equations. To achieve this, the operating conditions in each reactor are first divided into k disjunctive models, and the optimizer decides to choose one model. We know that, each disjunctive model represents a combination of Severity and S/HC ratio. Therefore, selection of feed rate to a particular disjunctive model decides the operating condition in that reactor. In other words, the flow through each disjunctive model will reflect the selected operating condition. If the fraction of flow

is equal to 1 for a particular disjunctive model, it means that only this model (operating condition) is selected. Alternatively, if more than one disjunctive models share the fraction of flow, then the operating condition can be calculated by interpolation. A schematic is shown in Figure 4-3.

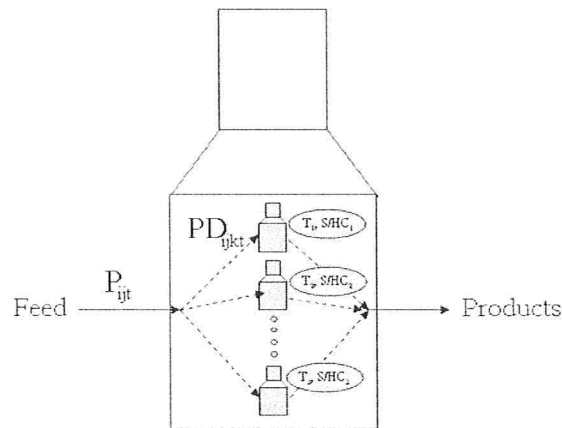


Figure 4-3: Disjunctive reactor conditions

Disjunctive operation is modeled as equation (4.7).

$$\sum_k PD_{ijkt} = P_{ijt} \quad \forall i, j, t \quad (4.7)$$

The flow through disjunctive models is used in the yield model to calculate the amount of products produced as shown below.

Product flow rates

Based on the disjunctive model flowrates, production rates of the components are obtained by the product of disjunctive model flowrates times the component yields as shown in equation (4.8). The yield data is taken from curves similar to Figure 3-4; the data used for the disjunctive models is reported in Appendix A. The amount of product produced from all the reactors at any time is given by equation (4-9).

$$PRate_{ijkct} = PD_{ijkt} \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (4.8)$$

$$\text{Pr od}_{ct} = \sum_i \sum_j \sum_k \text{PRate}_{ijkct} \quad \forall c, t \quad (4.9)$$

Fraction of flow through disjunctive reactors

The fraction of flow for each disjunctive operation is required in the coking model. As stated earlier, each disjunctive model is related to a particular operating condition and hence to a particular coking rate. To calculate the coking rate associated with the selected disjunctive operation, we need to calculate the fraction of flow through the disjunctive reactors. It can be modeled as shown in equation (4-10). Unfortunately, equation (4.10) is nonlinear.

$$\text{PD}_{ijkt} = x_{ijkt}^d \cdot P_{ijt} \quad \forall i, j, k, t \quad (4.10)$$

Since our aim is to develop a linear MIP, we propose an approximation scheme here that maintains model linearity with minimal effect on the model accuracy. Equations (4.11 – 4.16) replaces equation (4.10) and enforces the procedure to calculate the fraction of flow.

$$\text{PD}_{ijkt} = x_{ijkt}^d \cdot P_{ij}^{\text{max}} \quad \forall i, j, k, t \quad (4.11)$$

$$\sum_k x_{ijkt}^d \leq 1 \quad \forall i, j, t \quad (4.12)$$

$$x_{ijkt}^d + s_{ijkt}^d = \sigma_{ijkt}^{\text{disj}} \quad \forall i, j, k, t \quad (4.13)$$

$$\sum_k \sigma_{ijkt}^{\text{disj}} = 1 \quad \forall i, j, t \quad (4.14)$$

$$\sum_k s_{ijkt}^d = \sum_k \sigma_{ijkt}^{\text{disj}} - \sum_k x_{ijkt}^d \quad \forall i, j, t \quad (4.15)$$

$$0 \leq s_{ijkt}^d \leq 1 \quad \forall i, j, k, t \quad (4.16)$$

First, the fraction of flow through each disjunctive model is calculated relative to the maximum processing rate as shown in equation (4.11). Second, additional variables are introduced in the form of slack variables (s_{ijkt}^d) and new disjunctive model flow fraction variables (σ_{ijkt}^{disj}) that will be used in the coking model. Note that it is not necessary to penalize these slacks variables in the objective function as they are used to ensure model feasibility. They are related to (x_{ijkt}^d) as shown in equation (4.13) while also observing equation (4.14); therefore, the new variables sum to one. Finally, the bounds on the slack variables are decided by equations (4.15 and 4.16). Hence, variables (σ_{ijkt}^{disj}) are the approximate fractions of flow through the disjunctive models.

As long as a single disjunctive model (or operating condition) is picked by the optimizer, this model ensures that there is no error in this approximation, i.e., x_{ijkt}^d equals σ_{ijkt}^{disj} . However, whenever multiple disjunctive models are picked by the optimizer, there is a small error in the fraction that is processed at each disjunctive reactor operating conditions (σ_{ijkt}^{disj}). The maximum error was found to be approximately 0.05%, which leads to an error of 1 hr for a 30 day run length. This is negligible for the scheduling horizon (90 days) considered in the model.

Equations (4.11 – 4.16) provide a conceptual approach to approximate the fraction of flow through each disjunctive model using linear constraints. However, to comply with feedstock allocation constraints, equation (4.12) should be replaced by equation (4.17), and to comply with decoke model constraints and guarantee model feasibility, equation (4.16) must be replaced by equations (4.18, 4.19).

$$\sum_k \sigma_{ijkt}^{disj} \leq W_{ijt} \quad \forall i, j, t \quad (4.17)$$

$$0 \leq s_{ijkt}^d \leq x_{ijkt}^d + \delta_{jt}^{decoke} \quad \forall i, j, k, t \quad (4.18)$$

$$0 \leq s_{ijkt}^d \leq W_{ijt} \quad \forall i, j, k, t \quad (4.19)$$

Coking and Tube wall temperature

Coking model constraints

The amount of coke in a reactor at any time t , is modeled as the coke present at time $t-1$ plus the coke accumulated during the current time interval. This constraint is modeled as equation (4.20). The coking rate depends upon the disjunctive operation. Therefore, the amount of coke accumulated during any time interval t is calculated using the selected severity and the corresponding coking rate data. This is written as equation (4.21).

$$\text{Coke}_{jt} = \text{Coke}_{j,t-1} + \sum_i \sum_k \Delta \text{Coke}_{ijkt} \quad \forall i, j, t \quad (4.20)$$

$$\Delta \text{Coke}_{ijkt} = (\text{Rcoke}_{ik} \cdot \sigma_{ijkt}^{\text{disj}}) \cdot \Delta t \quad \forall i, j, k, t \quad (4.21)$$

Equation (4.21) is the reason that we needed to evaluate the flow fraction variables ($\sigma_{ijkt}^{\text{disj}}$). It is assumed that coke is additive in two disjunctive models. Also, note that in this model coke is not proportional to the reactor hydrocarbon feed rate.

Tube wall temperature constraints

Since coke cannot be measured directly, the industrial practice is to infer its value using the tube wall temperature measurement. Tube wall temperature depends upon the current reactor coke and the disjunctive operation that is achieved adjusting the reactor outlet temperature to give the required severity or conversion. It increases with the accumulated coke in a reactor. Therefore, it is correlated with the accumulated coke and the clean tube wall temperature as equation (4.22).

$$Tw_{jt} = \sum_i \sum_k (Tw_{ik}^{clean} \cdot \sigma_{ijkt}^{disj}) + Tw^{const} \cdot Coke_{jt} \quad \forall j, t \quad (4.22)$$

Threshold limits

These are the limits that are imposed on the accumulated coke and the tube wall temperature to trigger a decoke operation. They are basically the upper bounds on the accumulated coke and the tube wall temperature of a reactor, which should not be violated in the model. These restrictions can be posed as equations (4.23 and 4.24).

$$Coke_{jt} \leq Coke_j^{max} \quad \forall i, j, t \quad (4.23)$$

$$Tw_{jt} \leq T_j^{max} \quad \forall i, j, t \quad (4.24)$$

These limitations require that a furnace be decoked before the bound has been violated.

Energy requirement constraints

The amount of energy required for cracking in furnace j at time t is modeled as equation (4.25) and the energy required by a compressor (in a single train compression system) at time t is modeled as equation (4.26). It should be noted that in this model, furnace energy required depends on the disjunctive model (operating condition) selection.

$$E_{jt}^{furnace} = \sum_i \sum_k PD_{ijkt} \cdot E_{ijk} \quad \forall j, t \quad (4.25)$$

$$E_t^{compressor} = \sum_i \sum_j \sum_k \sum_c \left(\frac{PRate_{ijkct}}{MW_c} \right) * E^{comp} \quad \forall t \quad (4.26)$$

Energy of compression assumes a constant compressibility and efficiency and constant inlet and outlet pressures. Therefore, it is a linear function of molar flow rate.

High pressure (HP) and Medium pressure (MP) steam flowrates

Hot cracked gases exiting from the reactors at 800-900⁰ C are immediately cooled in the transfer line exchangers (TLE's) to quickly reduce the temperature so that no further reactions takes place. During this cooling process, heat is recovered to generate HP and MP steam that is used for various purposes within the plant. The generated steam flow rates are related to the processing rates in the reactors as shown in equations (4.27, 4.28).

$$F_{ijt}^{HP\text{steam}} = P_{ijt} \cdot G^{HP\text{steam}} \quad \forall i, j, t \quad (4.27)$$

$$F_{ijt}^{MP\text{steam}} = P_{ijt} \cdot G^{MP\text{steam}} \quad \forall i, j, t \quad (4.28)$$

Decoking constraints

The time required for decoking is considered to be 1 day. Decoking can be performed at anytime when the tube wall temperature and the accumulated coke in the reactors are within the threshold limits. However, while scheduling a decoke operation, it is important to ensure that at any time, no more than one reactor is taken offline for maintenance. This will ensure that there is sufficient uninterrupted and continuous product flow in the plant at all times. The decoke decision is modeled using binary variables with the above described constraint posed as equation (4.29). Also one should ensure that when a reactor is decoked, (i) the hydrocarbon flow through the reactor is zero, and (ii) the accumulated coke is completely cleaned. These constraints are posed as equations (4.30) and (4.31) respectively. The accompanying variables in equation (4.31) are described in equations (4.32) and (4.33).

$$\sum_j \delta_{jt}^{\text{decoke}} \leq 1 \quad \forall t \quad (4.29)$$

$$P_{ij}^{\min} \cdot (1 - \delta_{jt}^{\text{decoke}}) \leq P_{ijt} \leq P_{ij}^{\max} \cdot (1 - \delta_{jt}^{\text{decoke}}) \quad \forall i, j, t \quad (4.30)$$

$$\text{Coke}_{jt} = \text{Coke}_{j,t-1} + \sum_i \sum_k \Delta \text{Coke}_{ijkt} - \Delta \text{Decoke}_{jt} + s_{jt}^c \quad \forall i, j, t \quad (4.31)$$

$$M \cdot \delta_{jt}^{\text{decoke}} \leq \Delta \text{Decoke}_{jt} \leq M \cdot \delta_{jt}^{\text{decoke}} \quad \forall i, j, t \quad (4.32)$$

$$0 \leq s_{jt}^c \leq M \cdot \delta_{jt}^{\text{decoke}} \quad \forall i, j, t \quad (4.33)$$

It is clear from these constraints that at any time t , when a reactor j is decoked, $\delta_{jt}^{\text{decoke}} = 1$ and therefore $\Delta \text{Decoke}_{jt}$ takes a value equal to M from equation (4.32), where M is a sufficiently large value chosen to eliminate the accumulated coke in the reactor, i.e., to make the variable Coke_{ijt} in equation (4.31) equal to 0. A slack variable s_{ijt}^c is added to ensure that Coke_{ijt} exactly takes a value equal to 0. Since coke accumulation is bounded to be non-negative, the decoke task cannot reduce coke below 0; since an economic debit occurs for any coke accumulation, the coke at the end of a decoke task will always be 0. Alternatively, when no reactor is decoked, $\delta_{jt}^{\text{decoke}}$ is 0 and both $\Delta \text{Decoke}_{ijt}$, s_{ijt}^c are 0; thus, equation (4.31) becomes equation (4.20). Therefore, equation (4.31) and not (4.20) is used in the scheduling optimizer.

Product inventory and sales constraints

The products obtained from the plant are transported through pipelines for sale and any excess amounts are stored in the inventory tanks. The model for the product inventory is given by equation (4.34) whereas the bounds on the inventory are given by equation (4.35). Additional flexibility can be added to the inventory by proposing either hard constraints or soft constraints. The sales depend on the predicted demands.

The plant cannot produce a constant rate of products because of periodic furnace decokes. Therefore, the sales are specified as total production over a period, which for this study in the output horizon of 90 days. Bounds on the integrated sales are shown in equation (4.36).

$$Inv_{ct} = Inv_{ct-1} + Prod_{ct} - Sales_{ct} \quad \forall c, t \quad (4.34)$$

$$Inv_c^{\min} \leq Inv_{ct} \leq Inv_c^{\max} \quad \forall t \quad (4.35)$$

$$Demand_c^{\min} \leq \sum_t Sales_{ct} \leq Demand_c^{\max} \quad \forall c \quad (4.36)$$

In ethylene plants products are stored as gas in an underground cavern or in liquefied form in a tank. In all our case studies, no inventory (or storage) of products was considered. Inventory (Inv_{ct}) in equation (4.34) was assumed to be zero at all times. This means that in this model, all the products are sold as they are being produced. Equation (4.36) is included to define the integrated product demand.

End point conditions

End conditions are the requirements that are imposed at the end of the time horizon. In the current study, end conditions are related to the amount of coke accumulated in the reactors. From computational experience, it was clearly evident that the optimal solution was unrealistic without the end conditions. Therefore, the end conditions described in this sub-section were always included in the scheduling model (with the exception of one case study to demonstrate the need for the end conditions).

There are two end conditions on the coke. The first condition is to ensure a feasible operational state at the end of the horizon, so that future operation remains feasible. This condition will make sure that two or more reactors do not require decoking during the first time period after the optimisation horizon ends i.e., ensuring that no two reactors are completely filled with coke at the end of the time horizon. A rigorous way of modelling this condition would require additional binary variables. Therefore, an alternative approach that reduces flexibility slightly using only continuous variables is proposed. This approach involves a hard constraint that must be strictly met for feasibility as shown in equation (4.37). This equation ensures that no two reactors are ready for

decoke at the end of the time horizon, thus enabling feasible operation beyond the specified time horizon. The value for $Coke_{\text{endcondition}}^{\text{max}}$ is calculated based on the number of furnaces in operation to allow feasible operation beyond the time horizon, as shown in equation (4.38).

$$Coke_{jNT} \leq Coke_{\text{endcondition}}^{\text{max}} \quad \forall j \quad (4.37)$$

$$Coke_{\text{endcondition}}^{\text{max}} = Coke^{\text{max}} - (Nfrs - 1) * Coke_{\text{accum/period}}^{\text{max}} \quad (4.38)$$

where, Nfrs is the number of furnaces in service, $Coke^{\text{max}}$ is the maximum coke allowed in a reactor before decoking, and $Coke_{\text{accum/period}}^{\text{max}}$ is the maximum coke accumulated during one time period.

The second end condition addresses the coke build up that will ultimately require decoking after the optimiser horizon. To define this end condition, a soft constraint is imposed by penalizing the amount of coke accumulated at the end of time horizon in the objective function. The penalty term as shown in equation (4.39) adds a cost that is proportional to the coke accumulation at the end of the optimiser horizon.

$$\text{Penalty}^{\text{coke}} = \frac{\sum_j Coke_{jNT}}{Coke_{\text{max}}} \cdot (\text{Cost}_{\text{decoke}}^{\text{energy}} + \text{Cost}_{\text{decoke}}^{\text{profitloss}}) \quad (4.39)$$

Typically, the cost associated with furnace decoke is the cost of energy required to completely cleanup coke. However, for instance if a furnace is scheduled to operate at full production capacity (and at its maximum severity), to meet the required product demand, a decoke under such a circumstance can incorporate a downtime of 1 day, leading to production loss, thus loss of profit. Both these terms are the costs associated with furnace decoke (i.e. to completely clean the coke ($Coke_{\text{max}}$) in the furnace); therefore, they are included in the penalty term as a cost proportional to the coke accumulation at the end of optimizer horizon. The energy costs are always present in the

penalty term; however, the costs related to profit loss are scenario specific. The profit loss is zero for scenarios where the integrated demand over the scheduling horizon can be met without operating the furnace at its full production capacity. The costs associated with both these terms for all the scenarios considered in this thesis are provided in Appendix B.

Sample optimisation results with and without penalty function (equation (4.39)) are shown in Figure 4-4. It is clear that without penalty, the optimizer avoids a second decoke at the end of the horizon. It does so by selecting a low severity (low temperature) for the reactor. This strategy is optimal for the fixed horizon, but it results in the decoking cost immediately after the horizon and lower overall profit. A more complete case study on the importance of end conditions is discussed in Section 4.5.1.1.

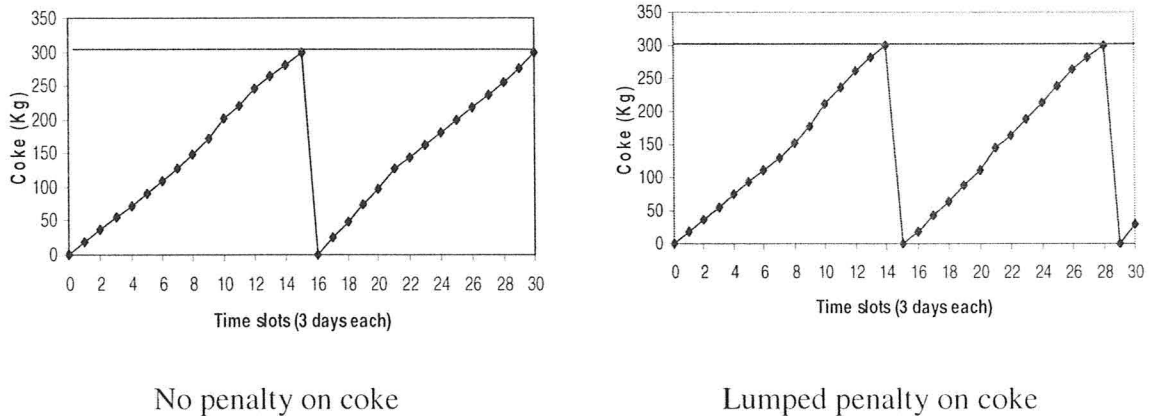


Figure 4-4: Sample results to highlight the importance of end conditions

Objective function

Since, the objective of this scheduling problem is to **maximize** the plant profit, an economic objective function is formulated in the model that is expressed as the plant profit less the penalties on coke and recycle feed inventory as shown in equation (4.40).

The plant profit is expressed in terms of the value of products, cost of feeds and other utility costs as shown in equation (4.41):

$$\text{Objective function} = \text{Plant Profit} - \text{Penalty}^{\text{Coke}} - \text{Penalty}^{\text{Recy_Inv}} \quad (4.40)$$

$$\begin{aligned} \text{Plant Profit} = & \text{Value of products} - \text{Cost of feedstocks} - \text{Cost of dilution} \\ & \text{steam} - \text{Cost of furnace energy} - \text{Cost of compressor energy} + \text{Value of} \\ & \text{HP and MP steam generated at TLE's} - \text{Cost for furnace decoke.} \end{aligned} \quad (4.41)$$

Details of each term in the profit equation are given as follows:

$$\text{Value of products} = \sum_t \sum_c \text{Sales}_{ct} \cdot \text{Cost}_c^{\text{product}} \quad (4.41a)$$

$$\text{Cost of feedstocks} = \sum_t \sum_i F_{it} \cdot \text{Cost}_i^{\text{feed}} \quad (4.41b)$$

$$\text{Cost of dilution steam} = \sum_t \sum_i \sum_j \sum_k \text{PD}_{ijkt} \cdot \rho_{ik}^{\text{S/HC}} \cdot \text{Cost}_{\text{steam}}^{\text{dilution}} \quad (4.41c)$$

$$\text{Cost of furnace energy} = \sum_t \sum_j E_{jt}^{\text{furnace}} \cdot \text{Cost}_{\text{energy}}^{\text{furnace}} \quad (4.41d)$$

$$\text{Cost of compressor energy} = \sum_t E_t^{\text{compressor}} \cdot \text{Cost}_{\text{energy}}^{\text{compressor}} \quad (4.41e)$$

$$\begin{aligned} \text{Value of HP and MP steam} = & \sum_t \sum_i \sum_j F_{ijt}^{\text{HPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{HP}} + \sum_t \sum_i \sum_j F_{ijt}^{\text{MPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{MP}} \\ & \quad (4.41f) \end{aligned}$$

$$\text{Cost for furnace decoke} = \sum_t \sum_j \delta_{jt}^{\text{decoke}} \cdot \text{Cost}_{\text{energy}}^{\text{decoke}} \quad (4.41g)$$

$$\text{Penalty}^{\text{Rcy_Inv}} = \lambda \cdot \sum_t \sum_i \text{Rcy_Inv}_{it} \quad (4.41h)$$

The objective function and all the constraints discussed so far forms the basic formulation of the scheduling model. The problem size for a case study involving 3 feedstocks and 5 reactors results in 3100 binary variables, 297794 continuous variables, 308629 linear constraints for a scheduling horizon of 90 days with 90 time intervals. When this MILP was attempted to solve using CPLEX, version 10.1, the solver initially had difficulties finding a feasible solution and eventually was unable to find the optimal solution in 100 hrs. This could be mainly attributed to the presence of large number of binary variables. Therefore, to enhance the computational time and make the model suitable for online computation, some constraints were reformulated and few tightening constraints were proposed. Details are discussed in the following sections.

4.3.2 Reformulated constraints

A couple of constraints were reformulated and included in the model. This was done to avoid the constraint structure that led to computational problems.

Feedstock allocation

Feedstock allocation is a discrete decision which should be made only when a cleaned reactor becomes available. Therefore, an alternative allocation constraint is modeled that can propagate the feedstock allocation decision during the normal plant operation and makes the allocation decision only when a cleaned reactor is available. This constraint as shown in equation (4.42) is included in the model . Furthermore, this constraint also ensures that there is no feedstock switching during the normal plant operation. Upon introducing this constraint, a logical modification has to be made for equation (4.1), as shown in equation (4.43). Therefore, equation (4.1) is replaced by equation (4.43) in the model.

$$W_{ijt} + \sum_{i' \neq i} W_{i'jt-1} \leq 1 \quad \forall i, j, t \quad (4.42)$$

$$\sum_i W_{ijt} \leq 1 \cdot (1 - \delta_{jt}^{\text{decoke}}) \quad \forall j, t \quad (4.43)$$

In equation (4.42), the summation is over all feedstocks (i) except the feedstock currently being processed in the reactor. The benefit of this constraint is to substantially reduce the feasible region, which should speed the branch and bound search.

Decoking model

As pointed out earlier, constraints (4.31 – 4.33) are used to model the cleaning of accumulated coke during a decoke operation. They have slack variables and big-M type constraints which were found to be computationally expensive from various trial runs. Therefore, those constraints are replaced by equations (4.44 – 4.46) to reduce computational time. This is done by eliminating the slack variables (s_{ijt}^c) and modifying the big-M type constraints.

$$\text{Coke}_{jt} = \text{Coke}_{jt-1} + \sum_k \Delta \text{Coke}_{jkt} - \Delta \text{Decoke}_{jt} \quad \forall j, t \quad (4.44)$$

$$0 \leq \Delta \text{Decoke}_{jt} \leq M \cdot \delta_{jt}^{\text{decoke}} \quad \forall j, t \quad (4.45)$$

$$0 \leq \text{Coke}_{jt} \leq \text{Coke}_{ij}^{\text{max}} \cdot (1 - \delta_{jt}^{\text{decoke}}) \quad \forall j, t \quad (4.46)$$

Since the economics require a decoke to remove all coke and negative coke accumulation is not possible, the slack was found to be unnecessary. It was found that the value of M in equation (4.45) affected the computational time. Experience has shown that large values of M needed more computational time. This made sense because large values of M result in larger feasible region; thus, requiring more time for the search. Therefore, in the model, the value of M was chosen to be no more than the maximum value of coke, i.e., 300 kg.

4.3.3 Tightening constraints

Several tightening constraints were formulated that incorporated process knowledge about the process and economics of an ethylene plant into the scheduling model. From computational experience these constraints were found to be very effective. Note that no additional assumptions are required when applying these constraints, except for the last constraint.

Minimum run length (η days) constraint

In general, operating a reactor at high severity leads to shorter run lengths and low severity leads to longer run lengths. Accordingly, if the maximum severity of operation in a reactor is known, it is possible to calculate the minimum run length for that reactor. In other words, one can estimate the minimum number of days (say η) a furnace should be in operation without decoking. This also means that only one decoke is possible in every (η) days.

The constraint, as shown in equation (4.47) is modeled as a rolling time window which assures that over the entire time horizon, at any time only one decoke is possible in η days. This is an important and very efficient tightening constraint, because it reduces the tree search significantly. For example, say the minimum run length is estimated as 20 days. If, a decoke is triggered at day 1, then this constraint will enforce the binary decoke variables in the next 19 days to take a no decoke value, thus reducing the feasible region and search time considerably.

$$\sum_{t'=t}^{t+\eta} \delta_{jt'}^{\text{decoke}} \leq 1 \quad \forall j, t \quad (4.47)$$

where, $\eta = \frac{\text{Coke}^{\text{max}} - \text{Coke}^{\text{clean}}}{\text{RCoke}^{\text{max}}}$ and $\text{RCoke}^{\text{max}}$ is the coking rate corresponding to maximum reactor severity.

(β) decokes in the defined time horizon

Once the minimum run length η is known, we can further calculate the maximum number of decokes possible for a reactor in the defined scheduling time horizon. This estimate can then be used to restrict the number of decokes, as shown in equation (4.48). Similar to the previous constraint, this one also increases the efficiency of tree search by pruning out the unnecessary node searches.

$$\sum_t \delta_{jt}^{\text{decoke}} \leq \beta \quad \forall j \quad (4.48)$$

where, $\beta = \frac{\text{TH}}{\eta}$, TH = Time Horizon (days)

No decokes in first (γ) days

Based on the initial coke present in the reactors, we can calculate the minimum number of days the reactors should operate without triggering a decoke operation, based on the heuristic that a decoke will not occur before required for feasibility. This estimate can be used to fix some of the binary variables in the beginning of the tree search thus reducing the search time. This constraint is more effective when the initial coke present in the reactor is small, thus allowing more number of binary variables to be fixed. This constraint is posed as shown in equation (4.49).

$$\sum_{t=1}^{t+\gamma} \delta_{jt}^{\text{decoke}} \leq 0 \quad \forall j \quad (4.49)$$

where, $\gamma = \frac{\text{Coke}^{\text{max}} - \text{Coke}^{\text{initial}}}{\text{RCoke}^{\text{max}}}$ and $\text{RCoke}^{\text{max}}$ is the coking rate corresponding to maximum reactor severity.

Force decoke within the first (α) days

If the typical minimum severity of operation is known, it is possible to calculate the maximum time within which a decoke must occur. This constraint adds less flexibility by forcing a decoke during the first (α) days, posed as equation (4.50).

$$\sum_{t=1}^{t+\alpha} \delta_{jt}^{\text{decok}} \geq 1 \quad \forall j \quad (4.50)$$

Where, $\alpha = \frac{\text{Coke}^{\text{max}} - \text{Coke}^{\text{initial}}}{\text{RCoke}^{\text{min}}}$ and $\text{RCoke}^{\text{min}}$ is the coking rate corresponding to minimum reactor severity. The value of α must be rounded.

Decoke possible only after a predefined condition

More frequent decokes decreases the life of the reactors. This information is not included in the model; therefore, if the optimum requires frequent decoking, the optimizer would select many decokes. To utilize the minimum number of decokes, a parameter is added to the model, which can ensure that decoking is triggered only after exceeding the limit on the accumulated coke ($\text{Coke}_{\text{allowed}}^{\text{decok}}$). This constraint is posed as shown in equation (4.51).

$$\text{Coke}_{jt-1} \geq \text{Coke}_{\text{allowed}}^{\text{decok}} \cdot \delta_{jt}^{\text{decok}} \quad \forall j, t \quad (4.51)$$

This constraint was found to be very useful in the model as it reduced the computational time greatly. However, it causes conflicts in few scenarios where premature decokes were advantageous due to changing demand during the horizon. Therefore, it was removed from the model while dealing with such cases. For example, this constraint was not included in the model for the scenario described in Section 4.6.1.2. The use of this constraint would depend on the engineer's insight; if the user is not sure that the heuristic is valid, the constraint should not be included.

4.4 Solution heuristic

Solution heuristics are required when it becomes difficult to solve large scale scheduling problems using standalone optimization solvers. Several aggregation and decomposition heuristics have been proposed in the literature (e.g., Pekny et al., 2000 and Kelly, 2005) to deal with difficult MIP's and solve them in a reasonable amount of time. A review of literature on solution heuristics is provided in Section 2.1.1.3. Typically, aggregation techniques rely on the idea of aggregating the time periods within the specified horizon in order to reduce the dimensionality of the problem leading to a coarse model and decomposition techniques rely on the idea of decomposing a large problem into several small problems and solving them sequentially.

Using the aggregation and decomposition heuristics, we proposed a two-stage temporal decomposition heuristic that was found to be very effective for solving the furnace scheduling problem. This heuristic is always used within our scheduling model and applied for all-the case studies discussed in this chapter.

4.4.1 Two-stage temporal decomposition heuristic

This is a time based decomposition heuristic which is designed to solve the scheduling model in two stages instead of solving in a single stage. In the first stage, a coarse grid model is formulated based on aggregation of time periods to reduce the dimensionality of the problem and solved. The results obtained from this stage are used to the binary (decoke) decisions in the next stage. In the second stage, many binary variables in the fine grid model are fixed based on the first stage solution. Finally, the fine grid model is solved to obtain a fine tuned solution. A schematic of this idea is shown in Figure 4-5.

The main difference between coarse grid and fine grid models with respect to the furnace scheduling model is the length of each time period. The fine grid model has more

(finer) time periods, whereas the coarse model has fewer (aggregated) time periods. Essentially both these models represent the same set of constraints and objective function with the exception of length of each time period in the scheduling horizon.

For example, consider the scheduling time horizon to be 90 days. In a fine grid model, the length of each time period is considered to be 1 day, resulting in 90 time periods over the entire horizon. The length of each time period for a coarse model is considered to be 3 days; therefore, the total number of time periods over the entire horizon is equal to 30. This reduction in dimensionality reduces the problem size to approximately $(1/3^{\text{rd}})$ of the size of fine grid model. Therefore, instead of solving the scheduling (fine-grid) model directly using a standalone solver in a single stage, this heuristic solves the scheduling model in two stages to be computationally efficient. The details of the heuristic are provided as follows.

In stage1, a coarse grid model is solved to obtain an approximate solution. This model is obtained by aggregating the time intervals in the defined scheduling horizon leading to a smaller scheduling model. The solution from this model yields three-day intervals within which the decoking occurs.

In stage2, the solution from stage1 is used to fix the binary (decoking) decisions in fine grid region where decoking may occur and definitely does not occur. As shown in Figure 4-5, the binary variables in the un-shaded time periods are fixed because decoking is not possible in this region as reflected in the coarse grid solution. Thus, the binary variables in the shaded time periods are the only active binary variables in the model to make decoking decisions. By searching the neighbourhood (9 time periods), this heuristic provides extra flexibility around the decoking three-day period selected at stage1. Finally, the fine grid model is solved to obtain a fine tuned decoking solution.

This heuristic is completely automated so that the optimization model need not be interrupted between the stages to fix the decisions. Fixing the logical decisions in the model is achieved by forcing the decoke decisions to take a particular integer value. Since this heuristic leads to smaller problem sizes in stage1 (due to aggregation of time periods) and stage2 (due to fixing binary variables), the solution can be obtained much more quickly.

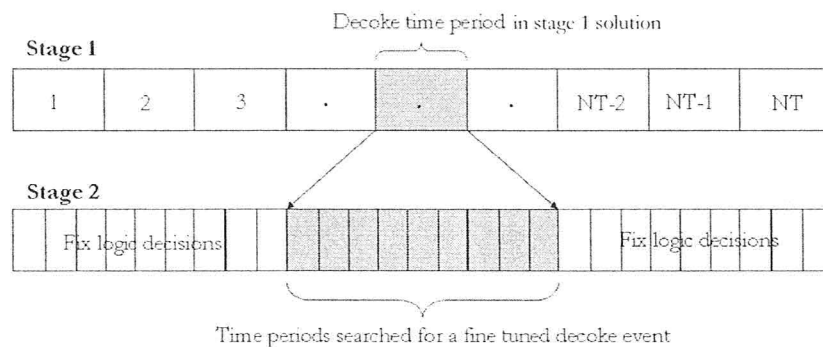


Figure 4-5: Illustration of two-stage decomposition heuristic

This heuristic was found to be very effective in reducing the computational time. The optimum using this heuristic was identical to the optimum using only fine grid in cases small enough that we could solve the optimisation problem in one stage with a fine grid. Naturally, a global optimum cannot be guaranteed when this heuristic is employed for large scheduling problems. As will be discussed in next section, this heuristic has improved the computational time substantially.

4.4.2 Issues with the coarse grid model

From the above discussion, it is clear that the solution of coarse grid model forms the basis for fine grid solution search because many of the binary variables in the fine grid model are fixed based on the coarse grid solution. For instance, if the coarse grid

model is incorrectly posed, that could mislead the fine grid model solution. Therefore, proper care should be taken while posing the coarse model.

In a coarse grid model, the length of each time period is equal to 3 days; when the optimizer chooses a reactor to decoke, it would be shutdown for one time period (i.e., 3 days). For a plant decoking time period of 1 day, this would result in 2 days of production loss and no coke accumulation. Over a scheduling horizon of 90 days, this would propagate inconsistency to the future decoking schedule due to incorrect interpretation of production and coke accumulation in the cracking coils. Furthermore, the condition that only one reactor could be decoked in a single time period holds good for a fine grid model, but could be misleading when used in a coarse grid model because for a reactor to shutdown, it would have to inevitably wait for 3 days (one time period) after any other reactor is shutdown.

In order to address these issues and model a 1 day decoke in a 3 day time period, few additional constraints have to be added to the coarse grid model. These constraints are added only to the coarse grid model and not to the fine grid model. The constraints are intended to (i) allow multiple (up to three) reactors to decoke in a single time period, (ii) accommodate two days of production when a furnace is decoked in a 3 day decoke period, and (iii) account for coke build up in a reactor during a 3 day decoke event. Details of these constraints are provided in the following sub-sections.

4.4.2.1 Decoking multiple reactors

Equation (4.29) ensures that only one reactor can be shutdown for maintenance at any time period. However, to allow multiple reactors to decoke within a single time period, equation (4.29) is replaced with equation (4.52) in the coarse grid model. The maximum number of reactors allowed to decoke (τ) in a single time period is calculated based on the length of time period and the maintenance period. The condition that only one reactor should be decoked at any time period can be taken care by the fine grid model in the second stage of the solution heuristic.

$$\sum_j \delta_{jt}^{\text{decoke}} \leq \tau \quad \forall t \quad (4.52)$$

where, $\tau = \frac{\Delta t}{\Delta t^{\text{decoke}}}$, is the number of reactors that can be docoked during each time period. For the coarse grid model in this study, $\tau = 3$.

4.4.2.2 Accommodate production in the decoke time period

In order to accommodate two days of production in a 3 day decoke time period, an additional (new) set of production constraints similar to those in the basic scheduling model are used. The variables in these constraints have star as a superscript to differentiate them from the variables in the basic scheduling model. These constraints are used to model production only during a decoke event in a coarse grid model. Therefore, during normal operation (periods without a decoke), these constraints are effectively eliminated based on the decoke binary variables (i.e., production variables are forced to be zero) using equation (4.53).

$$P_{ij}^{\min} \cdot \delta_{jt}^{\text{decoke}} \leq P_{ijt}^* \leq P_{ij}^{\max} \cdot \delta_{jt}^{\text{decoke}} \quad \forall i, j, t \quad (4.53)$$

During a decoke event, the logic variable $\delta_{jt}^{\text{decoke}} = 1$ and the processing rate variables are activated according to equation (4.53). During normal plant operation, $\delta_{jt}^{\text{decoke}} = 0$ and the variables are forced to take zero values according to the same equation.

The feed balance constraint is shown as equation (4.54). Disjunctive reactor model constraint is shown as equation (4.55) and the production rates are calculated using equations (4.56 to 4.58). To account for appropriate material balance, the production during these two days is added to the production variable in the main scheduling model as shown in equation (4.58a).

$$F_{it}^* = \sum_j P_{ijt}^* \quad \forall i, t \quad (4.54)$$

$$\sum_k PD_{ijkt}^* = P_{ijt}^* \quad \forall i, j, t \quad (4.55)$$

$$PRate_{ijkt}^* = PD_{ijkt}^* \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (4.56)$$

$$Pr od_{ct}^* = \sum_i \sum_j \sum_k PRate_{ijkt}^* \quad \forall c, t \quad (4.57)$$

$$Sales_{ct}^* = Pr od_{ct}^* \quad \forall c, t \quad (4.58)$$

$$Pr od_{ct} = Pr od_{ct} + Pr od_{ct}^* \cdot (\Delta t - \Delta t^{decoke}) \quad \forall c, t \quad (4.58a)$$

These equations account for production during all decoke periods. Note that equation (4.53) governs the equations (4.54 to 4.58). During normal operation, equation (4.53) is inactive and so all the production variables are forced to zero. The profit during the two day production period is calculated as shown in equation (4.61) which should be added to the objective function (equation 4.40) while solving the coarse grid model. The profit calculation is shown in equation (4.61). This profit is added to the objective function as shown in equation (4.62).

$$\begin{aligned} \mathbf{profit}^* = & \left(\sum_c Sales_{ct}^* \cdot Cost_c^{product} - \sum_i F_{it}^* \cdot Cost_i^{feed} - \sum_i \sum_j \sum_k PD_{ijkt}^* \cdot \rho_{ik}^{S/HC} \cdot Cost_{steam}^{dilution} \right. \\ & - \sum_i \sum_j \sum_k PD_{ijkt}^* \cdot E_{ijk} \cdot Cost_{energy}^{furnace} - \sum_i \sum_j \sum_k \sum_c \left(\frac{PRate_{ijkt}^*}{MW_c} \right) \cdot E_{compressor} \cdot Cost_{energy}^{compressor} \\ & \left. + \sum_i \sum_j F_{ijt}^{HPsteam^*} \cdot Cost_{steam}^{HP} + \sum_i \sum_j F_{ijt}^{MPsteam^*} \cdot Cost_{steam}^{MP} \right) \cdot (\Delta t - \Delta t^{decoke}) \quad (4.61) \end{aligned}$$

$$\text{Objective function} = \text{Plant Profit} - \text{Penalty}^{\text{Coke}} - \text{Penalty}^{\text{Recy_Inv}} + \text{profit}^* \quad (4.62)$$

4.4.2.3 Modifications to the coke model

While modelling a 1 day decoke in a 3 day time period, it is assumed that the first day is allocated for decoking and the next two days for production. The coke accumulated during the two days of production is added to the subsequent time periods to maintain consistency in the coking model. Therefore the coke model, described earlier as equation (4.44), should be replaced with equation (4.63) in the coarse grid model. The three terms identified in the equation are explained in the table below.

$$\text{Coke}_{jt} = \text{Coke}_{jt-1} + \sum_k \Delta\text{Coke}_{jkt} + \text{Coke}_{jt-1}^* - \Delta\text{Decoke}_{jt} \quad \forall j, t \quad (4.63)$$

Term	Description
1	Coke buildup during normal operation
2	Coke buildup during the 2 days in a 3 day decoke period. This term will add the 2 days of coke buildup to the next time step.
3	Term to eliminate coke during decoking

The tube wall temperature constraint is modified as shown in equation (4.64). The coke accumulated during the two days is calculated using equation (4.65) and used in equation (4.66) to calculate the change in the tube wall temperature during those two days.

$$Tw_{jt} = \sum_i \sum_k (Tw_{ik}^{\text{clean}} \cdot \sigma_{ijkt}^{\text{disj}}) + Tw^{\text{const}} \cdot \text{Coke}_{jt} \quad \forall j, t \quad (4.64)$$

$$\text{Coke}_{jt}^* = R_{\text{coke}}^* \cdot (\Delta t - \Delta t^{\text{decoke}}) \quad \forall j, t \quad (4.65)$$

where, R_{coke}^* is the coking rate chosen during the two days of production, $\Delta t = 3$ days for coarse grid model and $\Delta t^{\text{decoke}} = 1$ day.

All these constraints are used only in the coarse-grid model to account of 1 day decoke in a 3 day time period. A complete set of constraints and objective function for coarse-grid and fine-grid models used in this thesis to solve single feedstock and multiple feedstock scenarios are provided in Appendix C.

4.5 Computational improvement

By introducing the reformulated constraints, tightening constraints and the solution heuristic into basic scheduling model, the computational time was significantly reduced. For example, let us consider a simple scenario where one feed is cracked in 2 reactors (for a one-stage, fine grid model: 180 binary variables, 37080 continuous variables and 37884 linear constraints). When a stand alone solver (CPLEX 10.1) was used to solve the basic model, it took approximately 14000 seconds to solve the problem. However, when the model was solved by introducing reformulated constraints, tightening constraints and using the solution heuristic, it took approximately 350 seconds.

Improvement in the computational time as research progressed for this scenario is shown in Figure 4-6. It is clear that the computational time has reduced greatly with the introduction of tailored schemes such as solution heuristic, reformulated constraints and tightening constraints to the basic model, during the course of the research. Most notably, the computational time has been reduced by a factor of 40, which means that the improved scheduling model (with tailored schemes included) could be solved 40 times quicker than the basic scheduling model. In case of large models, the computational improvement was found to be even more. For a scenario with 3 feedstocks and 5 reactors (for a one-stage, fine grid model: 3100 binary variables, 297794 continuous variables and 308629 linear constraints), the computational efficiency was improved by over 240 times.

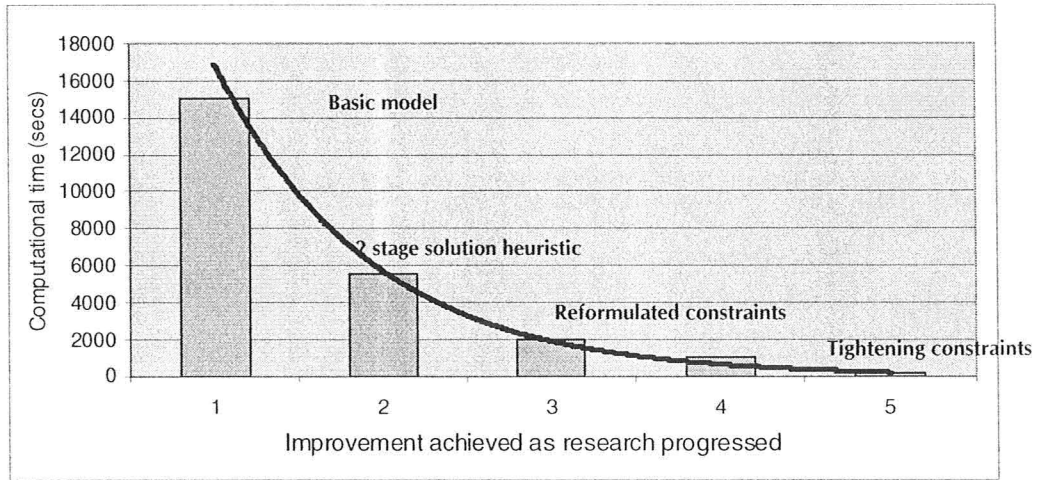


Figure 4-6: Computational improvement as research progressed

Label on x-axis	Additions to the basic model
1	Basic model
2	Two-stage temporal decomposition heuristic
3	Reformulated constraints
4&5	Tightening constraints

4.6 Open-loop case studies

Several case studies have been formulated and the results are discussed in this section. These case studies are designed to highlight the flexibility of the scheduler to handle various scenarios. The results obtained for every scenario are the predictions from the scheduler, i.e., the solution of the MILP without feedback to account for any model mismatch. (In the next chapter, the MILP will be the MPC controller in a feedback control system.) Several single feed and multi-feed scenarios are formulated; these scenarios are designed to show the importance of formulation features, to demonstrate the ability of the formulation to solve complex problems, and to evaluate the computing times. For all the cases, the formulation includes the two-stage solution heuristic, reformulated constraints and tightening constraints. A complete set of constraints and the objective function for coarse grid and fine grid models used to solve the open-loop case studies are provided in Appendix C.

4.6.1 Single feedstock scenarios

Scenarios formulated with a single feedstock are discussed here. Naphtha is the feedstock used for all the cases. Ethane, obtained in the products is not recycled back for further cracking; it is sold. The main optimization decisions are to obtain optimal flowrates, reactor operating conditions and decoke time periods. Yield profiles from naphtha feedstock for various reactor conditions are shown in Figure 4-7. Severities corresponding to propylene and ethylene peaks are highlighted in the figure as they are repeatedly used in the following discussion. Yield profiles from Ethane feedstock for various reactor conditions are shown in Figure 4-8. (For propane feedstock yield profiles, refer to Figure 3-4) .

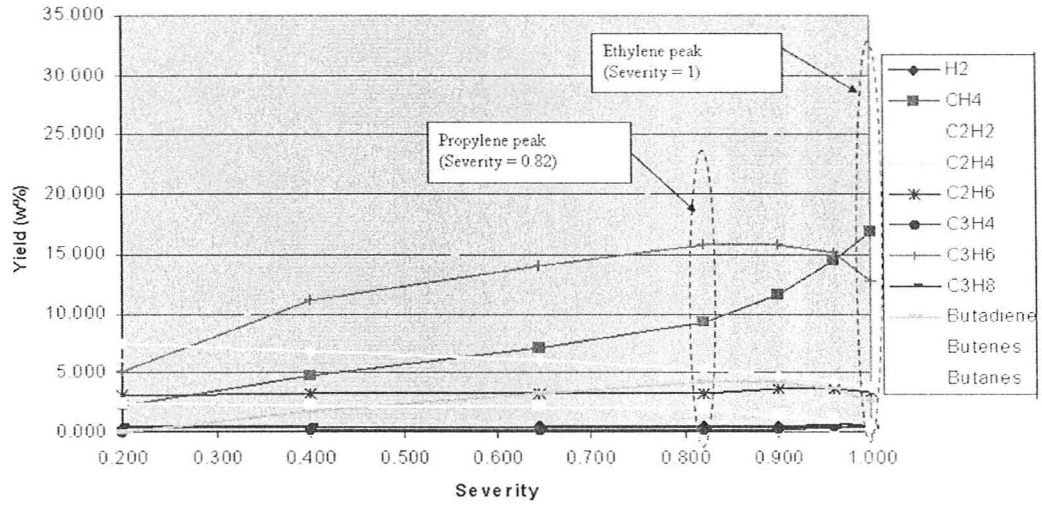


Figure 4-7: Yield profiles of naphtha feedstock

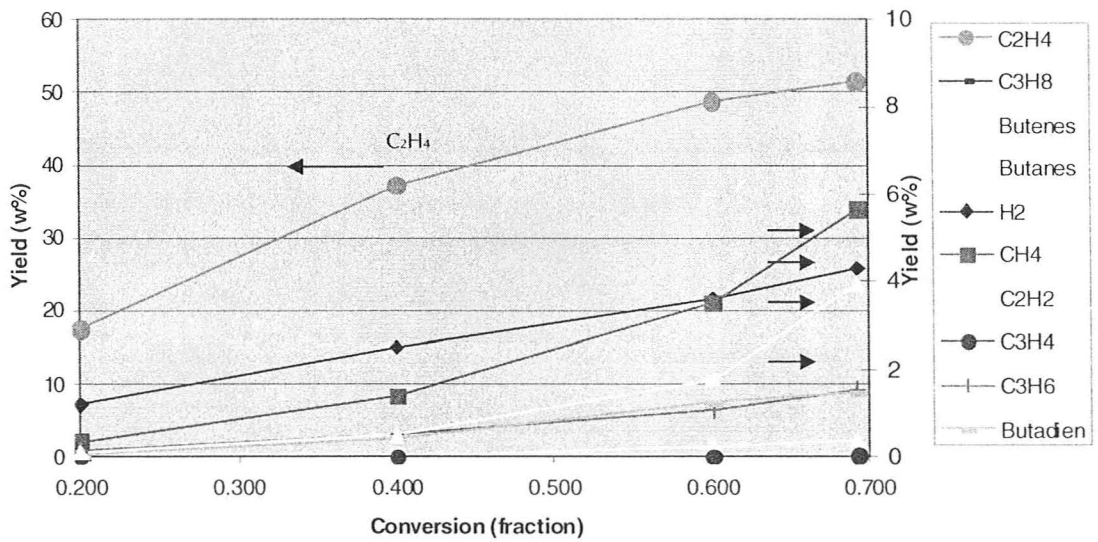


Figure 4-8: Yield profiles of Ethane feedstock

In Figure 4-8, only ethylene yield is plotted onto the primary y-axis, which is on the left hand side. All the remaining product yields are plotted onto the secondary y-axis shown on the right hand side of the graph.

4.6.1.1 Case 1 - End conditions

End conditions are the requirements that we decide must be met to ensure a feasible operational state at the end of time horizon. In this scenario, we study the effect of end conditions on the reactor operation and maintenance schedule. This is done by looking at the results from the scheduling model with end conditions and without end conditions. A brief description of the scenario parameters are tabulated as shown below.

Feedstock	Naphtha
Number of Reactors	2
Time horizon	90 days
Sales limit	Unlimited C ₂ H ₄ sales
Fresh feed	Unlimited amount available
Degrees of freedom	Processing rates, Severity, S/HC and decoke time periods

Discussion of results

Results obtained without end penalties in the model are shown in Figures 4-9 and 4-10. The production details of ethylene and propylene, maintenance schedule in the form of Gantt chart, coke accumulation details over the entire horizon are depicted in Figure 4-9. Severity and S/HC profiles for both the reactors are shown in Figure 4-10.

In general, for an unlimited ethylene sales scenario, the reactors should operate at high severity and S/HC ratios to produce as much ethylene as possible. From Figure 4-10, it can be seen that severities in both the reactors were high in the beginning; however, they gradually decrease towards the end of the horizon. On the other hand, both the reactors are completely filled with coke by the end of the horizon. This leads to a conclusion that the reactors have been operating at reduced severities to avoid a (third)

decoke towards the end of the horizon. Although it is an “optimal” solution for the horizon in the model, it leads to a situation where both the reactors have to be decoked in the future – immediately after the horizon ends. In such a situation, there would be no production in the plant until the maintenance is complete, and the plant would have to be shutdown at a large economic cost.

In order to overcome such situations, end penalties have been imposed in the model, and the results obtained after its implementation are shown in Figures 4-11 and 4-12. The new solution has an additional decoke for each reactor almost at the end of the horizon. The little coke accumulated in both the reactors at the end of the horizon provides scope for feasible operation in the future as can be seen from Figure 4-11. Also, there is no decrease in the severity levels as before; the reactors are operated consistently at expected levels. This leads to a very reasonable solution.

In conclusion, without end penalties the final operational state could be infeasible for future operation and the cost for coke present at end of the horizon would not be included in objective function. Since end conditions overcome such a situation, they are always embedded in the standard implementation of the scheduling model, including all further studies reported in this thesis.

Results without end conditions

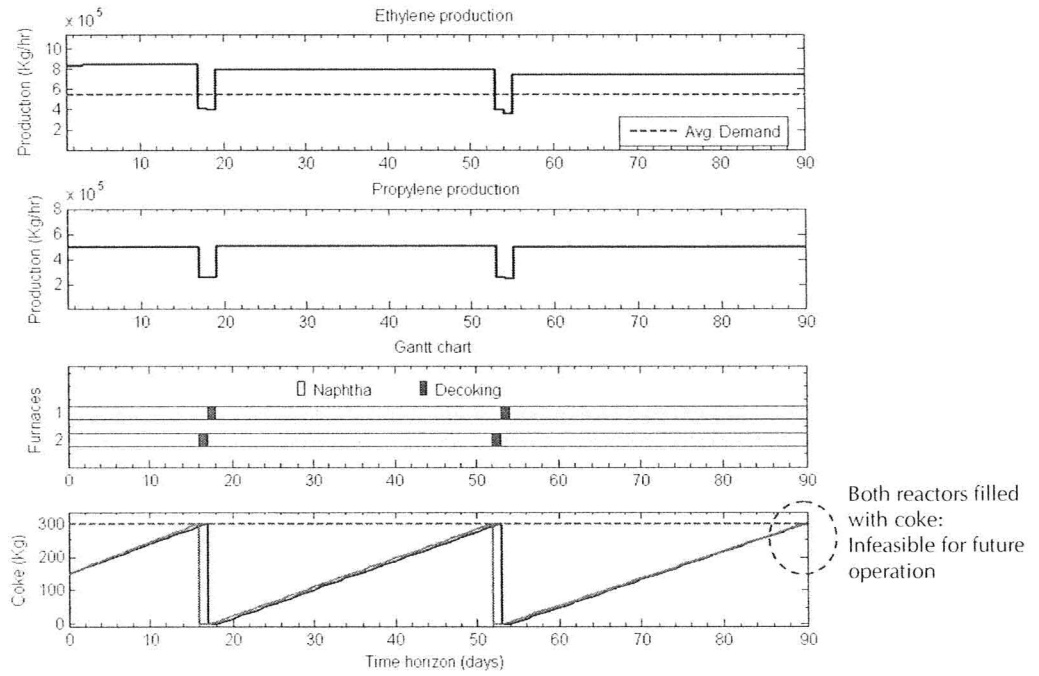


Figure 4-9: Case 1 - Gantt chart and Production details

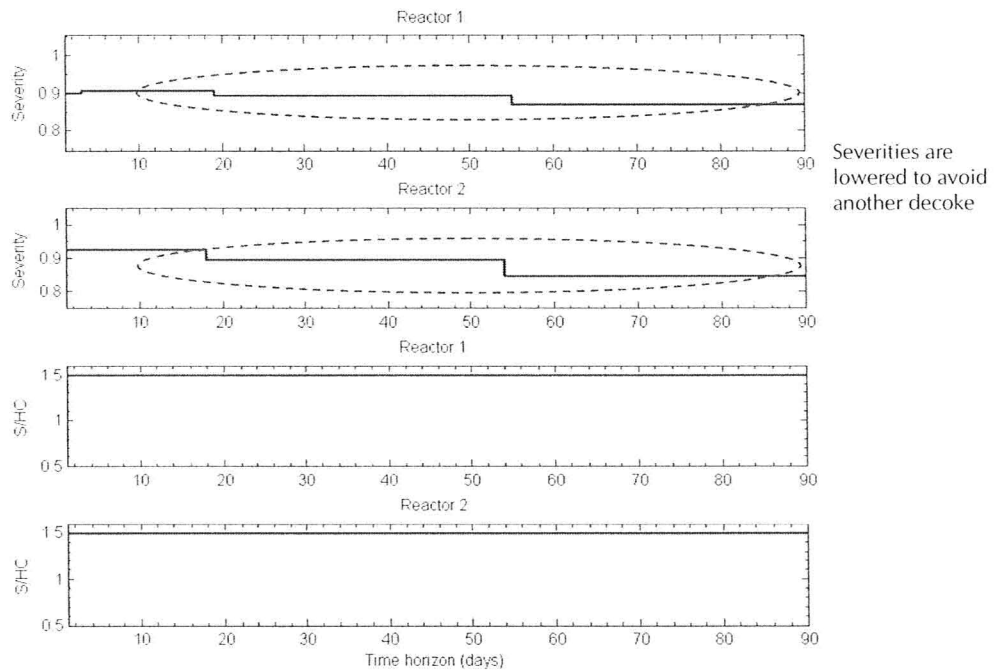


Figure 4-10: Case 1 - Severity and S/HC profiles

Results with End conditions

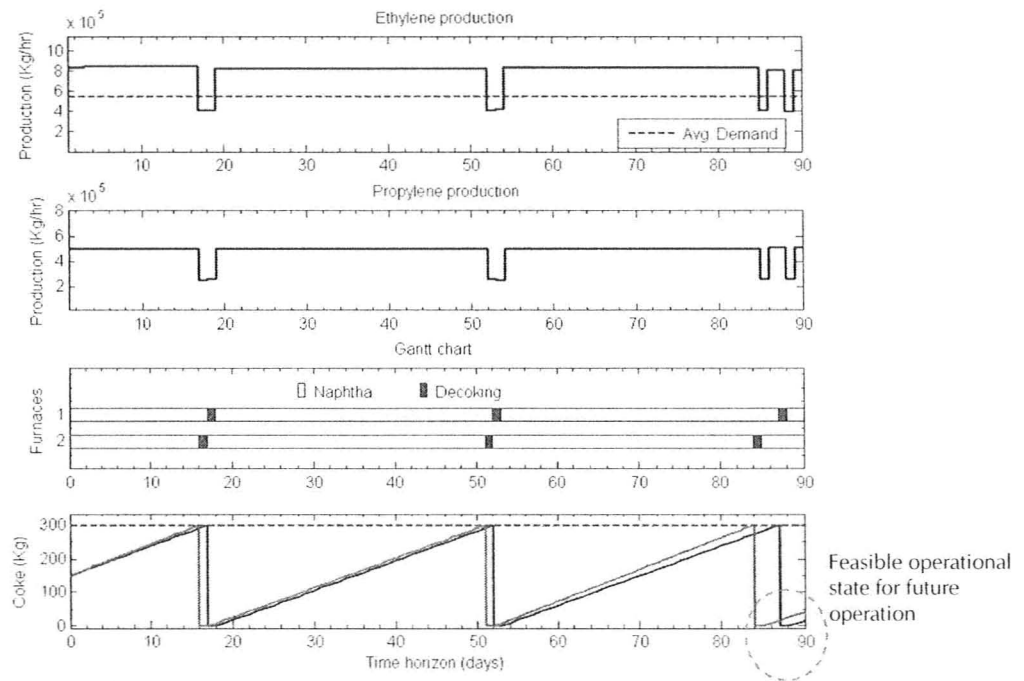


Figure 4-11: Case 1 - Gantt chart and Production details

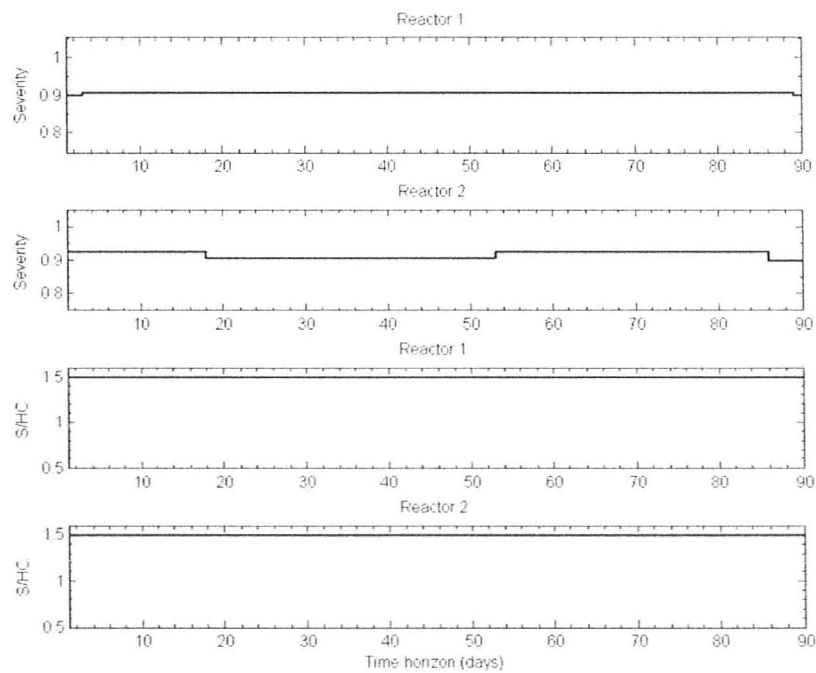


Figure 4-12: Case 1 - Severity and S/HC profiles

4.6.1.2 Case 2 - Variable sales limits

It is possible for the demands for certain products may vary over a 90 day period. Hence, the sales limits vary accordingly with the demand patterns since demand is interpreted in these cases as a maximum market sales. In this scenario, we highlight the flexibility of the optimizer to tackle such a varying demand situation. In this scenario, there is a sales limit on ethylene for the first 30 days, while there is no limit on ethylene sales for the remaining 60 days. A brief description of the scenario parameters are tabulated as shown below. We expect the optimizer to adapt to these changes by choosing operating conditions and decoke timings that are most profitable.

Feedstock	Naphtha
Number of Reactors	2
Time horizon	90 days
Integrated ethylene Demand	60% of the plant capacity for the first 30 days and unlimited sales for the last 60 days
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and decoke time periods

Discussion of Results

Results obtained for this scenario are shown in Figures 4-13 to 4-15. During the first 30 days, there is a limit on ethylene sales. Therefore, the optimizer chooses to operate both the reactors at the propylene peak corresponding to a severity of 0.82 and low S/HC of 0.5 as shown in Figure 4-14. The propylene peak is a profitable operating condition during normal reactor operation. At this peak, the reactors produce as much propylene as possible, while producing just enough ethylene to meet the ethylene demand. One can also see that the reactors have around 250 kg of coke accumulated.

During the last 60 days, there is no limit on ethylene sales. Therefore, the reactors can produce as much ethylene as possible during this period. Thus, the optimizer choose to operate both the reactors at the ethylene peak corresponding to a severity of 1 and S/HC ratio of 1.5. During this period of high severity operation, it is also desirable to

have as little down time as possible. This means that the number of reactor shutdowns for coke cleanup should be minimum. Therefore, as a solution the optimizer has chosen to prematurely decoke both the reactors before the 31st day, the day when the unlimited sales starts. It is clear from the Gantt chart as shown in Figure 4-13, that Reactor1 is cleaned on 29th day and Reactor2 is cleaned on the 30th day. Doing so, the optimizer made sure that both the reactors are clean and available for production at maximum capacity from the 31st day.

Numerical results obtained are shown in Table 4-2. The problem sizes, computational times, and so forth for both the temporal decomposition stages are highlighted. It can be seen that this problem was solved in less than 15 seconds in two stages.

Table 4-2: Case 2 - Numerical results

	Two Stage decomposition heuristic	
	Stage 1	Stage 2
Discrete time intervals	30	90
Integer variables	48	28
Continuous variables	14750	27066
Constraints	15114	27474
Computational time	4.86 secs	9 secs
Model Profit	38270551.8 \$	
Solver details	CPLEX 10.1	

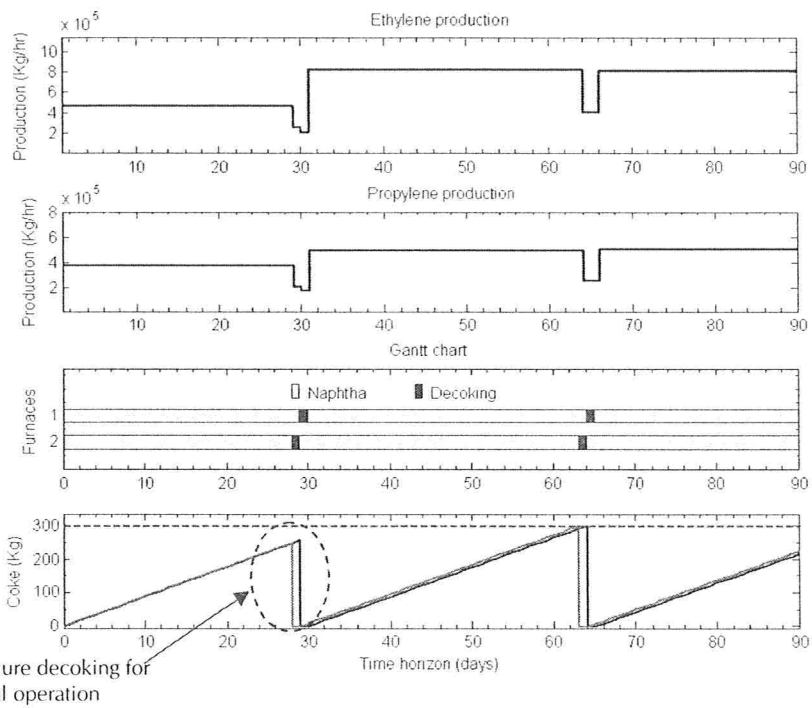


Figure 4-13: Case 2 - Gantt chart and Production details

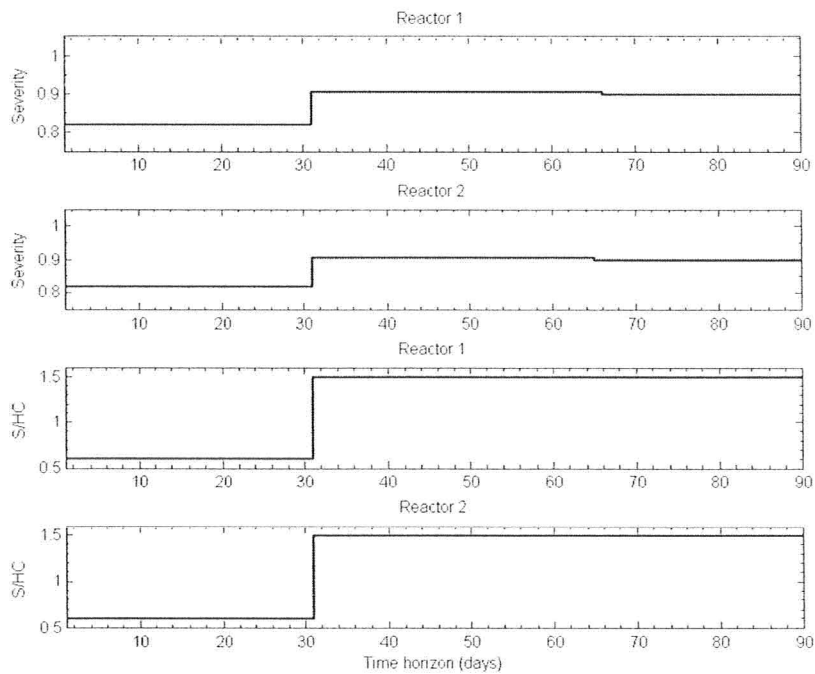


Figure 4-14: Case 2 - Severity and S/HC profiles

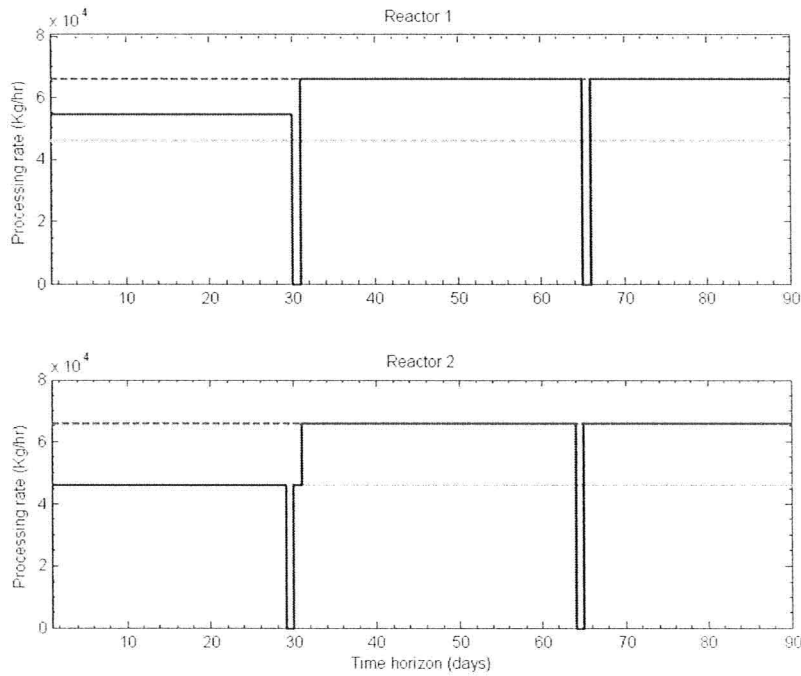


Figure 4-15: Case 2 - Processing rates

4.6.1.3 Case 3 - Reactors in service

Sometimes the demand for products may drop significantly. In such a case, it might be necessary to shutdown one or a few reactors to reduce production. In this scenario, we highlight the capability of the model to deal with a situation when there is low demand for ethylene. The main decisions are then to decide which reactors will be in service at what times during the time horizon. The constraints used to model this condition are discussed in Appendix B. A brief description of the scenario parameters are tabulated below.

Feedstock	Naphtha
Number of Reactors	2
Time horizon	90 days
Integrated ethylene Demand	40% of the plant capacity
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC, Decoke time periods and Number of furnaces in operation

Discussion of Results

In this scenario, the demand for ethylene is very low, which leads to a significant reduction in ethylene production due to sales limits. As an optimal solution, the optimizer has chosen to operate both reactors and shut them down intermittently. The results obtained for this scenario are shown in Figures 4-16 to 4-18. Due to the specified initial condition, both the reactors start to operate in the beginning. But after the 16th day, we can observe in the Gantt chart in Figure 4-16 that Reactor 2 remains in operation while Reactor 1 is taken offline. The processing rates of the reactors are shown in Figure 4-18. When the processing rate for a reactor is zero, it means that the reactor is not in service.

The optimizer could have chosen to operate both the reactors for certain period and then shutdown both of them once the demands were met. But in our formulation, we imposed an additional constraint that there should be a minimum feed flow into the reactors to maintain continuous downstream plant operation. Therefore, the optimizer has chosen to operate at least one reactor by allowing intermittent shutdowns.

Numerical results obtained are shown in Table 4-3. The problem sizes, computational times etc. for both the stages are highlighted. It can be seen that this problem was solved in 270 seconds in two stages. The integrated demand for ethylene was exactly met in this scenario.

Table 4-3: Case 3 - Numerical results

	Two Stage decomposition heuristic	
	Stage 1	Stage 2
Discrete time intervals	30	90
Integer variables	110	46
Continuous variables	16139	21341
Constraints	16615	19426
Computational time	258 secs	12 secs
Integrated C ₂ H ₄ Demand	30000000 Kg	
Ethylene produced	30000000 Kg	
Model Profit	22419400 \$	
Solver details	CPLEX 10.1	

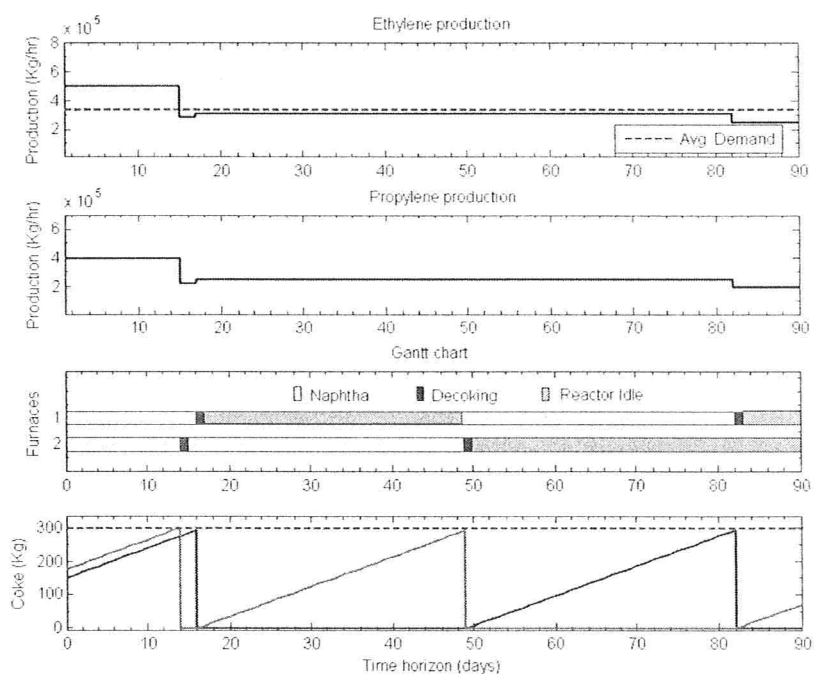


Figure 4-16: Case 3 - Gantt chart and Production details

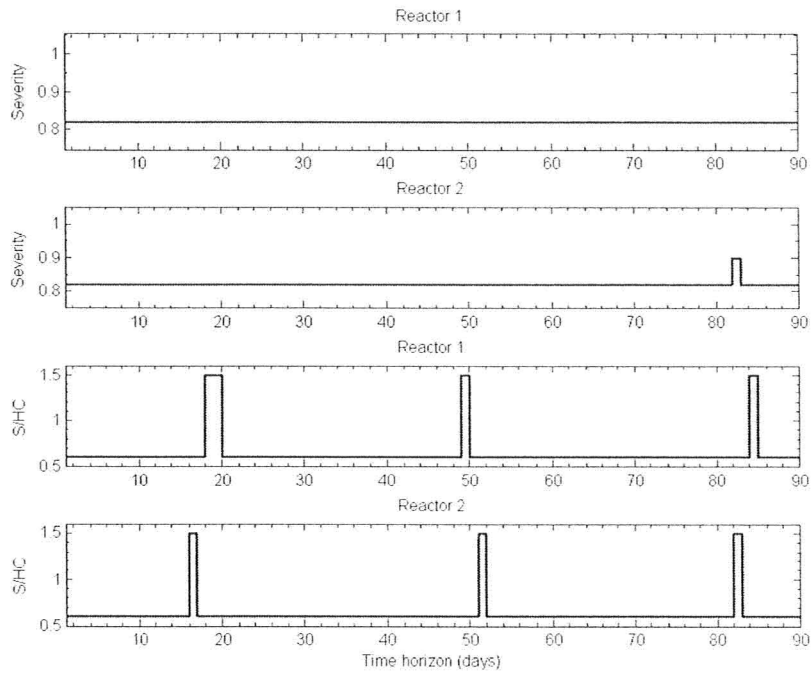


Figure 4-17: Case 3 - Severity and S/HC profiles

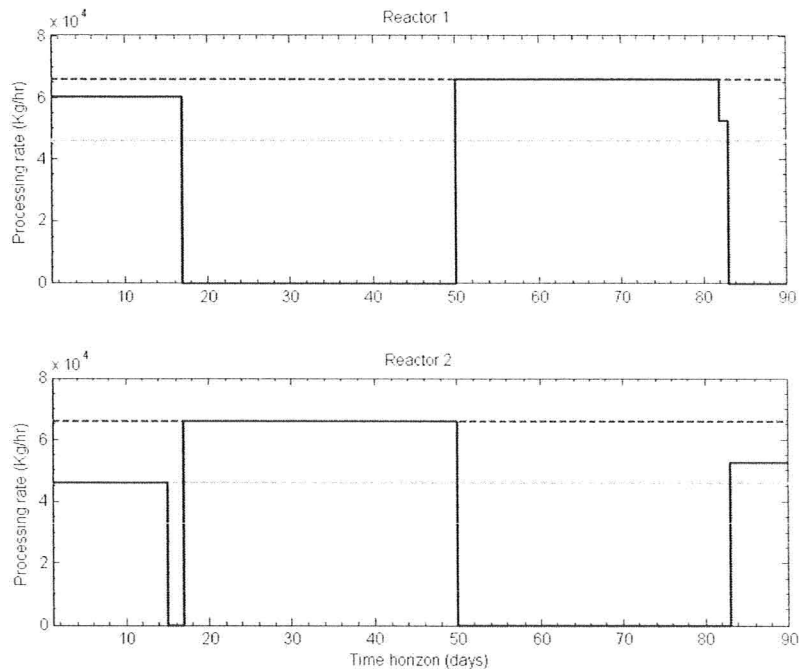


Figure 4-18: Case 3 - Processing rates

4.6.1.4 Case 4 - Coked reactors

In this scenario, both the reactors in operation initially have a large amount of coke (250 Kg) so that decoking is required in the near future. However, due to maintenance constraints only one reactor can be decoked on any particular day. Therefore, it becomes necessary to prematurely decoke (before reaching the decoke limits) one reactor to achieve feasible plant operation. Here, we highlight the flexibility of the optimizer to deal with such a situation and decide which reactors to prematurely decoke and which to operate at different periods of time. A brief description of the scenario parameters are tabulated as shown below.

Feedstock	Naphtha
Number of Reactors	2
Time horizon	90 days
Integrated ethylene Demand	66% of the plant capacity
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and Decoke time periods

Discussion of Results

The results obtained are shown in Figures 4-19 to 4-21. Figure 4-19 clearly shows that Reactor 1 is prematurely decoked. The maintenance schedule shown in the form of a Gantt chart shows a cyclic pattern for reactor shutdowns. The severities and S/HC ratios for reactors 1 and 2 are shown in Figure 4-20. The processing rates for all the reactors are clearly depicted in Figure 4-21 .

The results from the simulation study for the same scenario were discussed in Chapter 3 (Section 3.7). It appears that simulation results (which represent an engineer making all decisions) and optimal results are the same for reactor maintenance decision making (compare Gantt chart). However, there are differences in the ethylene production rates and hence demand met. In optimization it is assured that integrated demand conditions are exactly met, which could not be assured with manual decision making. Also, one should note that this is a simple scenario, therefore feasible operation was

achieved by easy simulation. However, for larger problems where the decisions to make are complicated, optimization based approach would provide faster optimal decisions.

Numerical results from the optimization based approach are shown in Table 4-4. The problem sizes, computational times etc. for both the stages are highlighted. It can be seen that this problem was solved in 12.4 seconds in two stages. The integrated demand for ethylene was exactly met in this scenario.

Table 4-4: Case 4 - Numerical results

	Two Stage decomposition heuristic	
	Stage 1	Stage 2
Discrete time intervals	30	90
Integer variables	48	28
Continuous variables	14750	27066
Constraints	15114	27474
Computational time	6.4 secs	6 secs
Integrated C₂H₄ Demand	49500000 Kg	
Ethylene produced	49500000 Kg	
Model Profit	36929999.06 \$	
Solver details	CPLEX 10.1	

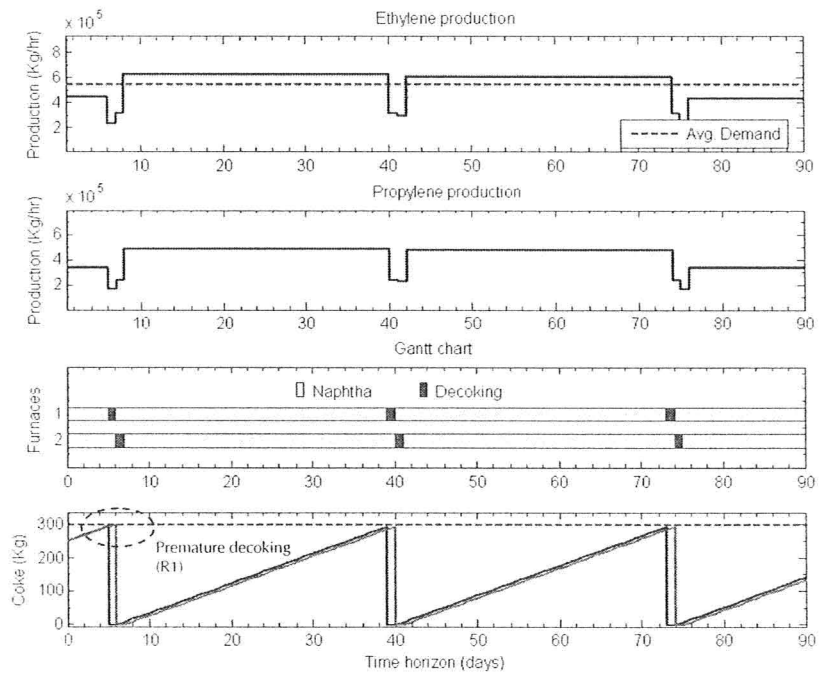


Figure 4-19: Case 4 - Gantt chart and Production details

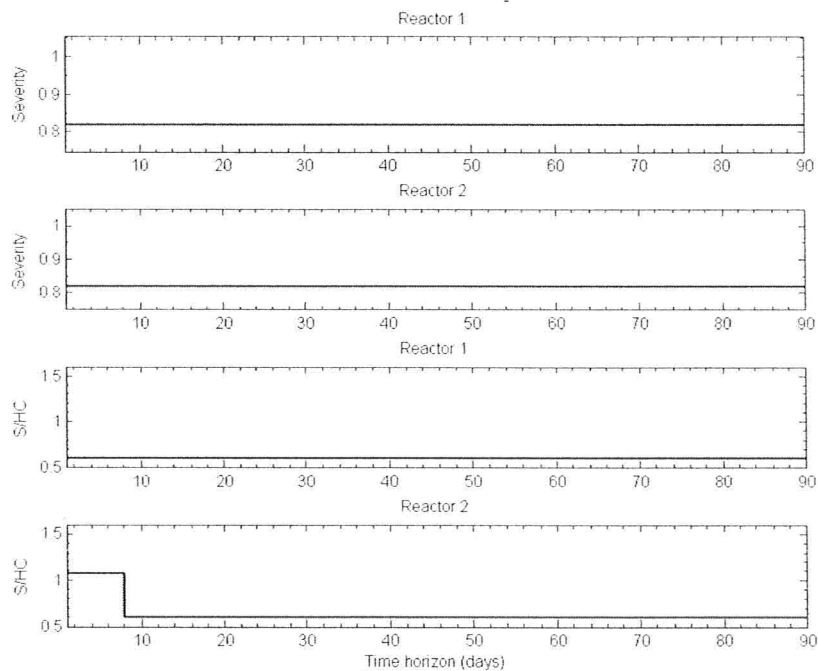


Figure 4-20: Case 4 - Severity and S/HC profiles

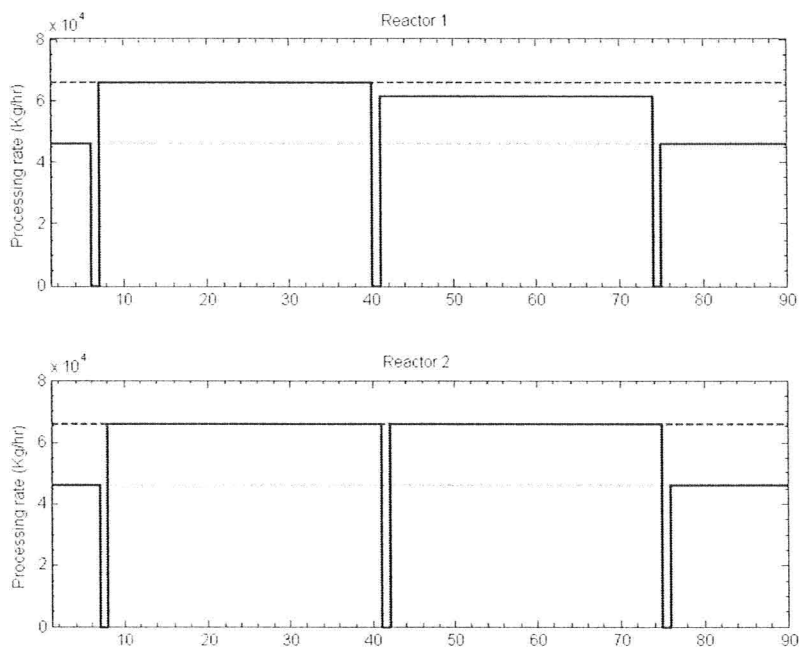


Figure 4-21: Case 4 - Processing rates

4.6.1.5 Case 5 - Large scale problem

This is a large scale ethylene furnace scheduling problem having the number of furnaces typical in a full-scale plant. In this scenario, the plant can crack naphtha feedstock in five reactors for a total plant capacity of 0.75 million MTA ethylene. Here, we highlight the model capability to handle large scale scheduling problems. To be more realistic, initial coke in the reactors is considered to be different for all the reactors. A brief description of the scenario parameters are tabulated as shown below.

Ethylene Plant Capacity	0.75 million MTA C ₂ H ₄
Feedstock	Naphtha
Number of Reactors	5
Time horizon	90 days
Integrated ethylene Demand	60% of the plant capacity
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and Decoke time periods

Discussion of Results

The results obtained for this scenario are shown in Figures 4-22 to 4-25. In general, the optimizer selects an optimal severity and S/HC for the reactors and manipulates the processing rates appropriately to meet the demands. The optimal severity is chosen to be 0.82 (Figure 4-23) and S/HC ratio to be 0.5 (Figure 4-24) for all the reactors during the entire horizon. The processing rates for the reactors are shown in Figure 4-25.

Severity of 0.82 corresponds to propylene peak in the product yields. At this peak, plant operates most profitably by producing more propylene and enough ethylene to meet the demand. S/HC ratio of 0.5 is the minimum steam required for reactor operation, which reduces furnace energy.

Schedule for maintenance of the reactors is shown in the Gantt chart as shown in Figure 4-22. It is clear that Reactor 1 has two decokes because of low coke at the initial condition and low severity chosen to maximize propylene yield, while all the others have three decokes during the horizon.

Numerical results are shown in Table 4-5. The problem sizes, computational times etc. for both the stages are highlighted. It can be seen that this problem took 453 seconds

in stage1 and 152 seconds in stage2 for a total of 705 seconds to solve the entire problem. The integrated demand for ethylene was exactly met in this scenario.

Table 4-5: Case 5 - Numerical results

	Stage 1	Stage 2
Discrete time intervals	30	90
Integer variables	136	94
Continuous variables	37412	64953
Constraints	38444	66075
Computational time	453 secs	152 secs
Integrated C₂H₄ Demand	123750000 Kg	
Ethylene produced	123750000 Kg	
Model Profit	92443061.13 \$	
Solver details	CPLEX 10.1	

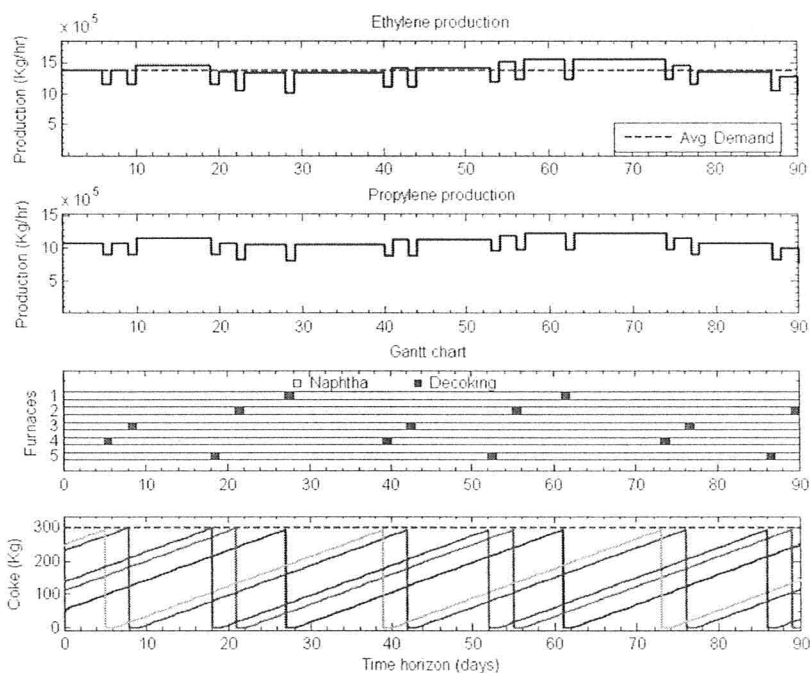


Figure 4-22: Case 5 - Gantt chart and Production details

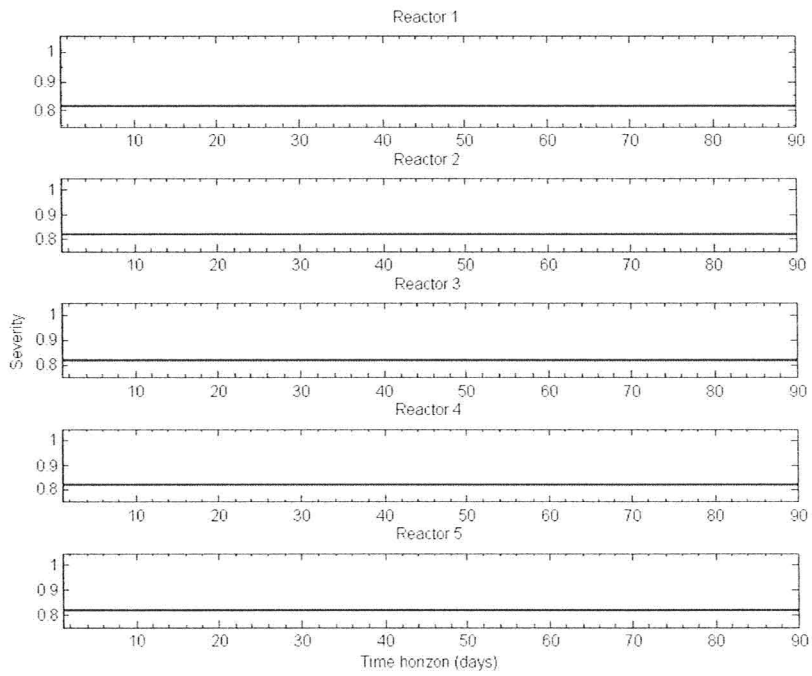


Figure 4-23: Case 5 - Severity profiles

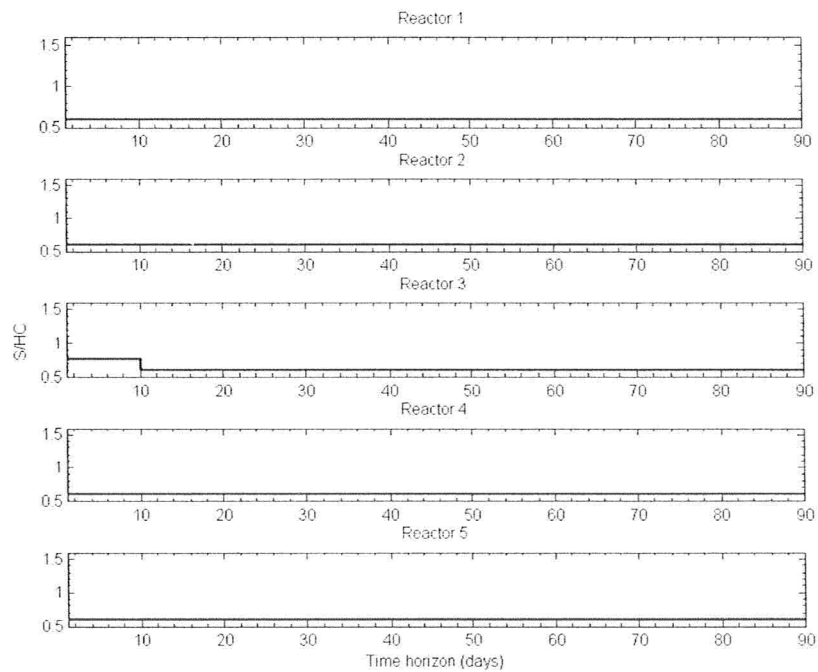


Figure 4-24: Case 5 - S/HC profiles

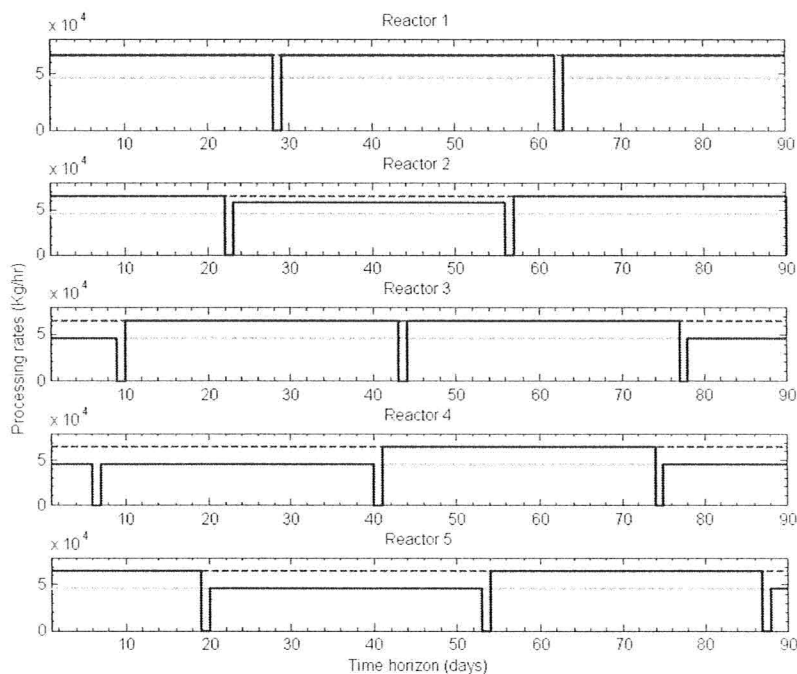


Figure 4-25: Case 5 - Processing rates

4.6.2 Multiple feedstock scenarios

The scenarios formulated with multiple feedstocks are discussed here. These scenarios have an additional decision to make over the single feed scenarios discussed earlier, which is to make an optimal allocation of feeds to the reactors. This decision is mainly based on the economics and the product demands.

Also, we have an additional condition for these scenarios that at least one reactor must crack the recycled ethane. Therefore, we have explicitly assigned Reactor 1 to crack ethane in all these scenarios, leaving the optimizer to select feedstocks for the remaining reactors. Details of the scenarios and results are discussed as follows.

4.6.2.1 Case 6 - Ethylene sales price higher than propylene

In this scenario, two feedstocks ethane and naphtha are available to be cracked in three reactors. Sales on ethylene are unlimited and the ratio of ethylene price to propylene is 1.46 (ethylene = 0.749 \$/kg and propylene = 0.511 \$/kg). Under this condition, the optimizer should choose the best feedstock to crack in the reactors for the given product pricing. Here we highlight the model capacity to make additional binary decisions (choosing appropriate feedstocks over time) besides the regular plant operating conditions and maintenance schedule. A brief description of the scenario parameters are tabulated as shown below.

Feedstocks	Ethane, Naphtha
Number of Reactors	3
Time horizon	90 days
Sales limits	Unlimited sales on all the products
Fresh feed	Unlimited feeds available
Degrees of freedom	Feedstock selection, Processing rates, Severity, S/HC and Decoke time periods

Discussion of Results

The results obtained for this scenario are shown in Figures 4-26 to 4-28. Since ethylene is sold for a higher price than propylene and no sales demands are active, it makes sense to operate the reactors at conditions giving the highest ethylene yields. Therefore, it is clear from the results that the optimizer has selected to crack ethane in all three reactors at their maximum severity, S/HC and processing rates so that the plant can produce as much ethylene as possible.

The schedule for maintenance of the reactors is depicted in the Gantt chart as shown in Figure 4.25. Clearly, all the reactors undergo three decokes during the entire horizon. The severities and S/HC ratios corresponding to the ethylene peak are shown in Figure 4-26.

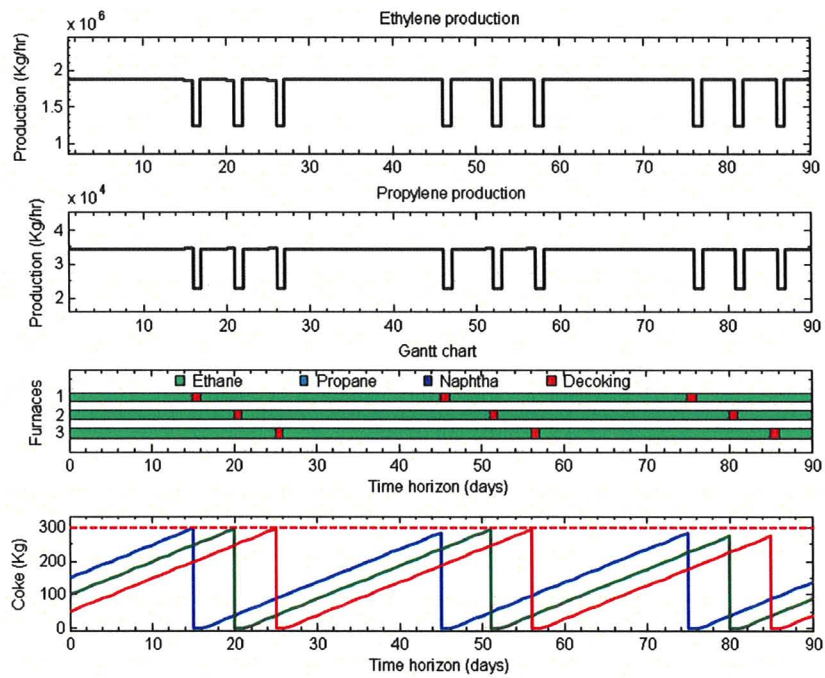


Figure 4-26: Case 6 - Gantt chart and Production details

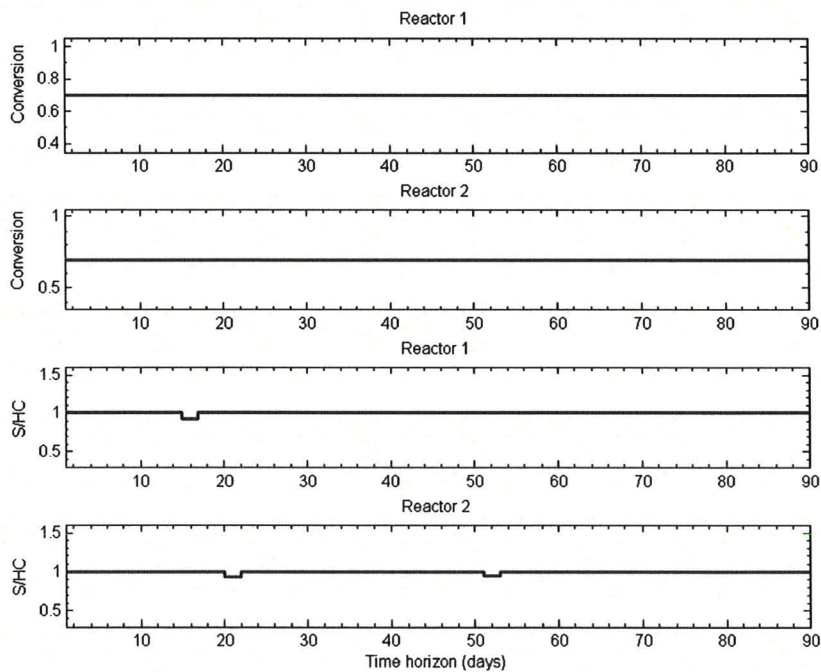


Figure 4-27: Case 6 - Severity and S/HC profiles

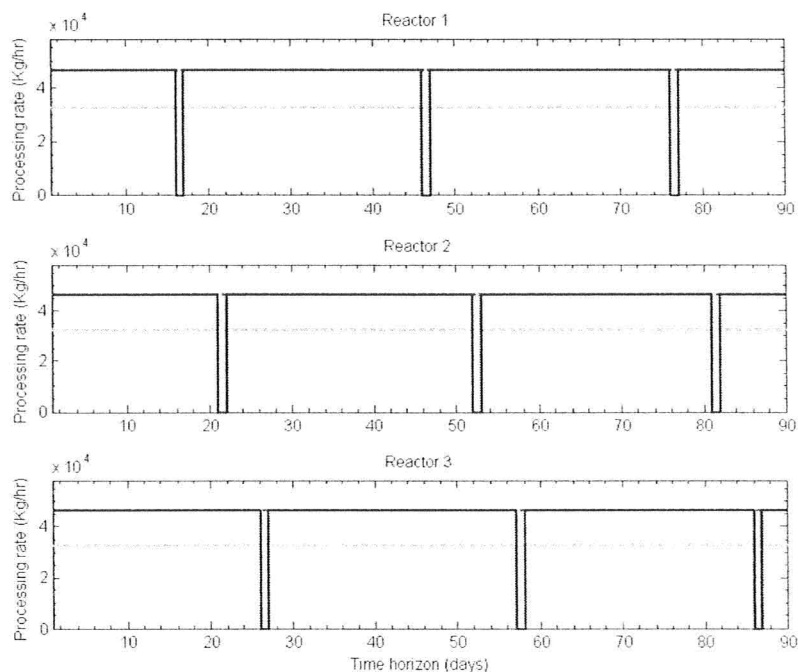


Figure 4-28: Case 6 - Processing rates

4.6.2.2 Case 7 - Propylene sales price higher than ethylene

This scenario is the same as Case 6 except for one pricing change; propylene is sold for a higher price than ethylene. The ratio of propylene price to ethylene is 1.46 (propylene = 0.749 \$/kg and ethylene = 0.511 \$/kg). Under this situation, the optimizer should obtain the best feedstock to be cracked in the reactors with optimal operating conditions and maintenance schedule. A brief description of the scenario parameters are tabulated as shown below.

Feedstocks	Ethane, Naphtha
Number of Reactors	3
Time horizon	90 days
Sales limit	Unlimited sales on all the products
Fresh feed	Unlimited feeds available
Degrees of freedom	Feedstock selection, Processing rates, Severity, S/HC and Decoke time periods

Discussion of Results

The scenario is the same as Case 6 except that the ratio of prices for ethylene and propylene are inverted so that propylene is more valuable than ethylene in the market. The main aim here is to find out which feedstock is profitable for ethylene plants under such a situation.

Reactor 1 is explicitly allocated to crack recycled ethane. Therefore, the optimizer has to decide on the feeds to be cracked only in Reactors 2 and 3. From the results, it is clear that the optimizer has chosen to crack naphtha in reactors 2 and 3 at the propylene peak. It makes sense to choose naphtha and crack at propylene peak because it has a much higher yield of propylene, which is the more valuable product in the market. This leads to a conclusion that when there is no limit on sales for the products and propylene is more valuable than ethylene, it is most profitable to crack naphtha in the plant.

The results obtained for this scenario are shown in Figures 4-28 to 4-30. The schedule for maintenance of the reactors is depicted in the Gantt chart as shown in Figure 4-28. Clearly, reactor 1 undergoes three decokes and reactors 2 and 3 undergo two decokes during the entire horizon. Severities corresponding to propylene peak are shown in Figure 4-29 and the processing rates are shown in Figure 4-30.

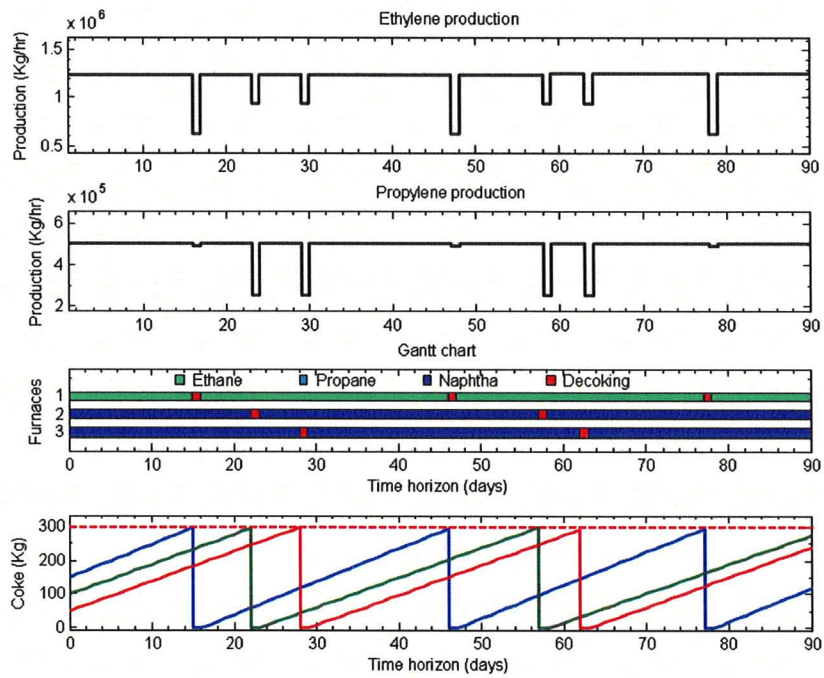


Figure 4-29: Case 7 - Gantt chart and Production details

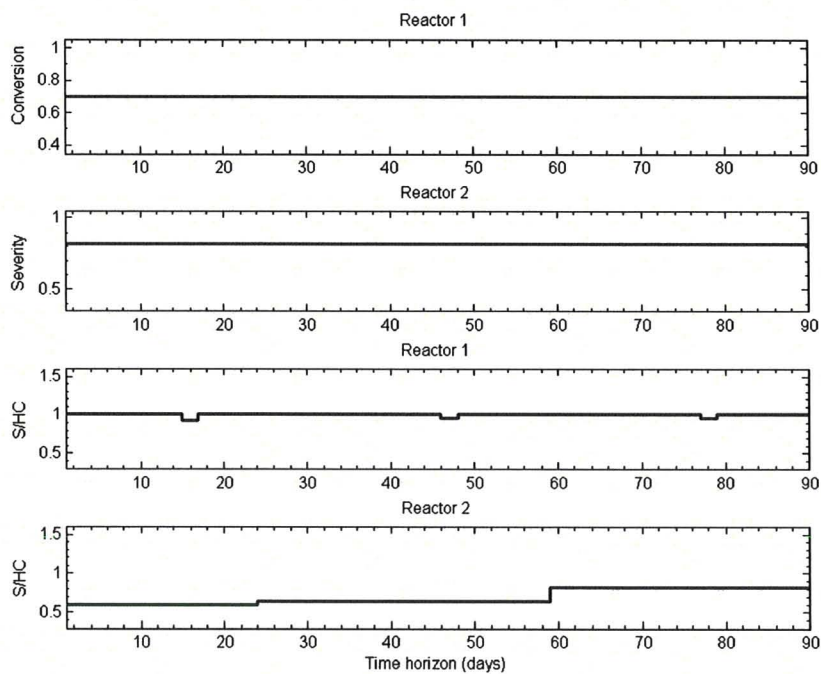


Figure 4-30: Case 7 - Severity and S/HC profiles

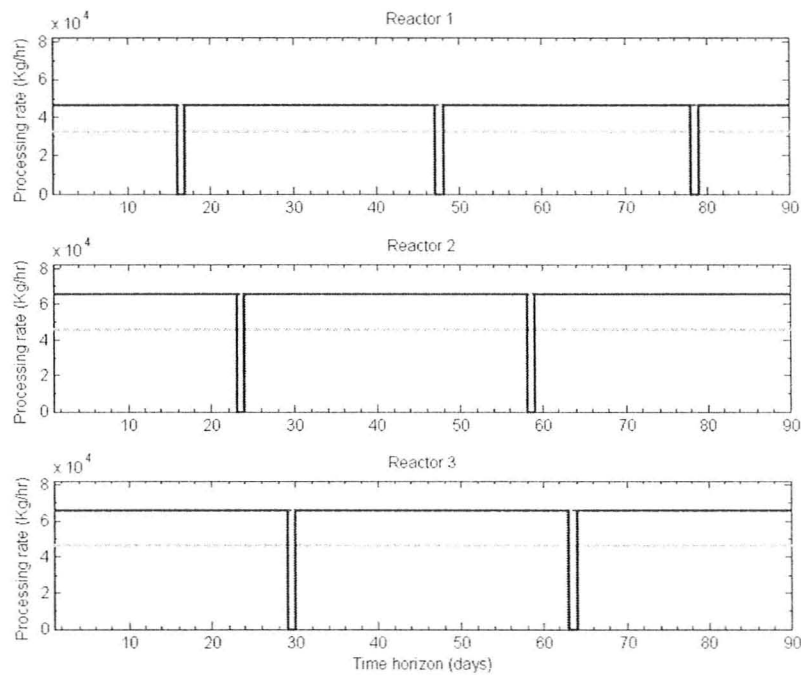


Figure 4-31: Case 7 - Processing rates

4.6.2.3 Case 8 - Large scale problem 1: Sales limit on Ethylene

This is a large scale scheduling problem encountered typical to those in a real plant. In this scenario, ethylene plant can crack ethane, propane and naphtha feedstocks for a total plant capacity of 0.8 – 1 Million MTA ethylene. Unlimited amounts of fresh ethane, propane and naphtha feeds are available for cracking. For a given ethylene demand scenario, the optimizer should process the best feedstock(s) to be cracked in the reactors over time with optimal operating conditions and maintenance schedule. A brief description of the scenario parameters are tabulated as shown below.

Feedstocks	Ethane, Propane and Naphtha
Number of Reactors	5
Time horizon	90 days
Sales limit	On ethylene: 60% of the plant capacity
Fresh feed	Unlimited feed available
Degrees of freedom	Feedstock selection, Processing rates, Severity, S/HC and Decoke time periods

Discussion of Results

For this scenario, the optimizer selects an appropriate feedstock, optimal severity and S/HC for the reactors and adjusts the processing rates appropriately to meet the demands. Reactor1 is explicitly allocated to crack recycled ethane. Therefore the optimizer has to allocate feeds to reactors 2 to 5. Although unlimited amounts of ethane, propane and naphtha feeds are available for cracking, optimizer selects naphtha feed for reactors 2 to 5. It is therefore clear that for the specified plant economics, it is most profitable to crack naphtha than ethane or propane.

The results obtained for this scenario are shown in Figures 4-31 to 4-34. The optimizer chooses to operate Naphtha crackers (i.e. Reactors 2 to 5) at the propylene peak corresponding to a severity of 0.82 and low S/HC of 0.5. At this peak, the reactors produce as much propylene as possible and enough ethylene to meet the ethylene demand and stay within the sales limits. The processing rates for all the five reactors are shown in Figure 4-34. The schedule for maintenance of the reactors is depicted in the form of a Gantt chart as shown in Figure. It is clear that reactors 1 to 4 undergo three decokes whereas reactor 5 has only 2 decokes.

Numerical results obtained from the two-stage temporal decomposition heuristic are shown in Table 4-6. It can be seen that this problem took 1263 seconds in stage1 and 284.25 seconds in stage2 for a total of 1547.25 seconds to solve the entire problem. This large problem could be solved in less than 30 minutes, which highlights the efficiency of the formulation.

Table 4-6: Case 8 - Numerical results

	Stage 1	Stage 2
Discrete time intervals	30	90
Integer variables	577	122
Continuous variables	106006	77086
Constraints	110533	71017
Computational time	1263 secs	284.25 secs
Integrated C₂H₄ Demand	142187500 Kg	
Ethylene produced	142187500 Kg	
Propylene produced	86850840 Kg	
Model Profit	104496482 \$	
Solver details	CPLEX 10.1	

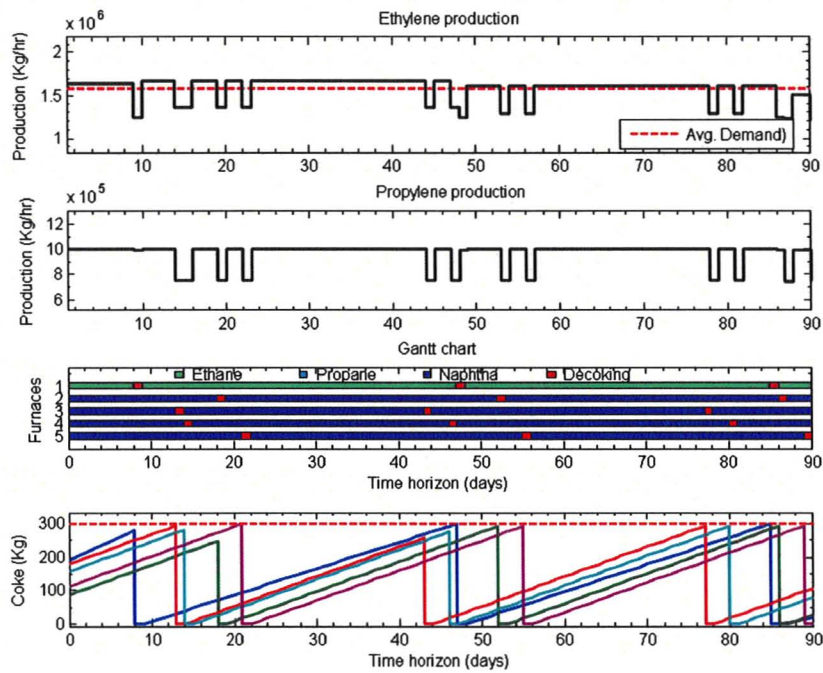


Figure 4-32: Case 8 - Gantt chart and Production details

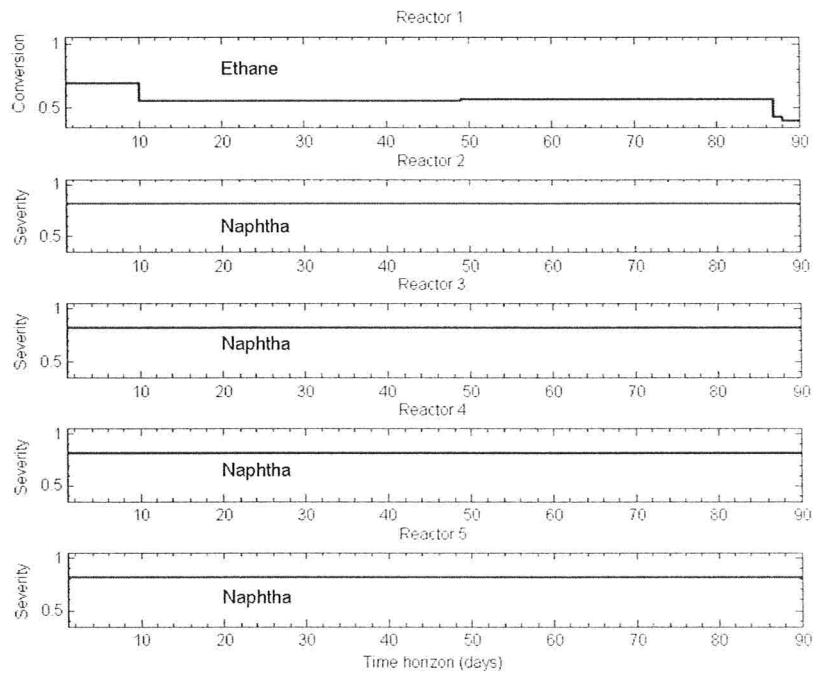


Figure 4-33: Case 8 - Severity profiles

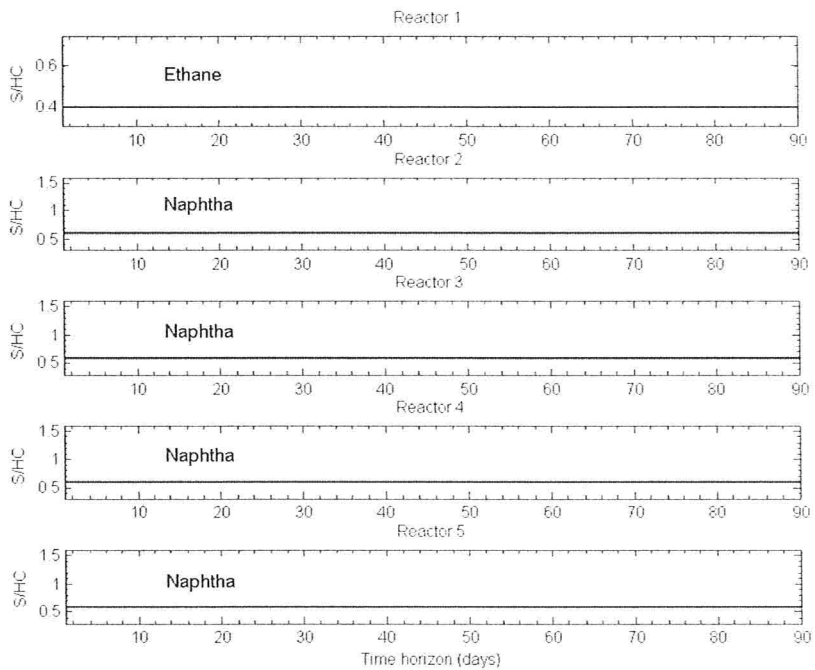


Figure 4-34: Case 8 - S/HC profiles

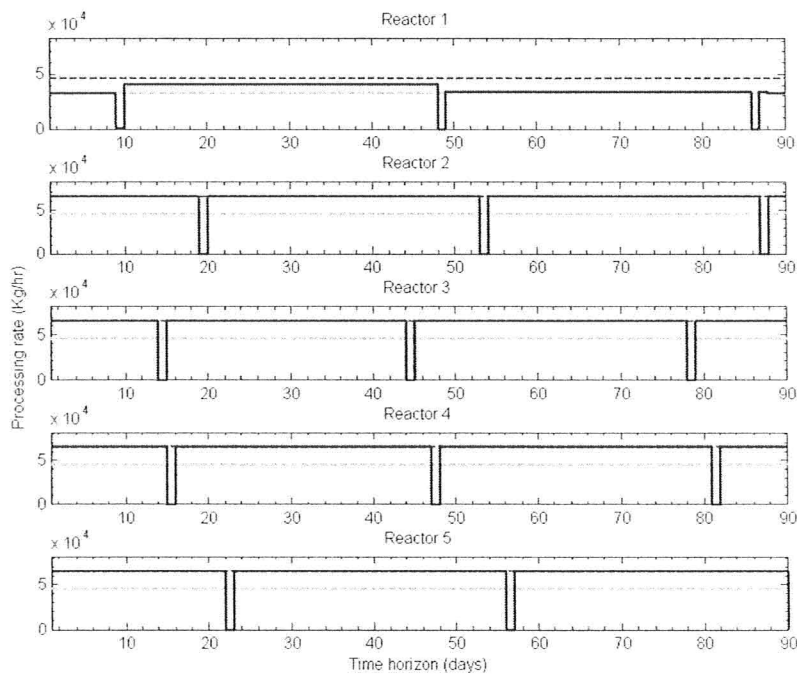


Figure 4-35: Case 8 - Processing rates

4.6.2.4 Case 9 - Large scale problem 2: Sales limit and Limited Naphtha feed

This is again a large scale scheduling problem similar to one discussed in Case 7. In this scenario, ethylene plant can crack ethane, propane and naphtha feedstocks for a total plant capacity of 0.8 – 1 Million MTA ethylene. An unlimited amount of fresh ethane and propane feeds are available, while limited naphtha feed is available. For a given ethylene demand scenario, the optimizer should obtain the best feedstock to be cracked in the reactors over time with optimal operating conditions and maintenance schedule. A brief description of the scenario parameters are tabulated as shown below.

Feedstocks	Ethane, Propane and Naphtha
Number of Reactors	5
Time horizon	90 days
Sales limit	On ethylene: 60% of the plant capacity
Fresh feed	Limited Naphtha and Unlimited Ethane and Propane available
Degrees of freedom	Feedstock selection, Processing rates, Severity, S/HC and Decoke time periods

Discussion of Results

Reactor1 is explicitly allocated to crack recycled ethane. Therefore the optimizer has to allocate feeds to reactors 2 to 5. In this scenario, limited amount of naphtha is available. We have seen in the Case 7 that naphtha is the most optimal feedstock. Since its availability is limited here, the optimizer has to choose between propane or ethane for cracking in the reactors. From the results, it is clear that the optimizer has selected to crack naphtha in two reactors and propane in two reactors. This again leads to a conclusion that propane is the next optimal feedstock after naphtha for this ethylene sales limited case study because it produces a variety of useful products that have good market value.

The results obtained for this scenario are shown in Figures 4-35 to 4-38. The optimizer chooses to operate Naphtha crackers (i.e. Reactors 3 and 5) at the propylene peak corresponding to a severity of 0.82 and low S/HC of 0.5. It also chose to operate propane crackers at its propylene peak corresponding to a severity of 0.8 and low S/HC ratio. For both naphtha and propane crackers, operating at propylene peak produces as much propylene as possible and enough ethylene to meet the ethylene demand and stay within the sales limits. The severity and S/HC for ethane cracker can also be seen from Figures 4-36 and 4-37. Processing rates for all the five reactors are shown in Figure 4-38.

The schedule for maintenance of the reactors is depicted in the form of a Gantt chart as shown in Figure 4-35. It is clear that reactors 2 and 4 cracking propane have two decokes and rest of the reactors undergo three decokes during the entire horizon. This schedule corresponds to a maximum plant profit.

Numerical results obtained from the two-stage temporal decomposition heuristic are shown in Table 4-7. The problem sizes, computational times etc. for both the stages are highlighted. It can be seen that this problem took 1254.5 seconds in stage1 and 782.92 seconds in stage2 for a total of 2037.42 seconds to solve the entire problem. This

large problem could be solved in less than 30 minutes, which highlights the efficiency of the formulation.

Table 4-7: Case 9 - Numerical results

	Stage 1	Stage 2
Discrete time intervals	30	90
Integer variables	147	138
Continuous variables	99796	164360
Constraints	100959	165727
Computational time	1254.5 secs	782.92 secs
Integrated C₂H₄ Demand	142187500 Kg	
Ethylene produced	142187500 Kg	
Propylene produced	87908886.43 Kg	
Model Profit	105467336.57 \$	
Solver details	CPLEX 10.1	

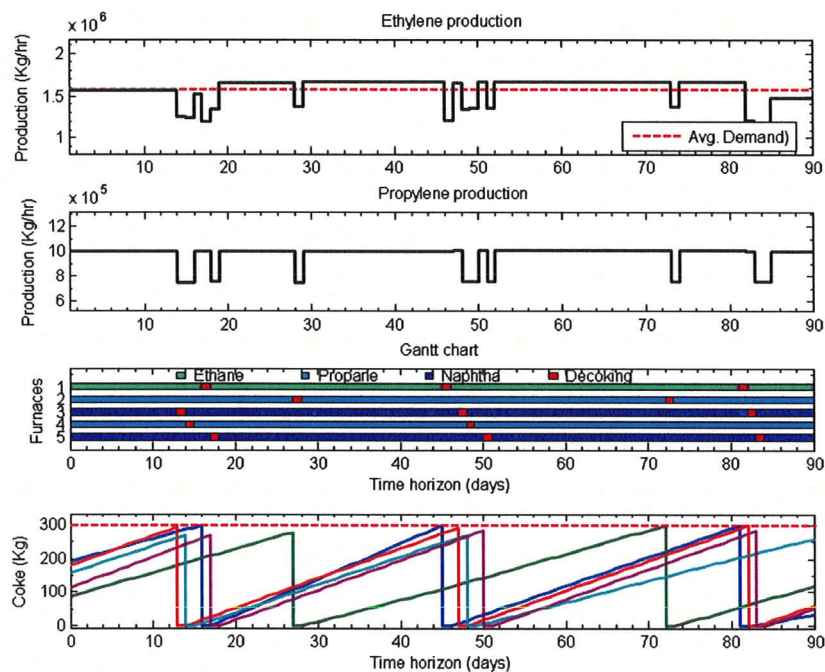


Figure 4-36: Case 9 - Gantt chart and Production details

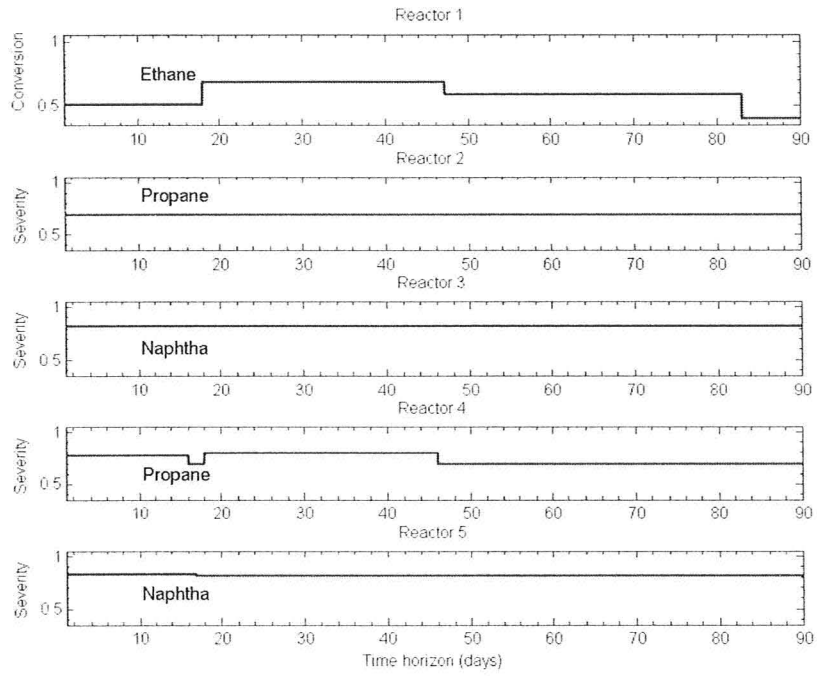


Figure 4-37: Case 9 - Severity profiles

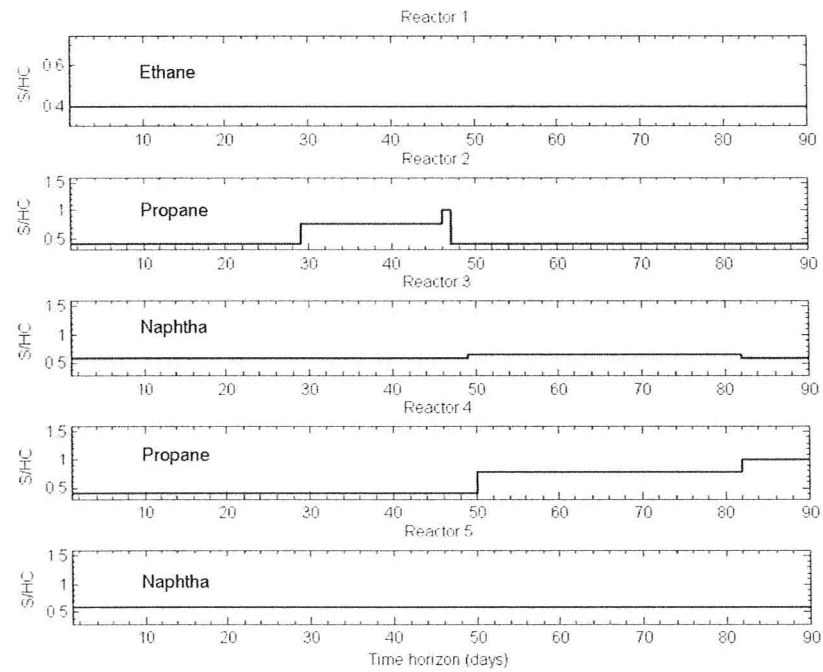


Figure 4-38: Case 9 - S/HC profiles

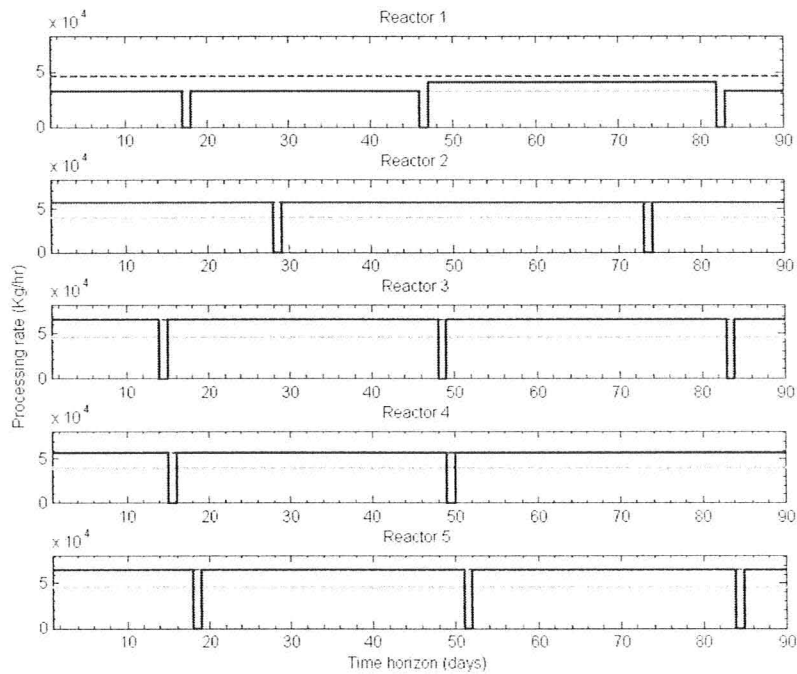


Figure 4-39: Case 9 - Processing rates

4.7 Summary

This chapter has covered the details of mathematical formulation of the scheduler (scheduling optimization model). The basic formulation leads to a large scale MILP (actual size depends on the scenario). It is important to know that the smallest problem (1 feed and 2 reactors) has a size of 180 binary variables, 37080 continuous variables and 37884 linear constraints. For a scenario representing a typical real size plant, the problem size was much larger. A stand alone solver (CPLEX 10.1) could not solve this problem to optimality.

Therefore, tailored schemes were proposed in the form of constraint reformulation, tightening constraints and solutions heuristics. This had reduced the computational time by approximately 40 times for small problems, which means that the scheduling model with tailored schemes was solved 40 times quicker than the basic scheduling model.

The scenarios for single feed and multiple feed were formulated to test the model adequacy and highlight the model capability under various circumstances. The problem was solved to optimality in reasonable times for an optimization that will be made daily in a plant. All results agree with qualitative process understanding, as covered in the discussions of the cases.

Chapter 5. Reactive (closed-loop) scheduling

This main focus of this chapter is on reactive scheduling framework and the implementation issues associated with it. The term “reactive scheduling” denotes a scheduling system that periodically measures selected variables in the plant and resolves the schedule; the results are implemented using a rolling horizon strategy. Thus, reactive scheduling is a feedback control system. Several closed-loop cases studies are presented in this chapter to assess the performance for the reactive scheduling system.

5.1 MPC framework for scheduling

Model predictive control (MPC) has been widely accepted by the process industries as a tool to effectively control multivariate systems with input and output constraints (Qin and Badwell, 2003, Marlin, 2000). MPC uses a plant model for predicting the effects of manipulated variables on output variables, and it solves a mathematical programming problem to optimize the future process behaviour to obtain optimal control moves. These control moves are implemented in the plant in a rolling horizon fashion. The plant model is periodically updated using the feedback information at each controller execution. This feedback mechanism compensates for prediction errors due to parametric and structural mismatch between the model and the plant, measurement errors and forecast errors.

Typical process scheduling methods currently optimize the open-loop behaviour of a system model. In practice, the methods are employed in a rolling horizon mode, with results for the current time period (or several time periods) implemented manually and the entire problem resolved in a batch manner by an engineer. Also, feedback information (e.g., inventories, feed properties, plant performance) is used to update the

model, but this feedback is added to the model manually by an engineer. Therefore, the current, manual scheduling optimization has a structure similar to MPC, and therefore, MPC framework is chosen as a basic framework for developing a closed-loop reactive scheduling system in this thesis.

5.1.1 Framework description

MPC framework for reactive scheduling is shown in Figure 5-1, with the set points, plant inputs, outputs and feedback shown. This structure is general and could be applied using many plant measurements to update numerous predictions. In this thesis, the feedback is limited to coke accumulation in each reactor. The scheduler is the optimizer which solves an open-loop scheduling optimization problem (MILP) at each scheduler iteration. The optimization results for the current time period (feed to each reactor, feed rate, reactor severity and S/HC ratio) are implemented in the plant. Note that the decisions on the number of reactors (furnaces) in operation are not included, since they should be made with manual review and are considered to be offline decisions. In addition, only single-feed type is considered, so that feed selection is excluded from this problem. Just before each scheduler execution, the outputs from the plant are measured and compared with the model outputs to obtain the bias term, which is used as a feedback to update the model, and the open-loop optimization problem is solved again. The set point is imposed on the product demand while obeying the terminal conditions.

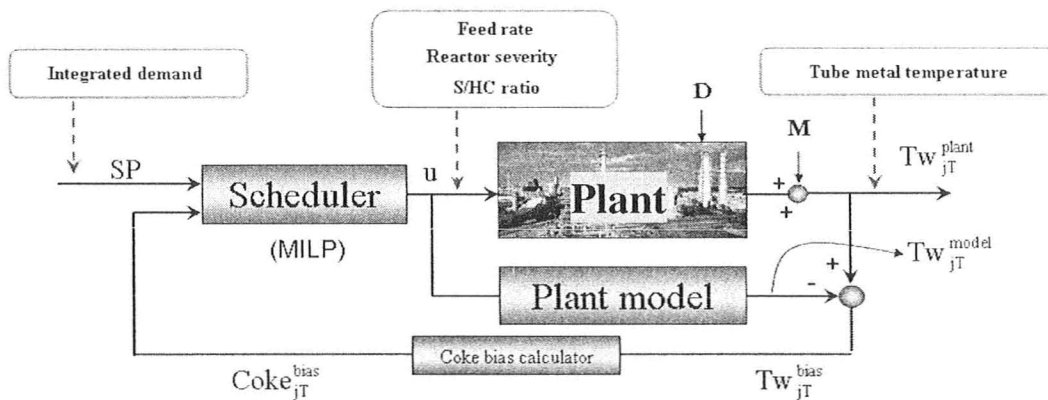


Figure 5-1: MPC framework for closed-loop scheduling

Disturbances entering the plant are represented as D , and the measurement errors are represented as M in the figure. Disturbances and measurement errors are very common in plants. Therefore, there is always a mismatch between the plant information and model prediction, mainly due to: (1) model error (parametric and structural mismatch in the model) (2) measurement error and (3) disturbances. This mismatch is often considered as uncertainty in the model. Any errors in the model prediction due to this uncertainty will be compensated through feedback model updating in the MPC framework.

For the closed-loop system considered in this thesis, as shown in Figure 5-1, the plant and the controller model are considered to be the same except for coke rate. Therefore, the model error is only in the coke build up and hence the tube metal temperature.

As a representation for the true plant, a plant simulation was performed (in AMPL) at every scheduler iteration. Therefore, the measurements obtained from the plant simulation represent the measurements from the true plant.

5.1.2 Available measurements and model updating

Typically, the measurements available from a plant are the production rates of the products and tube metal temperatures. Production rates are used to keep track of the demand met at every scheduler iteration, while tube metal temperatures are used to update the reactor model via feedback mechanism.

As discussed in Chapter 4 and shown here in equation (5.1), the tube metal temperature is modeled as a function of reactor coke. Therefore, as the coke deposited in the reactors changes, the tube metal temperature changes, as modeled by the following equation.

$$T_{jT}^{\text{model}} = \sum_i \sum_k (T_{ik}^{\text{clean}} \cdot \sigma_{ijkt}^{\text{disj}}) + T_{jT}^{\text{const}} \cdot \text{Coke}_{jT}^{\text{model}} \quad \forall j, T \quad (5.1)$$

where, the subscript T denotes time (days) in closed-loop implementation.

This model is used on-line to predict the tube metal temperatures at every scheduler iteration to compare with the measured plant values. Due to the model errors, there will always be a mismatch in the model prediction and the measured value. In order to compensate for those prediction errors in the tube metal temperatures, reactor coke is updated at every scheduler iteration. Reactor coke is not available as a direct measurement from the plant; however, it can be estimated from the plant measurement of tube metal temperature (Tw_{jT}^{plant}). The coke in each reactor is estimated prior to each scheduler execution. First, the error in the tube metal temperature model is calculated.

$$Tw_{jT}^{bias} = Tw_{jT}^{plant} - Tw_{jT}^{model} \quad \forall j, T \quad (5.2)$$

where, Tw_{jT}^{plant} is the tube metal (wall) temperature from plant simulation and Tw_{jT}^{model} is obtained from the controller/optimizer model. We know through equation (5.1) that tube metal temperature is modeled as a function of reactor coke and the reactor severity. Since the severity effect is the same in the model and plant, the mismatch is attributed to the coke, and the coke bias updating can be calculated as shown in the following.

$$Tw_{jT}^{bias} = Tw^{const} * Coke_{jT}^{bias} \quad \forall j, T \quad (5.3)$$

Finally, the coke model is updated as shown in the following equation.

$$Coke_{jT}^{model} = Coke_{jT}^{model} + Coke_{jT}^{bias} \quad \forall j, T \quad (5.4)$$

where $Coke_{jT}^{model}$ is the accumulated coke from the model. Note that this updated coke is used as the initial condition by the scheduler for the optimization. The formulation for the open-loop optimization performed in each MPC iteration is defined in section 5.3.

5.2 Modifications to scheduling optimization for closed-loop implementation

During closed-loop implementation, an open-loop optimization problem is solved at each scheduler iteration. In addition, very large, frequent changes in reactor operation may reduce the life of the furnaces, because of their operation near maximum metal temperatures. These fluctuations are undesirable; therefore, additional constraints should be included in the model so that changes in decision variables are penalised in order to ensure that closed loop response is smooth. Therefore, “move suppression” similar to process control MPC design is included in the scheduler to make it suitable for online implementation.

5.2.1 Move suppression

Move suppression on the process manipulated variables is important to ensure that the process operating conditions do not deviate excessively from their previous state in one controller iteration. It can be accomplished by penalizing the current optimization moves, i.e., the change from the previous optimization manipulated variables. This way, at each iteration, the optimization results remain “closer” to the previous optimization results, which ensures that there are no large changes (fluctuations) in the reactor operating conditions. This is important because these fluctuations affect the reactors and downstream processes and in turn the profitability of the plant.

A sample result is shown in Figure 5-2 (obtained for a scenario with two reactors and naphtha feedstock), where the effect of move suppression in the scheduling model is clearly demonstrated. One can see that without move suppression, the processing rates fluctuate excessively, which would be undesirable. With move suppression, the reactor feed rates are constant between decokes. Importantly, the profits for these two cases are the same; therefore, we see that the move suppression does not have an adverse effect on the profit.

The sharp decrease in the flows to zero is due to reactor decoke operation when the reactor should be shutdown, which is unavoidable. Therefore, while penalizing the moves in the move suppression model, additional care should be taken to make sure decoking moves are *not penalized*. Move suppression is implemented as a penalty appearing in the objective function. An appropriate value of the penalty coefficient is important to ensure a balance between the operational changes and plant profit.

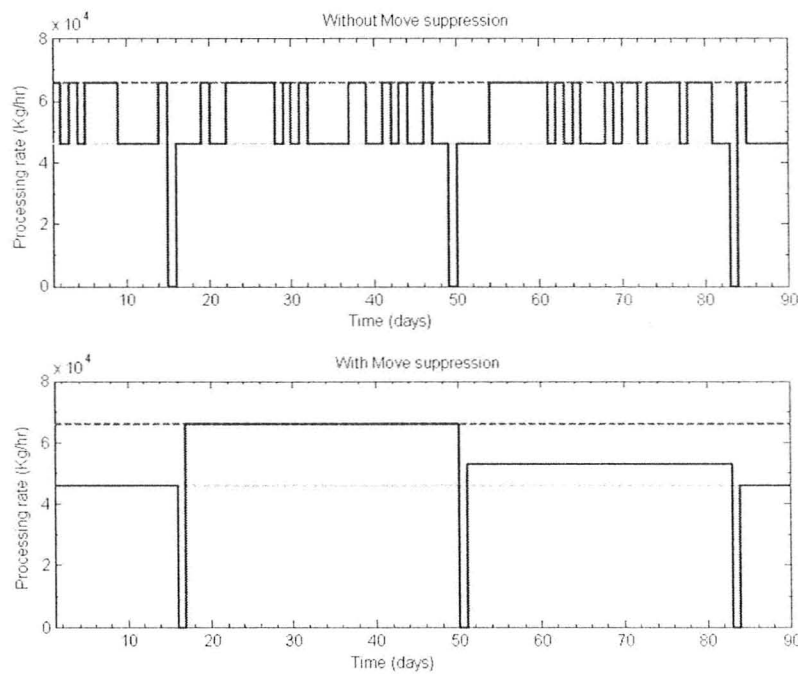


Figure 5-2: Effect of move suppression in closed-loop scheduling

5.2.2 Move suppression constraints

Move suppression in the closed-loop implementation is modelled as a soft constraint. This was accomplished by determining the change from the feed flows values to the disjunctive reactors in the previous optimal solution. The absolute difference between the disjunctive moves is obtained as shown in the following equation.

$$-\Delta m_{ijkT} \leq (PD_{ijkT} - PD_{ijkT-1}) \leq \Delta m_{ijkT} \quad \forall i, j, k, T \quad (5.5)$$

where, PD_{ijkT-1} is the previous optimization result, PD_{ijkT} is the current optimization result.

Move suppression could be accomplished by penalizing the summation of the moves $\sum_{ijk} \Delta m_{ijkT}$ in the objective function during each scheduler evaluation time T , to ensure a smooth response in the operating conditions. However, if we penalize $(\sum_{ijk} \Delta m_{ijkT})$ in the objective function, that will introduce a penalty for all moves, including the decoke moves. (Recall that a large change in the production rate during decoke is required.)

It is therefore necessary to modify the constraint in such a way that it suppresses all the moves except the decoke moves. A new set of variables ΔM_{ijkT} is defined as shown in equation (5.6).

$$\Delta M_{ijkT} \geq \Delta m_{ijkT} \cdot (1 - \delta_{jT} - \delta_{jT-1}) \quad \forall i, j, k, T \quad (5.6)$$

The left hand variables represent the absolute differences between the disjunctive models for all the moves except the decoke moves, including when the reactor is reduction for shutdown and the increase for starting up. Finally, $\sum_{ijk} \Delta M_{ijkT}$ is penalized in the objective function with an appropriate penalty coefficient. In equation (5.6), the left-hand side is zero for the times when the reactor is shutdown and started up; thus, the penalty is zero for these situations. (This constraint assumes that the reactors shall resume immediately after decoke.) The discussion on the penalty coefficient is covered in the next sub-section.

One can notice that equation (5.6) is nonlinear due to the product of continuous variables Δm_{ijkT} and binary variables δ_{jT} , δ_{jT-1} . A reformulation technique discussed by (Gueret et al., 2000) can exactly reformulate bilinear constraints, shown in equation (5.6), as a set of linear constraints. Details regarding the technique are discussed in Appendix B, while the reformulated constraints are provided here.

First, equation (5.6) can be re-written as shown in equation (5.7)

$$\Delta M_{ijkT} \geq \Delta m_{ijkT} - \Delta m_{ijkT}^x - \Delta m_{ijkT}^y \quad \forall i, j, k, T \quad (5.7)$$

where,

$$\Delta m_{ijkT}^x = \Delta m_{ijkT} \cdot \delta_{jT} \quad (\text{Non-linear}) \quad \forall i, j, k, T \quad (5.8)$$

$$\Delta m_{ijkT}^y = \Delta m_{ijkT} \cdot \delta_{jT-1} \quad (\text{Non-linear}) \quad \forall i, j, k, T \quad (5.9)$$

The exact linear reformulation of equations (5.8 and 5.9) are shown below with all continuous variables being non-negative.

Non-linear constraints	$\Delta m_{ijkT}^x = \Delta m_{ijkT} \cdot \delta_{jT}$	$\Delta m_{ijkT}^y = \Delta m_{ijkT} \cdot \delta_{jT-1}$
Exact linear reformulations	$\Delta m_{ijkT}^x \leq \Delta m_{ijkT} \quad (5.8a)$	$\Delta m_{ijkT}^y \leq \Delta m_{ijkT} \quad (5.9a)$
	$\Delta m_{ijkT}^x \geq \Delta m_{ijkT} - P^{\max} (1 - \delta_{jT}) \quad (5.8b)$	$\Delta m_{ijkT}^y \geq \Delta m_{ijkT} - P^{\max} (1 - \delta_{jT-1}) \quad (5.9b)$
	$\Delta m_{ijkT}^x \leq P^{\max} \cdot \delta_{jT} \quad (5.8c)$	$\Delta m_{ijkT}^y \leq P^{\max} \cdot \delta_{jT-1} \quad (5.9c)$
Where, P^{\max} is the maximum processing rate in the reactors		

Equations (5.5), (5.7), (5.8a, 5.8b, 5.8c) and (5.9a, 5.9b, 5.9c) constitute the move suppression constraints. These equations were added for every i, j, k and the summation of the penalties (ΔM_{ijkT}) were included in the objective function.

5.2.3 Penalty coefficient

It is important to select an appropriate penalty coefficient that considers the trade-off between operational changes and the plant economics. Obviously, if the penalty coefficient is higher the fluctuations will be reduced; however, the move suppression can result in lower profits because it reduces the operational flexibility. Figure 5-3 depicts the behaviour clearly. The term “number of fluctuations” used in the figure refers to the number of operational changes, i.e., the number of non-zero ΔM_{ijkT} . One can see that, when there is almost no penalty on the operational moves (i.e. penalty=1E-9), there are many fluctuations in the operating conditions and gradually they are reduced as the penalty increases. On the other hand, plant profit also decreased with the increasing penalty. From Figure 5-3, a penalty coefficient of 0.0001 appears to be a good choice that considers the trade-off between the number of operational changes (fluctuations) and plant profit. The closed-loop scenario (Case 12) was chosen to perform this analysis. Six different values of move suppression penalty coefficients were used in the closed-loop optimization to obtain this graph.

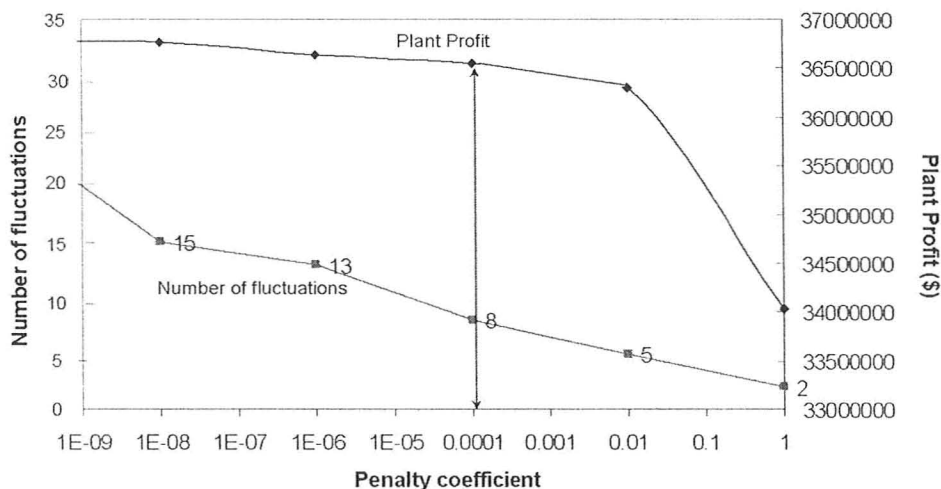


Figure 5-3: Effect of move suppression penalty coefficient on the plant profit and number of operational changes

5.3 Closed-loop scheduler details

The open-loop scheduler model (MILP) is solved every day during the online implementation. For performing a closed loop analysis, in this thesis, only single feed optimization model is considered for simplicity. Therefore, the constraints and objective function of the single-feedstock open-loop scheduler model used in the closed-loop analysis are listed here.

Constraints

Feed balance constraints and

$$F_{it} = \sum_j P_{ijt} \quad \forall i, t \quad (5.10)$$

Disjunctive reactor model constraints

$$\sum_k PD_{ijkt} = P_{ijt} \quad \forall i, j, t \quad (5.11)$$

Production rates

$$PRate_{ijkct} = PD_{ijkt} \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (5.12)$$

$$Prod_{ct} = \sum_i \sum_j \sum_k PRate_{ijkct} \quad \forall c \quad (5.13)$$

$$Sales_{ct} = Prod_{ct} \quad \forall c \quad (5.14)$$

Fraction of flow through disjunctive reactors

$$PD_{ijkt} = x_{ijkt}^d \cdot P_{ij}^{\max} \quad \forall i, j, k, t \quad (5.15)$$

$$\sum_k x_{ijkt}^d \leq 1 \quad \forall i, j, t \quad (5.16)$$

$$x_{ijkt}^d + s_{ijkt}^d = \sigma_{ijkt}^{disj} \quad \forall i, j, k, t \quad (5.17)$$

$$\sum_k \sigma_{ijkt}^{disj} = 1 \quad \forall i, j, t \quad (5.18)$$

$$\sum_k s_{ijkt}^d = \sum_k \sigma_{ijkt}^{disj} - \sum_k x_{ijkt}^d \quad \forall i, j, t \quad (5.19)$$

$$0 \leq s_{ijkt}^d \leq 1 \quad \forall i, j, k, t \quad (5.20)$$

Coking, Tube wall temperature and Decoking

$$Coke_{jt} = Coke_{j,t-1} + \sum_i \sum_k \Delta Coke_{ijkt} - \Delta Decoke_{jt} \quad \forall j, t \quad (5.21)$$

$$\Delta Coke_{ijkt} = (R_{coke_{ik}} \cdot \sigma_{ijkt}^{disj}) \cdot \Delta t \quad \forall i, j, k, t \quad (5.22)$$

$$Tw_{jt} = \sum_i \sum_k (Tw_{ik}^{clean} \cdot \sigma_{ijkt}^{disj}) + Tw^{const} \cdot Coke_{jt} \quad \forall j, t \quad (5.23)$$

$$0 \leq \Delta Decoke_{jt} \leq M \cdot \delta_{jt}^{decoke} \quad \forall j, t \quad (5.24)$$

$$0 \leq Coke_{jt} \leq Coke_{ij}^{max} \cdot (1 - \delta_{jt}^{decoke}) \quad \forall j, t \quad (5.25)$$

$$\sum_j \delta_{jt}^{decoke} \leq 1 \quad \forall t \quad (5.26)$$

$$P_{ij}^{min} \cdot (1 - \delta_{jt}^{decoke}) \leq P_{ijt} \leq P_{ij}^{max} \cdot (1 - \delta_{jt}^{decoke}) \quad \forall i, j, t \quad (5.27)$$

Threshold limits for decoking

$$Coke_{jt} \leq Coke_j^{max} \quad \forall i, j, t \quad (5.28)$$

$$Tw_{jt} \leq T_j^{\max} \quad \forall i, j, t \quad (5.29)$$

Energy constraints

$$E_{jt}^{\text{furnace}} = \sum_i \sum_k PD_{ijkt} \cdot E_{ijk} \quad \forall j, t \quad (5.30)$$

$$E_t^{\text{compressor}} = \sum_i \sum_j \sum_k \sum_c \left(\frac{PRate_{ijkct}}{MW_c} \right) * E^{\text{comp}} \quad \forall t \quad (5.31)$$

Steam generated

$$F_{ijt}^{\text{HPsteam}} = P_{ijt} \cdot G^{\text{HPsteam}} \quad \forall i, j, t \quad (5.32)$$

$$F_{ijt}^{\text{MPsteam}} = P_{ijt} \cdot G^{\text{MPsteam}} \quad \forall i, j, t \quad (5.33)$$

Tightening constraints

$$\sum_{t'=t}^{t+n} \delta_{jt'}^{\text{decoke}} \leq 1 \quad \forall j, t \quad (5.34)$$

$$\sum_t \delta_{jt}^{\text{decoke}} \leq \beta \quad \forall j \quad (5.35)$$

$$\sum_{t=1}^{t+\gamma} \delta_{jt}^{\text{decoke}} \leq 0 \quad \forall j \quad (5.36)$$

$$Coke_{jt-1} \geq Coke_{\text{allowed}}^{\text{decoke}} \cdot \delta_{jt}^{\text{decoke}} \quad \forall j, t \quad (5.37)$$

Integrated demand constraint

$$\sum_t Sales_{ct} \leq Demand_c \quad \forall c \quad (5.38)$$

Move suppression constraints

$$-\Delta m_{ijkT} \leq (PD_{ijkT} - PD_{ijkT-1}) \leq \Delta m_{ijkT} \quad \forall i, j, k, T \quad (5.39)$$

$$\Delta M_{ijkT} \geq \Delta m_{ijkT} - \Delta m_{ijkT}^x - \Delta m_{ijkT}^y \quad \forall i, j, k, T \quad (5.40)$$

$$\Delta m_{ijkT}^x \leq \Delta m_{ijkT} \quad \forall i, j, k, T \quad (5.41)$$

$$\Delta m_{ijkT}^x \geq \Delta m_{ijkT} - P^{\max} (1 - \delta_{jT}) \quad \forall i, j, k, T \quad (5.42)$$

$$\Delta m_{ijkT}^x \leq P^{\max} \cdot \delta_{jT} \quad \forall i, j, k, T \quad (5.43)$$

$$\Delta m_{ijkT}^y \leq \Delta m_{ijkT} \quad \forall i, j, k, T \quad (5.44)$$

$$\Delta m_{ijkT}^y \geq \Delta m_{ijkT} - P^{\max} (1 - \delta_{jT-1}) \quad \forall i, j, k, T \quad (5.45)$$

$$\Delta m_{ijkT}^y \leq P^{\max} \cdot \delta_{jT-1} \quad \forall i, j, k, T \quad (5.46)$$

Data on current operation

During closed-loop implementation, (i) coke accumulated in the cracking coils is updated through bias update, and (ii) the disjunctive flow rates from previous optimization are used for move suppression. Therefore, the data required for current operation are $Coke_{jT-1}$ in equation (5.21) and PD_{ijkT-1} in equation (5.39). As discussed earlier in section (5.1.2) coke ($Coke_{jT-1}$) is estimated from tube-metal temperature (Tw_{jT-1}) measurement.

Objective function

The objective function for every scheduler optimization is given as shown in equation (5.37).

$$Obj_T = Profit_T^{\text{plant}} - Penalty^{\text{coke}} - \omega \cdot \sum_i \sum_j \sum_k \Delta M_{ijkT} \quad (5.47)$$

Where, ω is the penalty coefficient for move suppression.

$$\text{Profit}_T^{\text{plant}} = \text{Value of products} - \text{Cost of feed stocks} - \text{Cost of dilution steam} - \text{Cost of furnace energy} - \text{Cost of compressor energy} + \text{Value of HP and MP steam generated at TLE's} - \text{Cost for furnace decoke.} \quad (5.48)$$

Details of each term in the profit equation are given as follows:

$$\text{Value of products/ Income} = \sum_t \sum_c \text{Sales}_{ct} \cdot \text{Cost}_c^{\text{product}} \quad (5.49a)$$

$$\text{Cost of feedstocks} = \sum_t \sum_i F_{it} \cdot \text{Cost}_i^{\text{feed}} \quad (5.49b)$$

$$\text{Cost of dilution steam} = \sum_t \sum_i \sum_j \sum_k \text{PD}_{ijkt} \cdot \rho_{ik}^{\text{S/HC}} \cdot \text{Cost}_{\text{steam}}^{\text{dilution}} \quad (5.49c)$$

$$\text{Cost of furnace energy} = \sum_t \sum_j E_{jt}^{\text{furnace}} \cdot \text{Cost}_{\text{energy}}^{\text{furnace}} \quad (5.49d)$$

$$\text{Cost of compressor energy} = \sum_t E_t^{\text{compressor}} \cdot \text{Cost}_{\text{energy}}^{\text{compressor}} \quad (5.49e)$$

$$\text{Value of HP and MP steam} = \sum_t \sum_i \sum_j F_{ijt}^{\text{HPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{HP}} + \sum_t \sum_i \sum_j F_{ijt}^{\text{MPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{MP}} \quad (5.49f)$$

$$\text{Cost for furnace decoke} = \sum_t \sum_j \delta_{jt}^{\text{decoke}} \cdot \text{Cost}_{\text{energy}}^{\text{decoke}} \quad (5.49g)$$

$$\text{Penalty}^{\text{Coke}} = \frac{\sum_j \text{Coke}_{jNT}}{\text{Coke}_{\text{max}}} \cdot (\text{Cost}_{\text{decoke}}^{\text{energy}} + \text{Cost}_{\text{decoke}}^{\text{profitloss}}) \quad (5.49h)$$

The equations (5.10) to (5.49) form the open-loop scheduler model (MILP), which is solved each day (T) during online implementation. At the end of every day, the coke model is updated as discussed earlier using equations (5.1) to (5.4), and the scheduler model is resolved the next day.

In order to evaluate the closed loop performance of the framework, only single feedstock and two reactors case studies were considered in this thesis. The solver CPLEX 10.1 was able to solve the problem in around 300 seconds without using the two-stage solution heuristics. Therefore, the two-stage decomposition heuristic was not used in the closed-loop implementation for all the case studies. However, when the closed-loop approach is applied to larger problems, the two-stage solution heuristic would have to be applied.

5.4 Closed-loop case studies

The closed-loop reactive scheduling is implemented daily using a rolling horizon approach for a 90-day horizon. For the first day, no feedback information is assumed available; therefore, an open-loop optimization problem (MILP) is solved. The results for the first day are implemented in the simulated plant, which can have mismatch from the model used in the scheduler. At the end of each subsequent day, the model (coke per reactor) is updated based on the plant measurement of tube metal temperature, and the scheduler open-loop optimization is solved. Again, the results for the first day are implemented in the simulated plant. Therefore, the results we see in this section are the plant operation for 90 days with daily reactive schedule update.

5.4.1 Single feedstock scenarios

For simplicity, only scenarios with a single feedstock and two reactors are considered in the case studies to study the effect of move suppression, measurement error and model error on the closed loop results. They are also used to highlight the capability of the closed-loop framework to handle model errors and disturbances via the feedback mechanism. Measurement error is considered in all the scenarios. A uniformly distributed white noise with mean 0 and standard deviation of (0.1) is used to simulate measurement error in the tube metal temperatures. No filtering was applied to the measurement before updating the coke model.

5.4.1.1 Case 10 - Perfect model without move suppression

This scenario is designed to highlight the importance of move suppression in closed-loop implementation. A perfect model (no model error) is considered and move suppression constraints are not included in the scheduling model. Naphtha is the only available feedstock. The main requirement is to exactly meet the integrated demand on ethylene by the end of the horizon i.e., by the 90th day. A brief description of the scenario parameters are tabulated as shown below.

Feedstock	Naphtha
Number of Reactors	2
Prediction horizon (open loop)	90 time steps
Time horizon (closed loop)	90 days
Integrated Ethylene Demand	4.95 E+7 Kg
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and Decoke time periods
Move suppression coefficient	0
Measurement error	Yes (Uniform white noise)
Plant-model mismatch	No
Disturbances	No

Discussion of Results

Results obtained without move suppression are shown in Figures 5-4 to 5-6. Ethylene production rates, maintenance schedule, coke accumulation over the horizon are depicted in Figure 5-4. Severity and S/HC profiles are shown in Figure 5-5 and the processing rates are shown in Figure 5-6.

As an optimal operating condition for this case, the optimizer selects operating the reactors at a severity corresponding to propylene peak and S/HC corresponding to its lower bound to save energy costs. The optimizer maintains this condition throughout the horizon without making any further changes. However, there are fluctuations in the processing rates which are highlighted as dotted circles in Figure 5-6. These fluctuations

are undesirable for plant operation as they affect the dynamics of the downstream processes by acting as continuous disturbances. It is therefore, necessary to reduce the fluctuations and remain as close as possible to the existing operating conditions. Implementing move suppression in the model can solve this problem.

The typical problem size of each open-loop optimization problem for this scenario is around 171 integer variables, 27906 continuous variables and 32889 constraints. The computational time required to solve an optimization problem of this size every day is around 285 seconds. The integrated ethylene demand was exactly met by the end of the horizon, and the resulting plant profit over the entire horizon is 36947005 \$.

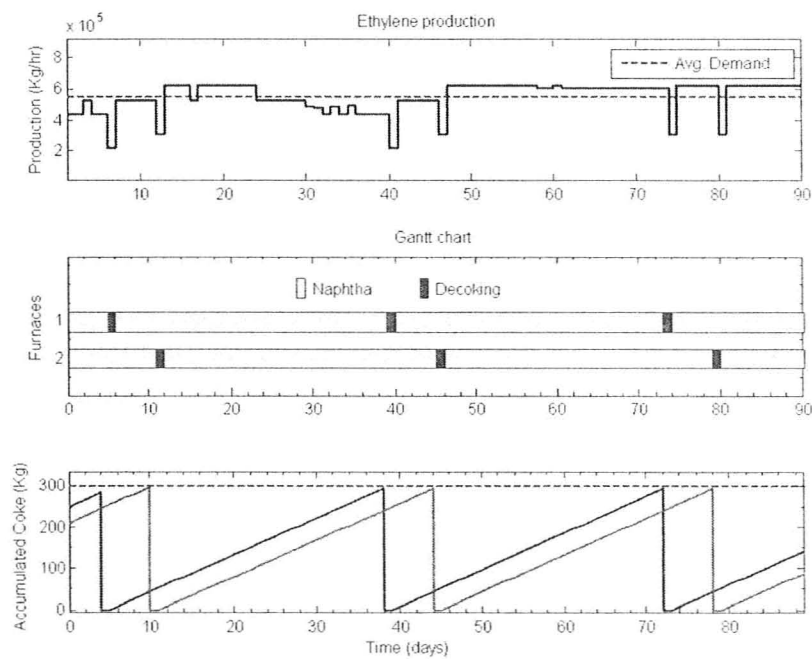


Figure 5-4: Case 10 - Gantt chat and production details

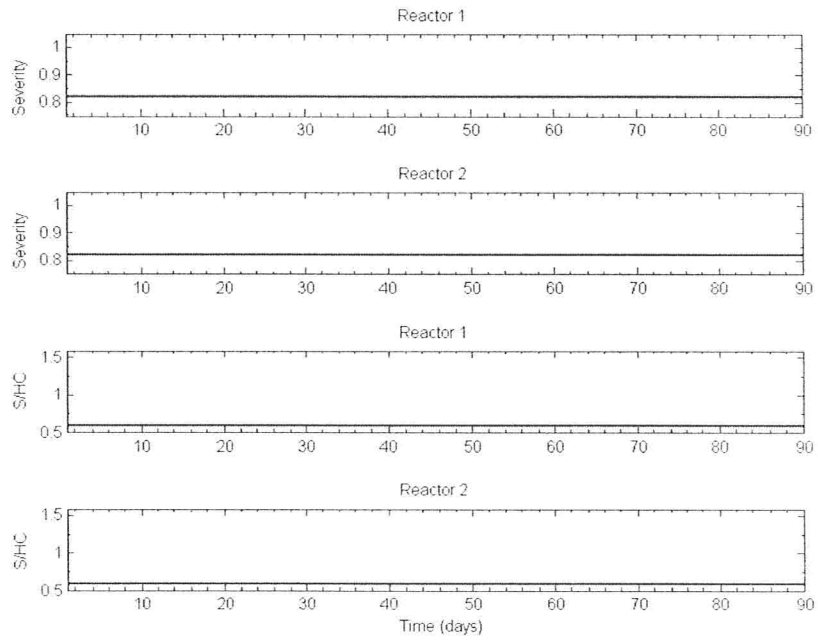


Figure 5-5: Case 10 - Severity and S/HC profiles

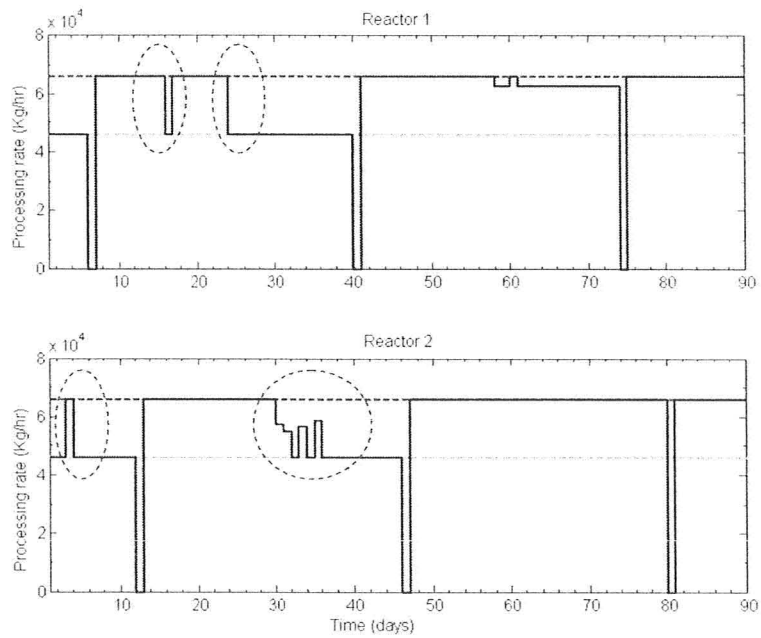


Figure 5-6: Case 10 - Processing rates

5.4.1.2 Case 11 - Perfect model with move suppression

Similar to the earlier scenario, a perfect model is considered but in addition move suppression constraints are implemented in the model. Naphtha is the available feedstock. The requirement is to exactly meet the integrated demand on ethylene by the end of the horizon i.e., by the 90th day. The results should show a smooth closed-loop response as apposed to the earlier scenario without move suppression. A brief description of the scenario parameters are tabulated as shown below.

Feedstock	Naphtha
Number of Reactors	2
Prediction horizon (open loop)	90 time steps
Time horizon (closed loop)	90 days
Integrated C₂H₄ Demand	4.95 E+7 Kg
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and Decoke time periods
Move suppression coefficient	0.0001
Measurement error	Yes (Uniform white noise)
Plant-model mismatch	No
Disturbances	No

Discussion of Results

Results obtained by implementing move suppression in the model are shown in Figures 5-7 to 5-9. Ethylene production details, maintenance schedule, coke accumulation over the horizon are depicted in Figure 5-7. Severity and S/HC profiles are shown in Figure 5-8 and the processing rates are shown in Figure 5-9.

The severity and S/HC ratio profiles are same as the solution without move suppression. However, we notice that after implementing move suppression, the fluctuations in the processing rates have disappeared and the response has smoothed a lot. This is the most desirable condition to operate a reactor. As a result, we remain close to the existing schedule without making any drastic changes in the schedule. Move suppression constraints are therefore, very important and should always be embedded in the scheduling model.

The typical problem size of each open-loop optimization problem for this scenario is around 171 integer variables, 30786 continuous variables and 38649 constraints. The computational time required to solve an optimization problem of this size at each iteration is on an average 296 seconds. The main requirement of meeting the integrated ethylene demand was exactly met by the end of the horizon and the resulting plant profit over the closed loop horizon (90 days) is 36947005 \$. It is important to notice that the profit remained the same as for Case10 . This result demonstrates that there are alternate solutions for this case study.

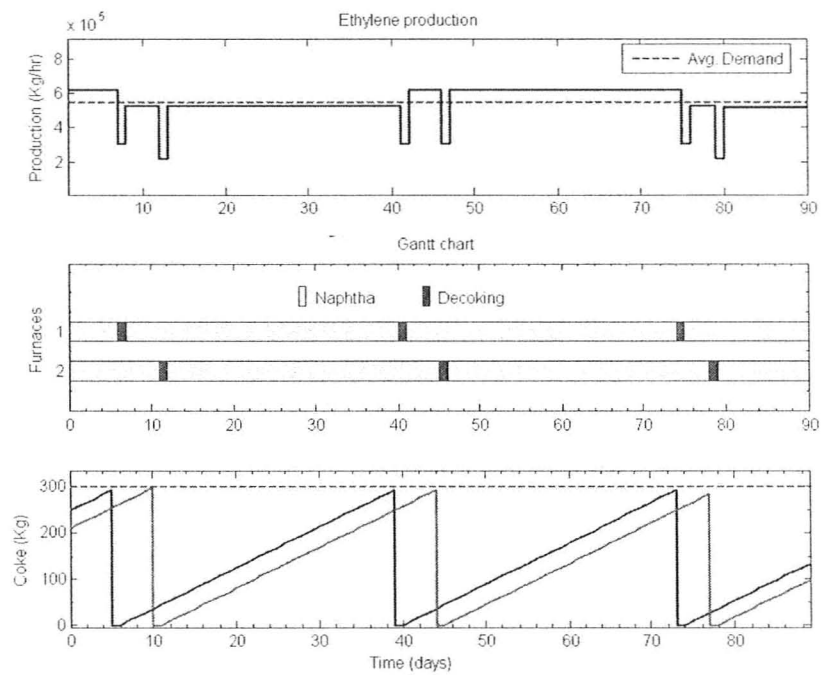


Figure 5-7: Case 11 - Gantt chart and Production details

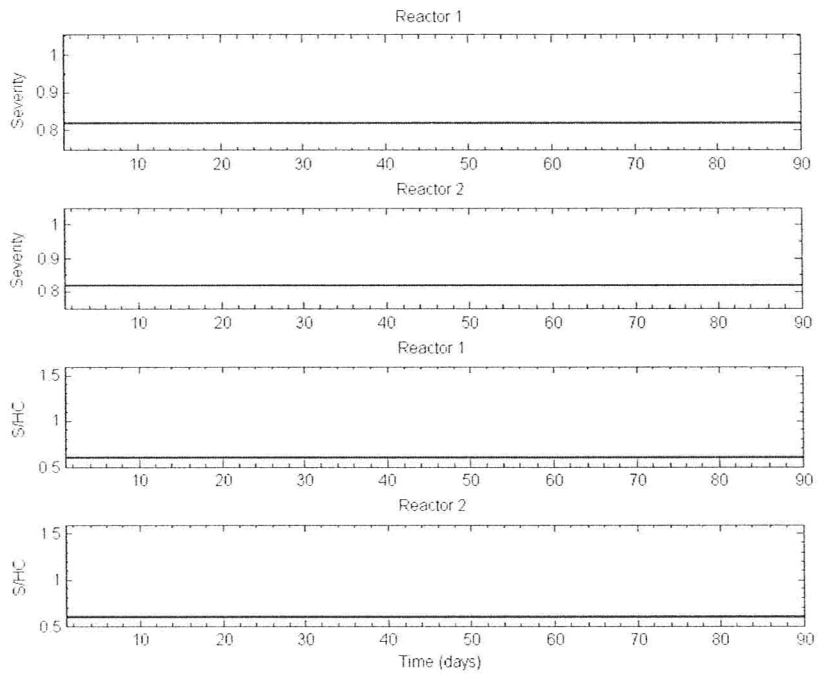


Figure 5-8: Case 11 - Severity and S/HC profiles

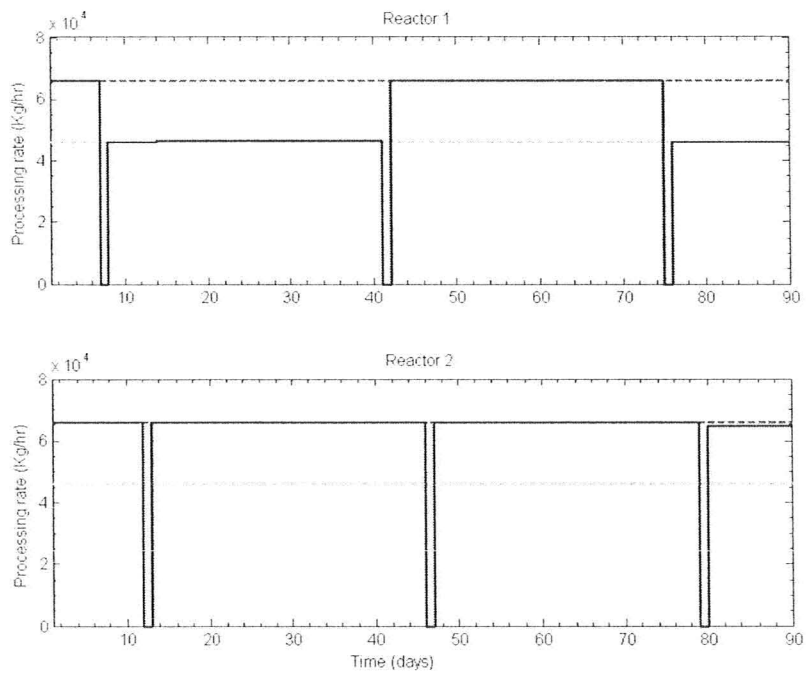


Figure 5-9: Case 11 - Processing rates

5.4.1.3 Case 12 - Plant-model mismatch case

This scenario is designed to study the effect of model error on the closed-loop results. The plant-model mismatch (model error) is considered due to the difference in the coking rates between model and plant. Naphtha is the available feedstock and the requirement in this scenario is to meet the integrated demand on ethylene by the end of the horizon. A brief description of the scenario parameters are tabulated as shown below.

Feedstock	Naphtha
Number of Reactors	2
Prediction horizon (open loop)	90 time steps
Time horizon (closed loop)	90 days
Integrated C₂H₄ Demand	4.95 E+7 Kg
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and Decoke time periods
Move suppression coefficient	0.0001
Measurement error	Yes (Uniform white noise)
Plant-model mismatch	Yes
Disturbances	No

Discussion of Results

In order to model the mismatch for this scenario, it was considered that the coking rates of the model used in the MPC are 5% lower than the coking in plant. The results obtained for this scenario are shown in Figures 5-10 to 5-12. These results are compared with the results of Case 11 to envision the differences.

Similar to Case 11, the optimizer chooses to operate both the reactors at propylene peak and low S/HC ratio as they are the optimum operating conditions. However, because of the model error, the coke prediction from model is different from actual coke deposited in the plant. This mismatch has altered the maintenance schedule by a small extent in comparison to that of Case 11.

In Case 11, Reactor 1 was decoked on 8th, 42nd and 76th days respectively, where as here they are decoked on 9th, 41st, and 75th days. Similarly, Reactor 2 was earlier decoked on 13th, 47th and 80th days whereas now it is decoked on 11th, 45th and 79th days. Clearly there is a change in the maintenance schedule.

The computational time required to solve an open-loop optimization problem at each iteration is around 300 seconds. The integrated ethylene demand was exactly met for this scenario and the resulting plant profit is 36946997 \$.

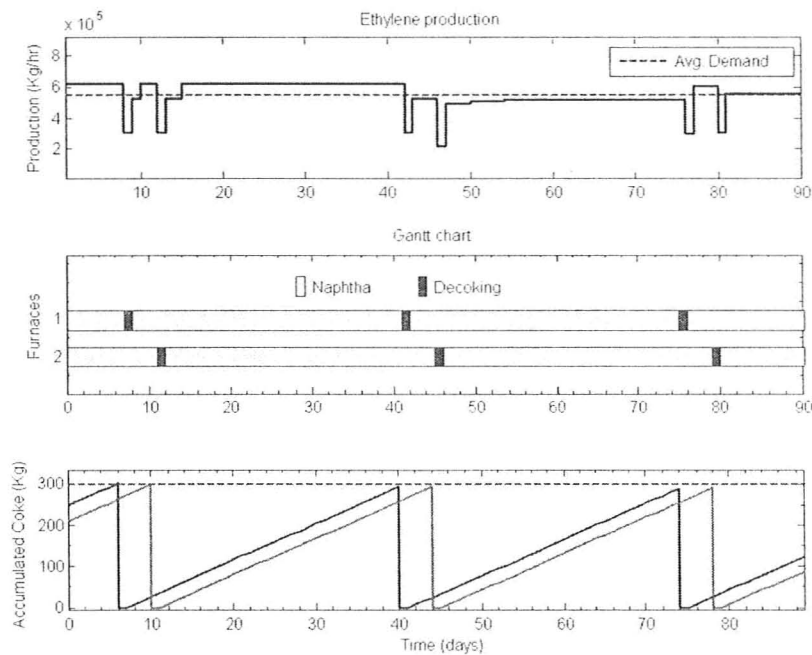


Figure 5-10: Case 12 - Gantt chart and Production details

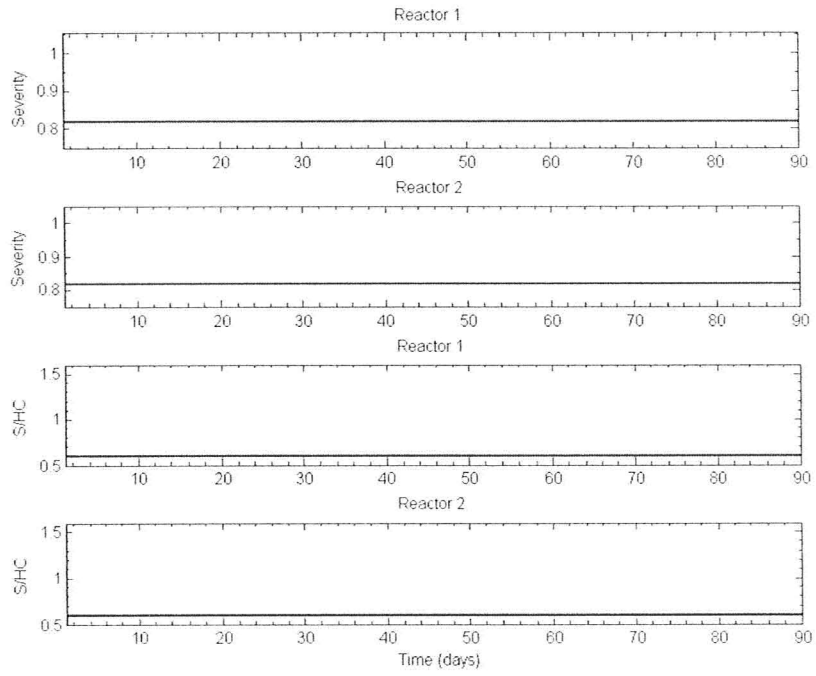


Figure 5-11: Case 12 - Severity and S/H/C profiles

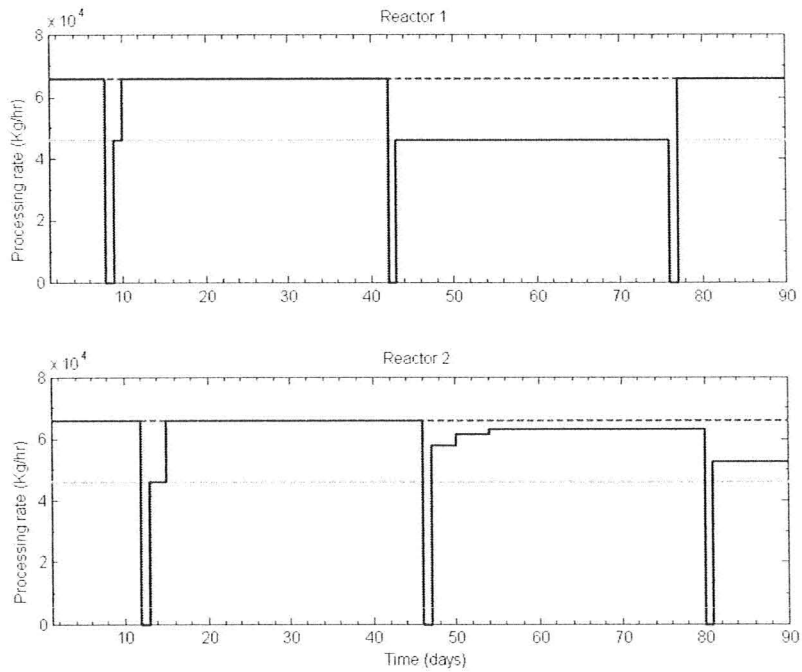


Figure 5-12: Case 12 - Processing rates

5.4.1.4 Case 13 - Plant-model mismatch and Disturbance effect

This is a more realistic scenario encountered in ethylene plants. It is formulated to study the effect of model error and disturbances on the closed-loop results. (1) Plant-model mismatch is modeled due to the difference in the coking rates between model and plant. (2) A disturbance is modeled as reduced available feedstock for a period of one month during the horizon (from 15th day to 45th day), i.e., during this period only 70% of the usual amount of feedstock was available for cracking. During the remaining days, unlimited feed is available. The scheduler is aware of the disturbance and its occurrence period on and after the 15th day, i.e., the optimizer has no prior knowledge of the disturbance. Limited feed availability is common in ethylene plants due to delay in the feedstock delivery or feed processing equipment problems.

Naphtha is the available feedstock and the requirement in this scenario is to meet the integrated demand by the end of the horizon. The results should highlight how the closed loop system reacts to the disturbances and model errors while meeting the integrated demand on ethylene. A brief description of the scenario parameters are tabulated as shown below.

Feedstock	Naphtha
Number of Reactors	2
Prediction horizon (open loop)	90 time steps
Time horizon (closed loop)	90 days
Integrated C₂H₄ Demand	4.95 E+7 Kg
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and Decoke time periods
Move suppression coefficient	0.0001
Measurement error	Yes (Uniform white noise)
Plant-model mismatch	Yes
Disturbances	Yes

Discussion of Results

The results are shown in Figures 5-13 to 5-15. From the results, it is clear that during the first 15 days, when no disturbance is anticipated (unlimited naphtha available), the severity, S/HC ratio and processing rate profiles show a smooth response. The optimizer is not aware of the disturbance till the 15th day. Therefore, it selects optimum operating conditions for the reactors in the form of propylene peak for severity and low S//HC as shown in Figure 5-14.

However, when disturbance enters on the 15th day, the operating conditions in the reactors are changed. From Figure 5-15, we can see that the flow rates are reduced due to the limited availability of naphtha feedstock. The optimizer reacts to this disturbance by increasing the severity in the reactors, shown in Figure 5-14, to compensate for the lower ethylene production due to reduced flow rates and to meet the ethylene demand. This behaviour is seen as long as the disturbance is present, i.e. until the 45th day.

Once the disturbance disappears, the plant returns to its normal operating state. The optimizer chooses to operate the reactors at the propylene peak and low S/HC ratio. However, during this period the processing rates are appropriately adjusted to meet the demands on ethylene exactly by the end of the horizon.

Numerical results have shown that during each iteration, the optimizer needed 305 seconds to solve an optimization problem. The main requirement of meeting the integrated ethylene demand was exactly met and the resulting plant profit is 36542227.6\$.

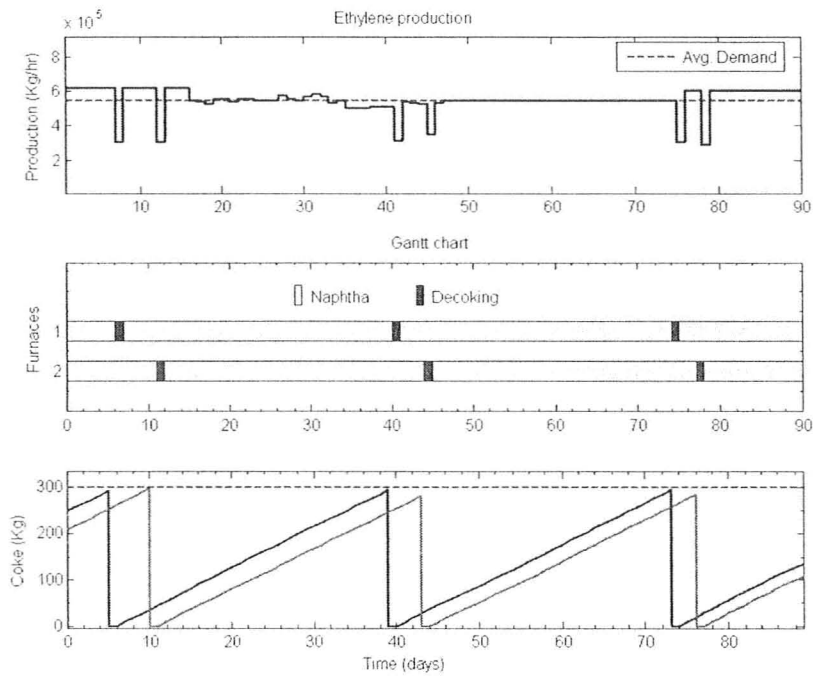


Figure 5-13: Case 13(a) - Gantt chart and Production details

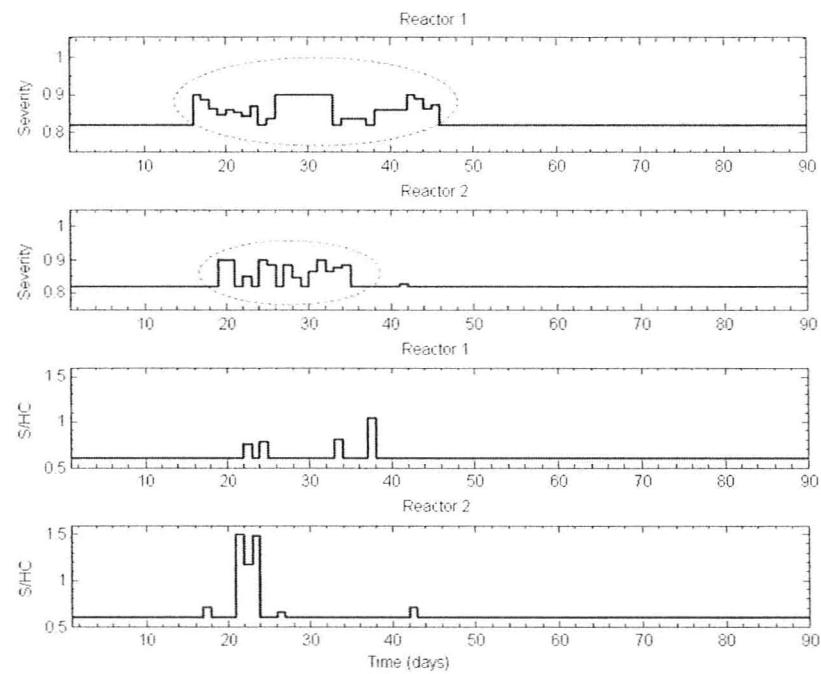


Figure 5-14: Case 13(a) - Severity and S/HC profiles

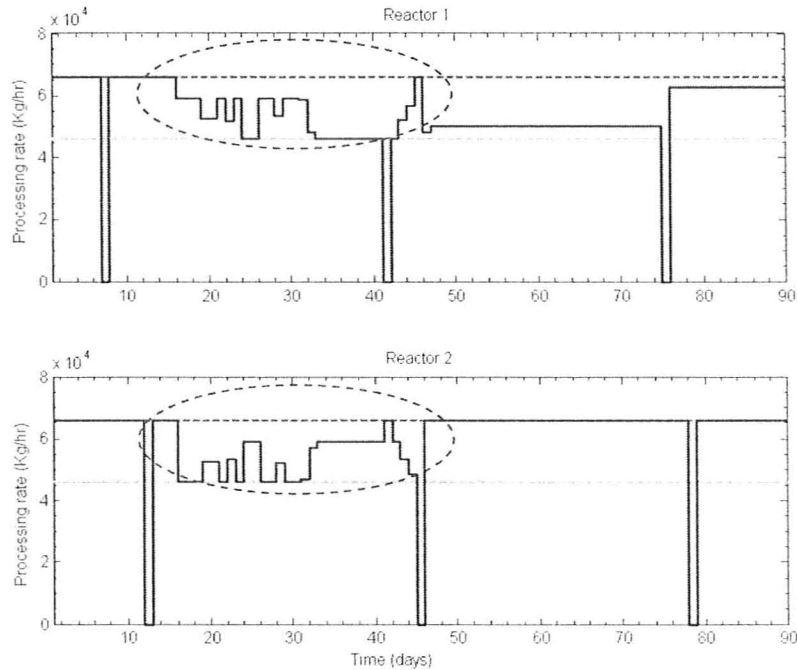


Figure 5-15: Case 13(a) - Processing rates

In Figures 5-14 to 5-15, the fluctuations in the operating conditions are encircled. These fluctuations may not be acceptable in a real plant. They can be reduced by adjusting the move suppression penalty coefficient; however, feed rate changes are required to satisfy the product demands. Results with a higher penalty coefficient (0.01) are shown in Figures 5-16 to 5-18. Although, the operating conditions are smooth here, the plant profit is reduced to 36298834.5\$. There is a trade-off between the operation performance and plant profit. One should understand that each plant has a different operating strategy. An engineer has to analyse the situation and select an appropriate trade-off. Therefore, it is up to an engineer to pick a suitable penalty coefficient.

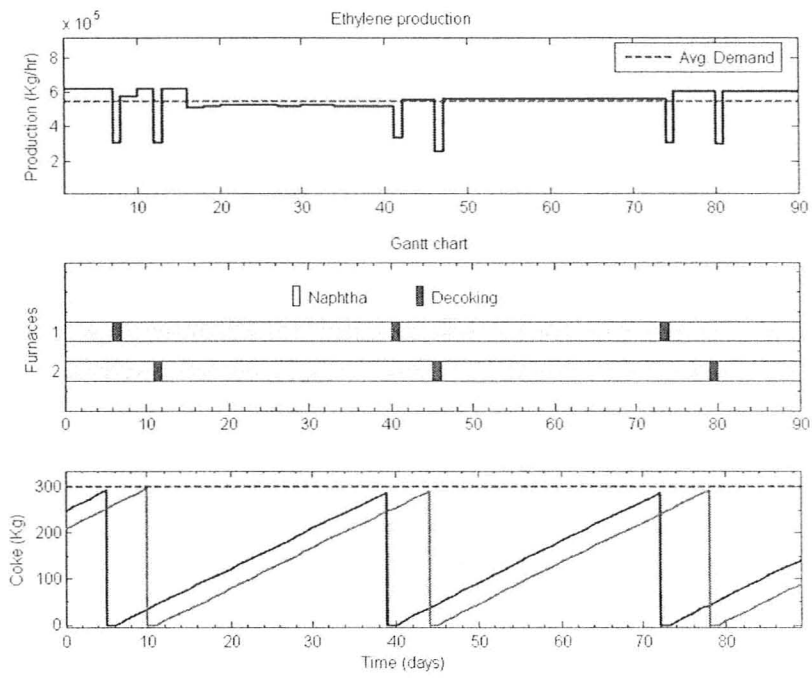


Figure 5-16: Case 13(b) - Gantt chart and Production details

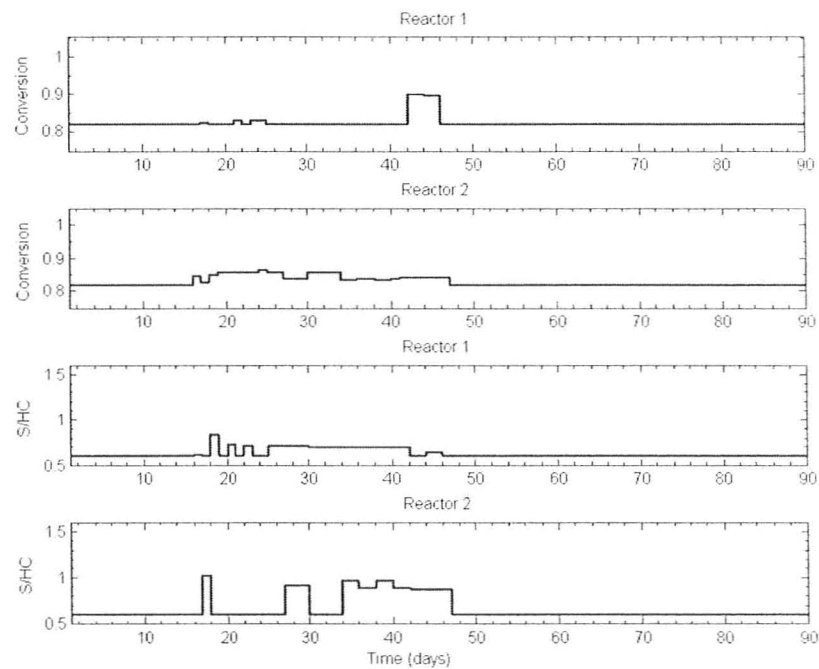


Figure 5-17: Case 13(b) - Severity and S/HC profiles

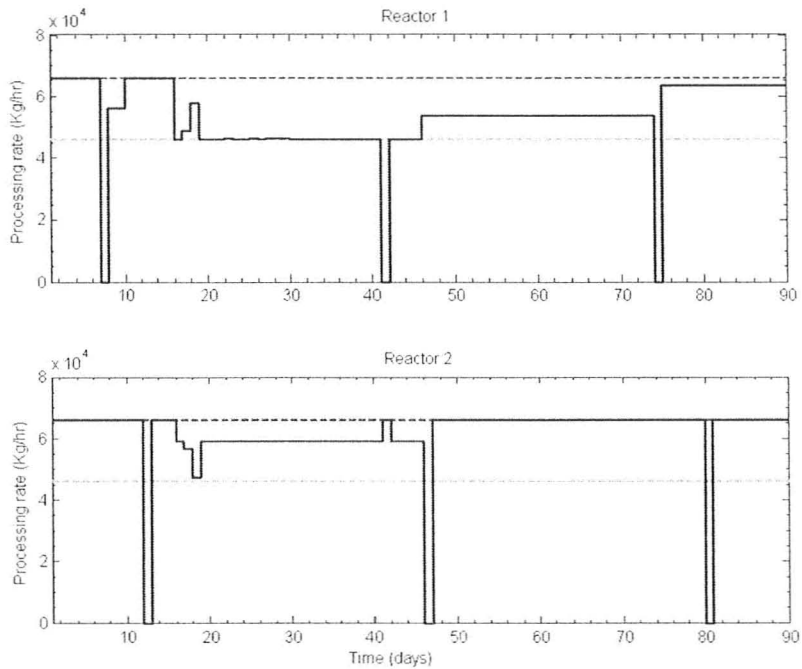


Figure 5-18: Case 13(b) - Processing rates

5.5 Summary

This chapter highlights the reactive scheduling framework and some online implementation issues. The open-loop schedule implementation structure resembles MPC; therefore, MPC framework has been chosen as the basic framework for developing the reactive scheduling system. The coke model was updated through a feedback mechanism just prior to every scheduler execution. The main advantage of this framework lies in its feedback model updating capability so that model prediction always remains close to the true plant behaviour.

The process variable trajectories should be smooth over the scheduling horizon. If not, the fluctuation will affect the operability of the plant and the plant profit in ways that are not included in the scheduler objective function. Therefore, move suppression constraints were developed as soft constraints which penalized all the moves except the decoke moves.

Several case studies were formulated to highlight the capability of the reactive scheduling system to handle the uncertainties in the form of measurement errors, model errors and disturbances. The case studies have shown that there are several alternate solutions for this problem. This was evident from the results of Case10 and Case11. The effect of measurement errors and model errors on the maintenance schedule was clearly seen by comparing Case 12 with Case11.

Finally, a more realistic case encountered in ethylene plants was considered in Case 13. During the presence of disturbance, the system modifies the operating conditions to compensate for the changes in the plant and to meet the integrated ethylene demand on time. It was found that the results of the scheduling system to handle the disturbances depends on appropriate penalty coefficient for move suppression. Since each plant has a different operating strategy, it is up to the engineer to consider the trade off between the operation performance and plant profit and use an appropriate penalty coefficient.

Chapter 6. Conclusions and Recommendations for future work

The main aim of this research work was to develop a reactive (closed-loop) scheduling system that automatically generates a schedule that can be implemented in the plant in real time. To develop such a system, the work was carried out in two phases. In the first phase, an open-loop scheduling model was formulated using rigorous optimization techniques. The goal was to ensure that the model can be solved in reasonable computing time, giving an optimal, feasible solution during the schedule horizon and leaving the plant in a state at the end of the horizon that provides the opportunity for feasible and continued profitable operation. In the second phase, this model was applied in a prototype closed-loop framework to develop a reactive scheduling system that can assist engineers to make appropriate decisions in a timely manner.

While these goals were successfully achieved, the technology (reactive scheduling system) developed in this thesis needs to be further improved before being directly applicable in the industry. The major conclusions and contributions of the research and the recommendations for future work are discussed in the following sections.

6.1 Conclusions

6.1.1 Open-loop optimization

- A comprehensive scheduling model has been developed in this thesis for scheduling the maintenance and operation of furnaces in ethylene plants. The model was formulated as a Mixed Integer Linear Programming problem

(MILP) using a discrete time representation and disjunctive modelling resulting in a large scale optimization problem.

- To preserve the linearity of the model, a disjunctive modelling approach was employed to formulate the nonlinear relationships in the reactor yields and coking rates as linear constraints. Also, the large number of binary variables associated with this approach was minimized by using only continuous variables in the disjunctive model. The results from the cases considered in the thesis have demonstrated that this approximation did not lead to any interpolation between the operating conditions, as unique solutions were obtained without integer variables. Although, this approximation is valid for this furnace scheduling problem, it may not be suitable for direct application to other problems without careful analysis during the model formulation stage.
- The combinatorial nature of the scheduling model (MILP) when accompanied by large problem size made it exceptionally difficult to solve in a reasonable amount of time. Therefore, to overcome these computational challenges, a tailored formulation was developed during the course of the work to improve the model structure and make it computationally tractable.
- Firstly, several reformulated constraints and tightening constraints were added to the scheduling model. Most notably these constraints reduced the integrality gap of the relaxed model (all continuous variables), thus making it a better model. Integrality gap is defined as the gap between the best current all-integer solution and the best current relaxed solution. Naturally, the smaller the integrality gap, the better is the formulation.
- Secondly, a two-stage temporal decomposition heuristic was proposed as an efficient solution strategy to solve the model in two-stages. Results have shown that even large models were easily solved using this heuristic which were unsolvable or needed excessive computational time. It was also confirmed (for a small problem: 1 feed, 2 reactors) that this heuristic did not

affect the optimal solution of the MILP when solved in two stages. Even if the heuristic affects the optimality for larger problems, it achieved a good feasible solution at all times, avoiding problems during online applications.

- Overall, the proposed tailored schemes had a profound effect on the computational time of the scheduling model as it improved the computational efficiency by over 240 times. For example, an industrial size furnace scheduling problem with 3 feedstocks and 5 reactors would end up in a problem size of 3100 binary variables, 297794 continuous variables and 308629 linear constraints for a scheduling horizon of 90 days. This model was unsolvable in 5 days of computation without the tailored schemes, whereas with them it was solved in about 2050 seconds (34 mins) with the reformulation.

The key contributions of the work in open-loop optimization are:

- **MILP model:** The open-loop scheduling model developed in this thesis is the first MILP formulation for furnace scheduling reported in the literature. This model enables the optimizer to make all key decisions (feed type, feed rate, reactor conditions, decoking) in an integrated manner. All the previous models are MINLP formulations (Schulz et al., 2006, Lim et al., 2006, Kelly, 2005 and Grossmann et al., 1998), which posed severe computational difficulties leading to many assumptions in the models as reported in Chapter 2.
- **Novel formulation:** A tractable formulation tailored to the furnace scheduling problem was developed in this thesis. The main features of this formulation include (a) Tractable disjunctive model, (b) Reformulated and Tightening constraints, and (c) Two-stage temporal decomposition solution heuristic.

6.1.2 Closed-loop optimization

- Model Predictive Control (MPC) framework was chosen for developing a closed-loop implementation of the scheduling model because of its feedback mechanism that compensates for model errors, measurement errors and disturbances. Since the open-loop scheduling model is an MILP, the closed-loop system resembled a hybrid MPC problem. During every closed-loop execution, a MILP was solved and the implementation was carried out in a rolling horizon manner. Since the open-loop model was tractably formulated using tailored formulation and solution schemes, the hybrid MPC problem was solved successfully, i.e., with reasonable computing times, acceptable manipulated variable behavior, and solved to optimality.
- During closed-loop implementation, fluctuations (large higher frequency changes) in the optimization results were observed. To eliminate these undesirable fluctuations, move suppression constraints were added to the model in the form of soft constraints. These constraints were tailored to the scheduling problem, penalizing all the moves except the large decoking moves, which are required during maintenance. The results have indicated that besides obtaining a smooth closed-loop response, the move suppression did not have a significant adverse effect on the closed-loop profit.
- The closed-loop implementation was tested for different scenarios over a 90-day scheduling horizon. The results demonstrated that the scheduling system is capable of adjusting the optimization results appropriately in real time when unexpected process disturbances affect the plant operation. The results also indicated that since every plant has different operational performance criteria, it is up to the engineers to use appropriate move suppression penalty coefficients to achieve significant economic benefits.

The key contributions of the work in closed-loop optimization are:

- **Hybrid MPC framework:** MPC framework was chosen as the prototype for implementing the closed-loop scheduling system. Since the open-loop scheduling model (MILP) had integer variables, the MPC framework with integer optimization at each optimizer execution would resemble a hybrid MPC problem. The main contribution in this context is related to successful implementation of the hybrid MPC framework over a 90-day period without encountering adverse dynamic behavior.

6.2 Recommendations for future work

In order to make the closed-loop scheduling system developed in this thesis ready for industrial application, some improvements have to be made to the scheduling model. The following are the recommendations for future work.

6.2.1 Better Furnace model

The furnace model used in this thesis is based on the data obtained from literature as reported in Appendix A. Since only limited information was available from the literature, the effects of the most important variables were considered in the model. For example, coking in the reactors was modelled only as a function of reactor severity and S/HC ratio. Feed flow rates also effect coking in the reactors, but this effect was not considered in the model due to limited available information. The section on modelling assumptions (Section 3.5) clearly states which variable effects were not included in the model. Therefore, in order to develop a scheduling system that is applicable in industrial practice, it is important to build a comprehensive furnace model that considers all the process variables and their effects on the furnace operation. Such a model can be developed by collaborating with an industrial partner. Plant engineers at ethylene plants could not only provide the data we require but also a lot of insight on the furnace

operation. Alternatively, vendors who develop process solutions (e.g. scheduling software) for industries such as Aspen Technology or Honeywell could also provide us some information from their state-of-the-art simulation tools.

6.2.2 Uncertainty

The scheduling model developed in this thesis is deterministic which assumes exact a priori knowledge of the model parameters (market demands, prices, feed characteristics). This is almost never the case in reality e.g., the market demand changes very often. In general, uncertainty is always prevalent in scheduling systems. The common sources of uncertainty arise due to fluctuations in the market prices, raw material qualities, customer demands, product specifications and plant-model mismatch. Measured disturbances occurring due to planned feed deliveries, product shipments, equipment maintenance and other causes can also be decisive in the optimal decision making process. In such highly uncertain environment, deterministic approaches have limitations for decision-making. Therefore, uncertainty handling capability should be included in the scheduling systems. Open-loop uncertainty and closed-loop uncertainty are the two main directions of research in this regard. Appendix D provides some literature on optimization under uncertainty, which is applicable for scheduling optimization.

6.2.3 Integration of Scheduling and Real Time Optimization

When automating the scheduling system, an important consideration is the integration of scheduling and real-time optimization. Closed-loop real-time optimizers (RTO) are becoming a standard in the olefins industry. Real-time optimizers are based on non-linear models and optimize plant operations on an hour-by-hour basis. Schedulers use a simplified model and are executed once a day to generate schedules for reactor operation and maintenance. These decisions have to be transferred to the RTO optimization layer, where they are fine tuned by the real time optimizer before implementing into the plant. Similarly, the scheduler would need some information from the real time optimizer to initialize the scheduling model, e.g. the operating conditions

that were implemented in the plant. Therefore, there is an exchange of information between these two layers. Proper integration of these two systems should resolve any conflicts arising during real time operation.

6.2.4 Relaxation of Binary Variables

In this application of MILP, many integer variables for selecting the disjunctive models were removed from the formulation. The result was a model that yielded solutions that could be implemented in the plant, closely or exactly matching the best integer solution, and could be computed in reasonable times. This approach was developed from “engineering insight” in this specific problem. A more fundamental method for recognizing when such a relaxation would be beneficial would be helpful for the engineer when building models. Also, a modified branch and bound strategy could perhaps take advantage of the solution obtained from the fully relaxed disjunctive integer variables by intelligently adding (a few) integer variables when the current approach did not yield an all-integer solution or a solution that could be interpolated, as discussed in Appendix B.

6.2.5 Move Suppression in Hybrid Models

Hybrid models have integer and continuous variables. The move suppression approach developed for MPC and used in this study penalizes changes in the manipulated variables from values in the previous solution. This approach is generally appropriate for process control, where it provides stability for moderate model mismatch and reduces manipulated variable variance. However, there are instances when a large fixed cost is incurred for any change in a manipulated variable; in other instances, changes in many contiguous time periods are unacceptable. Therefore, novel methods for modeling the cost of manipulation are needed in production scheduling, some of which might require integer variables.

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Appendix A

Summary of the data used in the model

A.1 Economics

The prices for the hydrocarbons used in the model were obtained from (Oil and Gas journal, 1992).

Component	Price (US\$/Kg)
Hydrogen (H ₂)	0.881
Methane (CH ₄)	0.220
Ethylene (C ₂ H ₄)	0.650
Ethane (C ₂ H ₆)	0.241
Propylene (C ₃ H ₆)	0.511
Propane (C ₃ H ₈)	0.260
Butadiene (C ₄ H ₆)	0.771
1Butene (C ₄ H ₈)	0.811
n-Butane (C ₄ H ₁₀)	0.300
Pentanes plus (C ₅ +)	0.401
Light Naptha	0.361
Gas oil	0.297

The prices of energy and steam (Campagne, 1981) used in the model are shown below. Since the price for energy was reported in \$/KJ, it is assumed to be the same for furnace energy and compressor energy.

Item	Price (US \$)
Furnace energy	3.5×10^{-6} \$/KJ
Compression energy	3.5×10^{-6} \$/KJ
Dilution steam	4.41×10^{-3} \$/Kg
High Pressure steam	9.02×10^{-3} \$/Kg
Medium Pressure steam	7.58×10^{-3} \$/Kg

A.2 Disjunctive reactor operation conditions

The disjunctive models for ethane, propane and naphtha feedstocks are shown here. The tables also contain information on Coil Outlet Temperature (COT), ethylene and propylene yields associated with the disjunctive models.

A.2.1 Ethane feedstock

Disjunctive models	S/HC (ratio)	Severity (% conversion)	COT ($^{\circ}$ C)	C=C yield	C3H6 yield
Ethane1	0.4	40	804.59	0.346	0.005
Ethane2	0.4	50	835.17	0.416	0.008
Ethane3	0.4	60	823.41	0.487	0.011
Ethane4	0.4	70	832.43	0.515	0.016
Ethane5	1	40	825.05	0.355	0.004
Ethane6	1	50	814.33	0.428	0.006
Ethane7	1	60	844.60	0.502	0.009
Ethane8	1	70	853.97	0.557	0.010

A.2.2 Propane feedstock

Disjunctive models	S/HC (ratio)	Severity (% conversion)	COT ($^{\circ}$ C)	C=C yield	C3H6 yield
Propane1	0.4	70	814.31	0.257	0.189
Propane2	0.4	80	825.85	0.301	0.175
Propane3	0.4	90	840.42	0.348	0.146
Propane4	0.4	95	851.37	0.370	0.106
Propane5	1	70	832.57	0.269	0.189
Propane6	1	80	844.50	0.321	0.175
Propane7	1	90	859.57	0.375	0.147
Propane8	1	95	870.91	0.399	0.107

A.2.3 Naphtha feedstock

Disjunctive models	S/HC (ratio)	Severity (% conversion)	COT ($^{\circ}$ C)	C=C yield	C3H6 yield
Naptha1	0.6	82	795.34	0.196	0.156
Naptha2	0.6	90	806.95	0.232	0.159
Naptha3	0.6	96	820.45	0.267	0.151
Naptha4	0.6	100	852.53	0.274	0.127
Naptha5	1.5	82	810.58	0.219	0.158
Naptha6	1.5	90	822.53	0.258	0.161
Naptha7	1.5	96	836.42	0.295	0.152
Naptha8	1.5	100	869.46	0.310	0.126

A.3 Product yield information

The product yields for ethane (Froment et al., 1976), propane (Vandamme et al., 1975) and naphtha (Plehiens et al., 1987) feedstocks associated with each disjunctive model are shown here.

A.3.1 Ethane feedstock

Disjunctive models	Ethane1	Ethane2	Ethane3	Ethane4	Ethane5	Ethane6	Ethane7	Ethane8
Conversion (w.fr.)	0.40	0.5	0.60	0.69	0.40	0.50	0.60	0.69
COT (C)	804.59	814.34	823.41	832.43	825.05	835.17	844.6	853.97
S/HC (ratio)	0.40	0.40	0.40	0.40	1.00	1.00	1.00	1.00
Yield (wt%)								
H2	2.50	3.05	3.60	4.30	2.50	3.06	3.62	4.30
CH4	1.40	2.46	3.51	5.64	1.25	2.00	2.75	3.21
C2H2	0.00	0.12	0.25	0.38	0.00	0.12	0.25	0.38
C2H4	34.57	41.64	48.70	51.45	35.48	42.84	50.20	55.74
C2H6	59.52	49.37	39.22	30.60	59.03	49.14	39.25	29.99
C3H4	0.00	0.01	0.01	0.02	0.00	0.01	0.01	0.02
C3H6	0.50	0.78	1.05	1.55	0.37	0.62	0.88	1.02
C3H8	0.01	0.07	0.14	0.20	0.01	0.07	0.14	0.20
C4H6	0.41	0.83	1.25	1.47	0.41	0.83	1.25	1.47
C4H8	0.19	0.20	0.22	0.23	0.19	0.21	0.22	0.23
C4H10	0.39	0.34	0.29	0.24	0.39	0.34	0.29	0.24
C5+	0.50	1.13	1.76	3.92	0.37	0.76	1.15	3.21

A.3.2 Propane feedstock

Disjunctive models	Propane1	Propane2	Propane3	Propane4	Propane5	Propane6	Propane7	Propane8
Conversion (w.fr.)	0.70	0.80	0.900	0.95	0.70	0.80	0.900	0.95
COT (C)	814.31	825.85	840.417	851.37	832.57	844.50	859.571	870.91
S/HC (ratio)	0.40	0.40	0.40	0.40	1.00	1.00	1.00	1.00
Yield (wt%)								
H2	1.38	1.60	1.649	1.72	1.31	1.50	1.750	1.86
CH4	16.79	20.10	23.716	26.76	16.34	19.40	24.000	25.52
C2H2	0.21	0.25	0.497	0.82	0.25	0.31	0.650	0.69
C2H4	25.73	30.10	34.760	36.99	26.93	32.10	37.500	39.88
C2H6	3.26	3.78	4.221	3.91	2.95	3.40	3.825	3.54
C3H4	0.25	0.29	0.328	0.36	0.25	0.29	0.330	0.35
C3H6	18.88	17.51	14.599	10.60	18.93	17.51	14.700	10.67
C3H8	29.13	19.70	9.405	4.65	28.86	19.51	9.155	4.69
C4H6	1.25	1.75	2.284	2.81	1.19	1.60	2.100	2.23
C4H8	0.78	0.74	0.685	0.65	0.81	0.75	0.600	0.55
C4H10	0.11	0.12	0.139	0.05	0.11	0.12	0.140	0.05
C5+	2.22	4.05	7.717	10.67	2.08	3.50	5.250	9.96

A.3.3 Naphtha feedstock

Disjunctive models	Naphtha1	Naphtha2	Naphtha3	Naphtha4	Naphtha5	Naphtha6	Naphtha7	Naphtha8
Conversion (w.fr.)	0.82	0.90	0.96	1.00	0.82	0.90	0.96	1.00
COT (C)	795.34	806.95	820.45	852.53	810.58	822.53	836.42	869.46
S/HC (ratio)	0.60	0.60	0.60	0.60	1.50	1.50	1.50	1.50
Yield (wt%)								
H2	0.54	0.60	0.68	0.73	0.55	0.61	0.69	0.73
CH4	9.17	11.63	14.47	16.86	9.29	11.77	14.53	16.79
C2H2	0.15	0.20	0.27	0.34	0.15	0.20	0.27	0.34
C2H4	19.63	23.18	26.67	27.37	21.87	25.80	29.46	30.95
C2H6	3.29	3.74	3.70	3.45	3.34	3.79	3.72	3.43
C3H4	0.17	0.27	0.42	0.62	0.18	0.27	0.42	0.62
C3H6	15.63	15.86	15.12	12.67	15.83	16.05	15.19	12.61
C3H8	0.46	0.45	0.46	0.44	0.46	0.46	0.46	0.44
C4H6	4.15	4.21	3.70	2.59	4.20	4.26	3.72	2.58
C4H8	5.31	4.82	4.40	3.77	5.38	4.87	4.42	3.75
C4H10	1.99	1.43	1.05	0.72	2.01	1.45	1.05	0.72
C5+	39.51	33.62	29.05	30.45	36.73	30.47	26.05	27.06

A.4 Coking rates

The coking rates used for ethane (Sundaram et al., 1981), propane (Sundaram et al., 1979) and naphtha (Kumar et al., 1985) feedstocks associated with each disjunctive model are shown here.

A.4.1 Ethane feedstock

Disjunctive models	Coking rate (Kg/day)
Ethane1	4.35
Ethane2	6.54
Ethane3	8.64
Ethane4	11.03
Ethane5	3.75
Ethane6	5.96
Ethane7	7.64
Ethane8	9.87

A.4.2 Propane feedstock

Disjunctive models	Coking rate (Kg/day)
Propane1	7.56
Propane2	9.63
Propane3	11.62
Propane4	12.61
Propane5	6.85
Propane6	8.51
Propane7	10.07
Propane8	10.86

A.4.3 Naphtha feedstock

Disjunctive models	Coking rate (Kg/day)
Naphtha1	8.88
Naphtha2	9.36
Naphtha3	11.43

Naptha4	14.41
Naptha5	7.84
Naptha6	8.65
Naptha7	10.31
Naptha8	12.66

A.5 Energy information

The calculations performed to obtain furnace energy and compression energy (Cengel & Boles (2001)) required in the model are shown here.

A.5.1 Furnace energy requirement

Since, enthalpy is a state property, the procedure followed to compute the necessary energy required in the furnace is shown in Figure A.1.

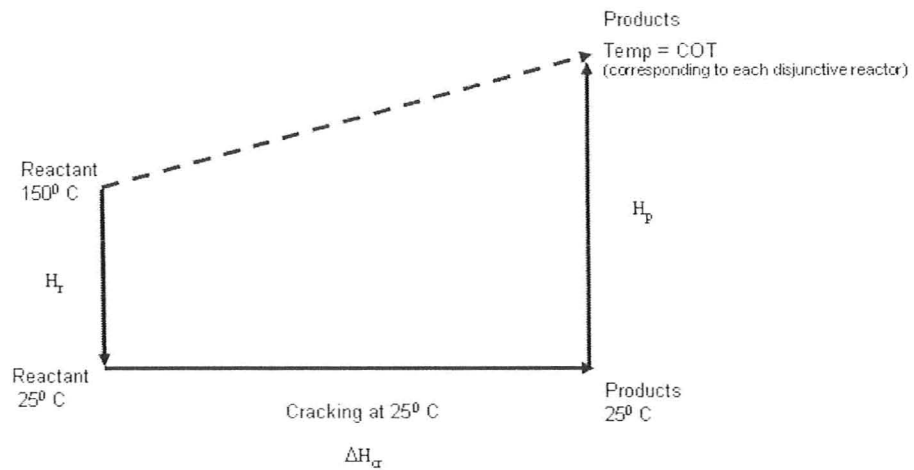


Figure A.1: Procedure for energy calculations

Where,

H_r = Energy released when cooling the feed from 150°C to 25°C

ΔH_{cr} = Heat of cracking; calculations carried out at 25⁰ C using the standard heats of formation

H_p = Energy required to heat the product mixture from 25⁰ C to corresponding coil outlet temperatures (COT) of each disjunctive model.

Therefore,

$$\text{Overall Heat requirement (cracking + heating product mixture)} = H_r + H_{cr} + H_p$$

(In addition, steam has to be heated from 150⁰ C to COT. Heat capacity data for steam was used to perform these calculations.)

H_r and H_p were calculated using the heat-capacity data. The following equations were used.

$$\Delta H = \langle C_p \rangle_H (T - T_0) \quad (\text{A.1})$$

$$\langle C_p \rangle_H = \text{Mean heat capacity, KJ/Kg K} \quad (\text{A.2})$$

$$\frac{\langle C_p \rangle_H}{R} = A + \frac{B}{2} T_0 (\tau + 1) + \frac{C}{2} T_0^2 (\tau^2 + \tau + 1) + \frac{D}{\tau T_0^2} \quad (\text{A.3})$$

$$\text{Where, } \tau = \frac{T}{T_0}$$

The variation of heat capacity with temperature is accounted for in these equations. The coefficients A, B, C and D for all the necessary hydrocarbons were obtained from (Cengel & Boles (2001)).

Heat of cracking (ΔH_{cr}) was calculated using the standard heats of formation of reactants and the products as follows:

$$\Delta H_{cr} = \Delta H_p - \Delta H_r \quad (A.4)$$

ΔH_{cr} = endothermic heat of cracking (KJ/Kg)

ΔH_p = heat of formation of the cracked products (KJ/Kg)

ΔH_r = heat of formation of the feed (KJ/Kg)

The standard heats of formation and molecular weights of the hydrocarbons were obtained from (Cengel & Boles (2001)).

These calculations were performed for all the feedstocks. Finally, the amount of energy required for cracking 1 kg of ethane, propane and naphtha feedstocks at various disjunctive operating conditions are reported here.

A.5.1.1 Ethane feedstock

Disjunctive model	Energy required (KJ/Kg)
Ethane1	4239.58
Ethane2	4706.85
Ethane3	5174.13
Ethane4	5536.37
Ethane5	4667.35
Ethane6	5141.53
Ethane7	5615.71
Ethane8	6106.56

A.5.1.2 Propane feedstock

Disjunctive model	Energy required (KJ/Kg)
Propane1	3828.79
Propane2	4092.44
Propane3	4428.75
Propane4	4617.61
Propane5	4257.32
Propane6	4531.93
Propane7	4818.56
Propane8	5084.98

A.5.1.3 Naphtha feedstock

Disjunctive model	Energy required (KJ/Kg)
Naphtha1	3785.24
Naphtha2	3894.26
Naphtha3	3968.43
Naphtha4	4183.26
Naphtha5	4370.82
Naphtha6	4500.21
Naphtha7	4581.41
Naphtha8	4713.48

A.5.2 Compression energy requirement

A five stage compression was considered in the model (Cengel & Boles (2001)). Details of the calculations are shown here.

Work done for adiabatic compression of ideal gases with constant heat capacities is given by:

$$W_c = \frac{RT}{\gamma - 1} \left[\left(\frac{P_2}{P_1} \right)^{(\gamma-1)/\gamma} - 1 \right] \quad (\text{A.5})$$

Multistage compression with inter-cooling can be used to reduce the compressor work. Therefore, for multistage compression with inter-cooling, the compression ratio that produces minimum work for a generalized case of n stages is given by:

$$\frac{P_2}{P_1} = \frac{P_3}{P_2} = \dots = \frac{P_{n+1}}{P_n} = \left(\frac{P_{n+1}}{P_1} \right)^{1/n} \quad (\text{A.6})$$

Assumption: No pressure drop across the cooler.

The corresponding work done for n stages can be calculated using,

$$W_c = \sum_{i=1}^{n-1} \frac{RT}{\gamma-1} \left[\left(\frac{P_{i+1}}{P_i} \right)^{(\gamma-1)/\gamma} - 1 \right] \quad (\text{A.7})$$

where,

$$\gamma = 1.3 (\text{polyatomic})$$

$$\eta = 0.7$$

$$T = 25^\circ \text{C} = 298.15^\circ \text{K}$$

$$R = 8.314 \frac{\text{J}}{\text{molK}}$$

With the known parameters, $P_1 = 1.5 \text{ atm}$ and $P_6 = 35 \text{ atm}$, the compression ratio that minimizes the work was estimated to be,

$$\frac{P_2}{P_1} = 1.8776$$

Using this ratio, pressures at each compressor were calculated. The values obtained are shown in the Figure A.2.

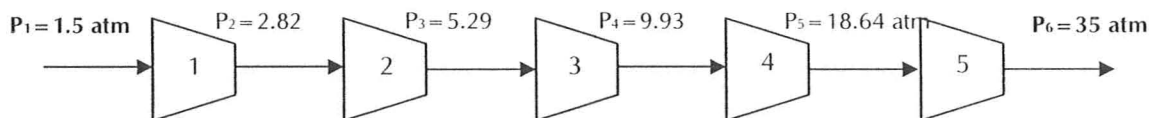


Figure A.2: 5-stage compression

Finally, for the 5-stage compression, amount of work done was estimated as follows:

$$W_c = \frac{RT}{\gamma-1} \times 5 \left[\left(\frac{P_2}{P_1} \right)^{(\gamma-1)/\gamma} - 1 \right]$$

$$W_c = 12006.197 \frac{\text{KJ}}{\text{Kmol}}$$

Therefore, the amount of compression energy required to compress 1Kmol of gaseous products is equal to 12006.2 KJ.

A.5.3 Molecular weights

Component	Molecular weight (Kg/Kmol)
H2	2.02
CH4	16.04
C2H2	26.04
C2H4	28.05
C2H6	30.07
C3H4	40.07
C3H6	42.08
C3H8	44.10
C4H6	54.09
C4H8	56.11
C4H10	58.12
C5+	100.00

Appendix B

**Valid disjunctive combinations, Solver specifications
and additional constraints**

B.1 Case studies: Binary variables for disjunctive model selection

Two scenarios are considered here to study the consequences of using binary variables for disjunctive reactor model selection on the computational time. These scenarios lead to a large number of binary variables and therefore are expected to experience computational difficulties. The results indicated that the small case study (Case B.1.1) was solved to optimality but the large case study (Case B.1.2) could not be solved even after 45 hours. The results and discussion for these scenarios are discussed as follows.

Case B.1.1 – Small case study: Binary variables for disjunctive model selection

This is a small case study with 1 feedstock and 2 reactors. The main requirement of this scenario is to meet the integrated demand by the end of the horizon while maximizing the plant profit. This case is considered to highlight the affect of using binary variables to make disjunctive model selection. A brief description of the scenario parameters are tabulated as shown below.

Feedstock	Naphtha
Number of Reactors	2
Time horizon	90 days
Integrated ethylene Demand	66% of the plant capacity
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and Decoke time periods

Discussion of Results

With binary variables for disjunctive model selection, the problem size for this scenario results in 1612 binary variables, 45160 linear variables and 48005 constraints. It can be observed that the binary variables for this scenario are approximately 10 times more than similar scenarios with continuous variable approximation for disjunctive model selection (refer to the single feedstock case studies in Chapter 4). Nevertheless, the optimal solution for this scenario was obtained in 150 seconds. Although, the scheduling

model for this scenario is tractable, the computational time is almost 12 times greater than the continuous approximation for disjunctive model selection. The results obtained are shown in Figures B-1 to B-3.

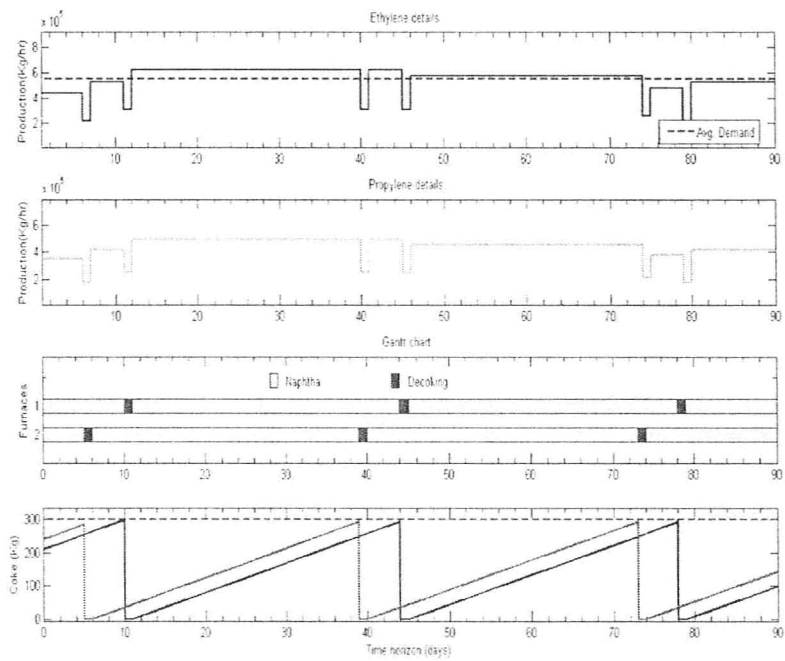


Figure B-1: Case B.1.1 - Gantt chart and Production details

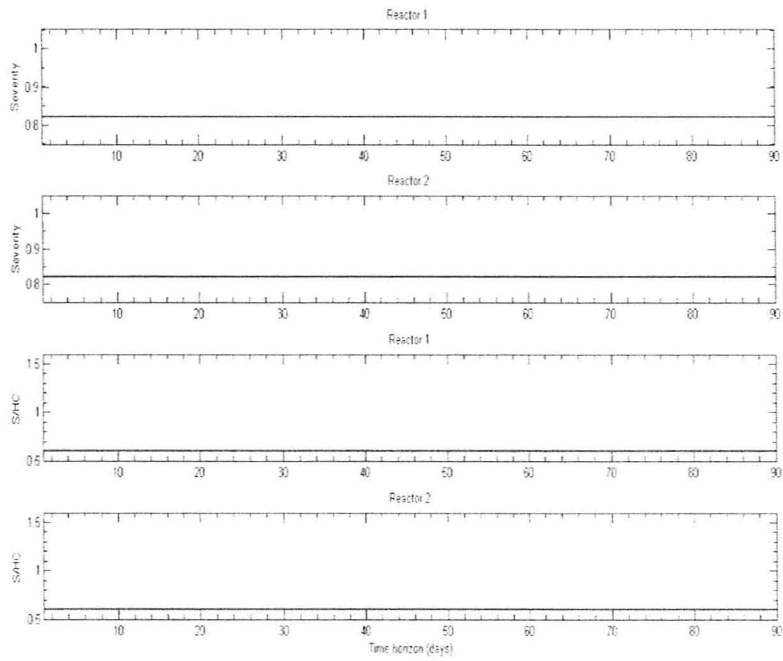


Figure B-2: Case B.1.1 - Severity and S/HC profiles

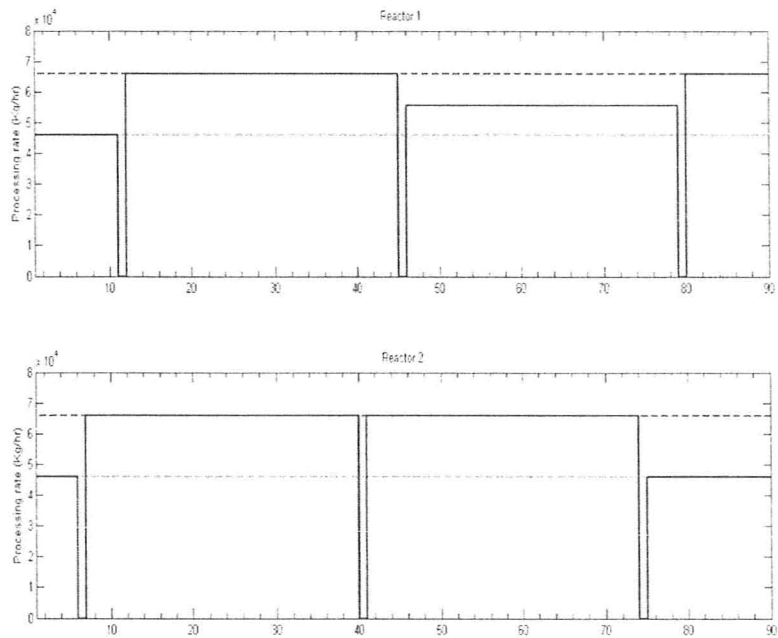


Figure B-3: Case B.1.1 - Processing rates

One should understand that MILP's are known for their combinatorial nature and exponential increase in the computational time with the number of binary variables. Although, this model was tractable for relatively large number of binary variables, further increase in the binary variables (number of furnaces) could make the model lose tractability. The results of such a case are discussed in the next case study.

Case B.1.2 – Large case study: Binary variables for disjunctive model selection

This is a large case study with 1 feedstock and 5 reactors representing a real single feed ethylene plant (similar to Case 5 of Chapter 4). The main requirement of this scenario is again to meet the integrated demand by the end of the horizon while maximizing the plant profit. Similar to the previous case, this is considered to highlight the affect of using binary variables to make disjunctive model selection. A brief description of the scenario parameters are tabulated as shown below.

Feedstock	Naphtha
Number of Reactors	5
Time horizon	90 days
Integrated ethylene Demand	66% of the plant capacity
Fresh feed	Unlimited Naphtha available
Degrees of freedom	Processing rates, Severity, S/HC and Decoke time periods

Discussion of Results

The scheduling model for this scenario results in 4050 binary variables, 296844 linear variables and 308629 constraints. From computational results, it was found that this model could not be solved to optimality in 45 hours. The best feasible solution obtained till this time had an objective function gap of 9 %, which cannot be considered as a good solution. Comparing the results with the previous case study, it is clear that the computational time increases exponentially with the increase in the number of binary variables. The computational time of 45 hrs or more for single optimization is not suitable for online applications. Therefore, using binary variables for disjunctive model selection is not a good option as it makes the scheduling model intractable.

B.2 Valid combinations of disjunctive models suitable for interpolation

As discussed in Chapter 4, continuous variables were used to make a disjunctive model selection. Consequently, the optimizer could select multiple disjunctive models instead of one single disjunctive model by sending non-zero feed rates to two or more yield models in the same physical reactor. If this occurs, the operating conditions would have to be interpolated, which in some cases (combinations of disjunctive models) would not be physically realizable. There are few valid combinations that allow a valid operating condition to be interpolated. These combinations are based on the adjacent disjunctive models corresponding to particular S/HC and severity. The valid combinations are listed here.

B.2.1 Ethane feedstock

S.No.	Valid combinations	Comment
1	(Ethane1, Ethane2)	Adjacent severities corresponding to S/HC = 0.4
2	(Ethane2, Ethane3)	
3	(Ethane3, Ethane4)	
4	(Ethane5, Ethane6)	Adjacent severities corresponding to S/HC = 1
5	(Ethane6, Ethane7)	
6	(Ethane7, Ethane8)	
7	(Ethane1, Ethane5)	Adjacent S/HC ratios corresponding to severities (0.4, 0.5, 0.6 and 0.7 respectively)
8	(Ethane2, Ethane6)	
9	(Ethane3, Ethane7)	
10	(Ethane4, Ethane8)	

B.2.2 Propane feedstock

S.No.	Valid combinations	Comment
1	(Propane1, Propane2)	Adjacent severities corresponding to S/HC = 0.4
2	(Propane2, Propane3)	
3	(Propane3, Propane4)	
4	(Propane5, Propane6)	Adjacent severities corresponding to S/HC = 1
5	(Propane6, Propane7)	
6	(Propane7, Propane8)	
7	(Propane1, Propane5)	Adjacent S/HC ratios corresponding to severities (0.7, 0.8, 0.9 and 0.95 respectively)
8	(Propane2, Propane6)	
9	(Propane3, Propane7)	
10	(Propane4, Propane8)	

B.2.3 Naphtha feedstock

S.No.	Valid combinations	Comment
1	(Naphtha1, Naphtha2)	Adjacent severities corresponding to S/HC = 0.6
2	(Naphtha2, Naphtha3)	
3	(Naphtha3, Naphtha4)	
4	(Naphtha5, Naphtha6)	Adjacent severities corresponding to S/HC = 1.5
5	(Naphtha6, Naphtha7)	
6	(Naphtha7, Naphtha8)	
7	(Naphtha1, Naphtha5)	Adjacent S/HC ratios corresponding to severities (0.82, 0.90, 0.96 and 1.0 respectively)
8	(Naphtha2, Naphtha6)	
9	(Naphtha3, Naphtha7)	
10	(Naphtha4, Naphtha8)	

Interpolation of the operating condition can be performed only between these combinations of disjunctive models. Our computational experience over all the case studies considered in this thesis has shown that during most of the time horizon an optimum operating condition corresponding to a single disjunctive model is selected with continuous variables without any difficulty. It is rarely that the optimizer selects more than one disjunctive model, just before a decoke event. This is done only to ensure feasibility of the model. Even when more than one disjunctive model was selected by the optimizer, at all times only valid combinations allowing interpolation were chosen by the optimizer.

B.3 Reactors in service

These constraints provide flexibility for when fewer than the maximum number reactors have to in operation due to limited product demands. In other words, these constraints allow the optimiser to decide the number of reactors (furnaces) in service at any point in time.

To be more realistic, we impose a condition that the reactors in service cannot be intermittently shutdown. It is possible to shut them down and bring in production only after the reactors are taken offline for maintenance (decoke). This condition is posed as shown in equation B.1.

Reactor shutdown possible only after a decoke

$$\delta_{jt}^{\text{shutdown}} \leq \delta_{jt}^{\text{decoke}} + \delta_{j,t-1}^{\text{shutdown}} \quad \forall j, t \quad (\text{B.1})$$

Also, when a furnace is shutdown there is no production. This is modeled using a constraint shown as equation (B.2).

No production during shutdown

$$P^{\min} \cdot (1 - \delta_{jt}^{\text{shutdown}}) \leq P_{ijt} \leq P^{\max} \cdot (1 - \delta_{jt}^{\text{shutdown}}) \quad \forall i, j, t \quad (\text{B.2})$$

Furthermore, the reactor model should also ensure that there is no coke deposition during the furnace shutdown. This condition is imposed using a set of constraints shown as equations B.3, B.4 and B.5. When a reactor is shutdown, equation B.4 ensures that Coke_{jt} is equal to zero. ΔDecoke_{jt} is always zero except during a decoke. Therefore, the only nonzero term in B.3 is the second term on the RHS. B.5 ensures that $\Delta\text{Nocoke_shutdown}_{jt}$ takes a large value during a shutdown, which erases the nonzero term in equation B.3. In this way, no coke build up is modeled during a shutdown.

No coke build up during shutdown

$$\text{Coke}_{jt} = \text{Coke}_{j,t-1} + \sum_i \sum_k (\text{Rcoke}_{ik} \cdot \delta_{ijkt}^{\text{disj}} \cdot \Delta t) - \Delta\text{Decoke}_{jt} - \Delta\text{Nocoke_shutdown}_{jt} \quad \forall j, t \quad (\text{B.3})$$

$$\text{Coke}_{jt} \leq \text{Coke}^{\max} \cdot (1 - \delta_{jt}^{\text{shutdown}}) \quad \forall j, t \quad (\text{B.4})$$

$$\Delta\text{Nocoke_shutdown}_{jt} \leq M \cdot (\delta_{jt}^{\text{shutdown}}) \quad \forall j, t \quad (\text{B.5})$$

It is important to understand that the use of this constraint would depend on the engineer's insight; if the user is not sure that the heuristic is valid, the constraint should not be included.

B.4 Costs associated with furnace decoke

The costs associated with furnace decoke are used in the coke penalty term used in the objective function to penalize coke accumulated at the end of time horizon. The two terms used in the penalty term are ($\text{Cost}_{\text{decoke}}^{\text{energy}}$) and ($\text{Cost}_{\text{decoke}}^{\text{profitloss}}$). The values of each term used for all the cases are listed below.

Case #	Decoke costs	
	Energy (\$)	Profit loss (\$)
Case 1	4500	0
Case 2	4500	206000
Case 3	4500	0
Case 4	4500	0
Case 5	4500	0
Case 6	4500	206000
Case 7	4500	206000
Case 8	4500	0
Case 9	4500	0
Case 10	4500	0
Case 11	4500	0
Case 12	4500	0
Case 13	4500	0

B.5 Product of a Binary and a Real variable: Linear reformulation technique

Gueret et al. (2000) introduces a linear reformulation technique when a nonlinear relationship (product of binary and a real variable) is encountered. The technique is elaborated here:

With two real variables, x and y , and a binary variable b , we want to model

$$y = b \cdot x \quad (\text{B.6})$$

Suppose we have some upper bound U on the value of x . Then consider the following constraints

$$y \leq x \quad (\text{B.7})$$

$$y \geq x - U \cdot (1 - b) \quad (\text{B.8})$$

$$y \leq U \cdot b \quad (\text{B.9})$$

If $b=0$, then (B.9) means that $y=0$. If $b=1$, then (B.9) simply imposes the upper bound constraint, and we have $y \leq x$ from (B.7) and $y \geq x$ from (B.8), i.e. $y=x$, which is what is desired.

B.6 Modeling language, Solver and Computer specifications

The solver and computer specifications used to carry out all the case studies in this thesis are provided here.

Modeling Language

- AMPL

Solver details

- Solver: CPLEX
- Version: 10.1
- Integrality gap = 0.00001

Computer specifications

- Processor speed: 3.2 GHz
- Memory (RAM): 2GB
- Operating system: Windows XP

Appendix C

Coarse-grid and Fine-grid scheduling models

C.1 Single feedstock scenarios

Naphtha is the feedstock used in these scenarios and no recycle is considered. The time horizon of 90 days is chosen for all the scenarios. A complete set of constraints and objective function for coarse-grid and fine-grid models used to solve the single feedstock scenarios are presented here.

C.1.1 Coarse-grid model

The length of each time period in a coarse-grid model is 3 days. Therefore, for a 90 day time horizon, the coarse-grid model has 30 time periods. This formulation reduces the problem size to approximately 1/3 of its original size (formulation with time period = 1 day). The time required for decoking is considered to be 1 day. Therefore, to model a 1-day decoke in a 3-day time period, we incorporated an additional set of constraints to accommodate decoking of multiple reactors and production for the remaining two days as discussed in Section 4.4.2. The constraints and the objective function of the coarse-grid model are presented as follows.

Constraints

Feed balance constraints

$$F_{it} = \sum_j P_{ijt} \quad \forall i, t \quad (\text{C.1})$$

Disjunctive reactor model constraints

$$\sum_k PD_{ijkt} = P_{ijt} \quad \forall i, j, t \quad (\text{C.2})$$

Production rates

$$PRate_{ijkct} = PD_{ijkt} \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (\text{C.3})$$

$$\text{Prod}_{ct} = \sum_i \sum_j \sum_k \text{PRate}_{ijkct} \quad \forall c \quad (\text{C.4})$$

$$\text{Sales}_{ct} = \text{Prod}_{ct} \quad \forall c \quad (\text{C.5})$$

Fraction of flow through disjunctive reactors

$$\text{PD}_{ijkt} = x_{ijkt}^d \cdot P_{ij}^{\max} \quad \forall i, j, k, t \quad (\text{C.6})$$

$$\sum_k x_{ijkt}^d \leq 1 \quad \forall i, j, t \quad (\text{C.7})$$

$$x_{ijkt}^d + s_{ijkt}^d = \sigma_{ijkt}^{\text{disj}} \quad \forall i, j, k, t \quad (\text{C.8})$$

$$\sum_k \sigma_{ijkt}^{\text{disj}} = 1 \quad \forall i, j, t \quad (\text{C.9})$$

$$\sum_k s_{ijkt}^d = \sum_k \sigma_{ijkt}^{\text{disj}} - \sum_k x_{ijkt}^d \quad \forall i, j, t \quad (\text{C.10})$$

$$0 \leq s_{ijkt}^d \leq 1 \quad \forall i, j, k, t \quad (\text{C.11})$$

Coking, Tube wall temperature and Decoking

$$\text{Coke}_{jt} = \text{Coke}_{jt-1} + \sum_i \sum_k \Delta \text{Coke}_{ijkct} + \text{Coke}_{jt-1}^* - \Delta \text{Decoke}_{jt} \quad \forall j, t \quad (\text{C.12})$$

$$\Delta \text{Coke}_{ijkct} = \left(\text{Rcoke}_{ik} \cdot \sigma_{ijkct}^{\text{disj}} \right) \cdot \Delta t \quad \forall i, j, k, t \quad (\text{C.13})$$

$$\text{Tw}_{jt} = \sum_i \sum_k \left(\text{Tw}_{ik}^{\text{clean}} \cdot \sigma_{ijkct}^{\text{disj}} \right) + \text{Tw}^{\text{const}} \cdot \text{Coke}_{jt} \quad \forall j, t \quad (\text{C.14})$$

$$\text{Coke}_{jt}^* = \text{Rcoke}^* \cdot \left(\Delta t - \Delta t^{\text{decoke}} \right) \quad \forall j, t \quad (\text{C.15})$$

$$\text{Tw}_{jt}^* = \text{Tw}^{\text{const}} \cdot \text{Coke}_{jt}^* \quad \forall j, t \quad (\text{C.16})$$

$$0 \leq \Delta \text{Decoke}_{jt} \leq M \cdot \delta_{jt}^{\text{decoke}} \quad \forall j, t \quad (\text{C.17})$$

$$0 \leq \text{Coke}_{jt} \leq \text{Coke}_{ij}^{\text{max}} \cdot (1 - \delta_{jt}^{\text{decoke}}) \quad \forall j, t \quad (\text{C.18})$$

$$P_{ij}^{\text{min}} \cdot (1 - \delta_{jt}^{\text{decoke}}) \leq P_{ijt} \leq P_{ij}^{\text{max}} \cdot (1 - \delta_{jt}^{\text{decoke}}) \quad \forall i, j, t \quad (\text{C.19})$$

Threshold limits for decoking

$$\text{Coke}_{jt} \leq \text{Coke}_j^{\text{max}} \quad \forall i, j, t \quad (\text{C.20})$$

$$\text{Tw}_{jt} \leq T_j^{\text{max}} \quad \forall i, j, t \quad (\text{C.21})$$

Decoking multiple reactors

$$\sum_j \delta_{jt}^{\text{decoke}} \leq \tau \quad \forall t \quad (\text{C.22})$$

$$\text{Where, } \tau = \frac{\Delta t}{\Delta t^{\text{decoke}}}$$

Accommodate lost production due to coarse time grid

$$P_{ij}^{\text{min}} \cdot \delta_{jt}^{\text{decoke}} \leq P_{ijt}^* \leq P_{ij}^{\text{max}} \cdot \delta_{jt}^{\text{decoke}} \quad \forall i, j, t \quad (\text{C.23})$$

$$F_{it}^* = \sum_j P_{ijt}^* \quad \forall i, t \quad (\text{C.24})$$

$$\sum_k PD_{ijk}^* = P_{ijt}^* \quad \forall i, j, t \quad (\text{C.25})$$

$$\text{PRate}_{ijkct}^* = PD_{ijk}^* \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (\text{C.26})$$

$$\text{Prod}_{ct}^* = \sum_i \sum_j \sum_k \text{PRate}_{ijkct}^* \quad \forall c, t \quad (\text{C.27})$$

$$\text{Sales}_{ct}^* = \text{Prod}_{ct}^* \quad \forall c, t \quad (\text{C.28})$$

$$\text{Prod}_{ct} = \text{Prod}_{ct} + \text{Prod}_{ct}^* \cdot (\Delta t - \Delta t^{\text{decoke}}) \quad \forall c, t \quad (\text{C.28a})$$

$$0 \leq \text{PD}_{ijkt}^* \leq P_{ij}^{\text{max}} \cdot \sigma_{ijkt}^{\text{disj}^*} \quad \forall i, j, t \quad (\text{C.29})$$

$$\sum_k \sigma_{ijkt}^{\text{disj}^*} \leq \delta_{jt}^{\text{decoke}} \quad \forall i, j, t \quad (\text{C.30})$$

Energy constraints

$$E_{jt}^{\text{furnace}} = \sum_i \sum_k \text{PD}_{ijkt} \cdot E_{ijk} \quad \forall j, t \quad (\text{C.31})$$

$$E_t^{\text{compressor}} = \sum_i \sum_j \sum_k \sum_c \left(\frac{\text{PRate}_{ijkct}}{\text{MW}_c} \right) * E^{\text{comp}} \quad \forall t \quad (\text{C.32})$$

Steam generated

$$F_{ijt}^{\text{HPsteam}} = P_{ijt} \cdot G^{\text{HPsteam}} \quad \forall i, j, t \quad (\text{C.33})$$

$$F_{ijt}^{\text{MPsteam}} = P_{ijt} \cdot G^{\text{MPsteam}} \quad \forall i, j, t \quad (\text{C.34})$$

Tightening constraints

$$\sum_{t'=t}^{t+\eta} \delta_{jt'}^{\text{decoke}} \leq 1 \quad \forall j, t \quad (\text{C.35})$$

$$\sum_t \delta_{jt}^{\text{decoke}} \leq \beta \quad \forall j \quad (\text{C.36})$$

$$\sum_{t=1}^{t+\gamma} \delta_{jt}^{\text{decoke}} \leq 0 \quad \forall j \quad (\text{C.37})$$

$$\text{Coke}_{j,t-1} \geq \text{Coke}_{\text{allowed}}^{\text{decoke}} \cdot \delta_{jt}^{\text{decoke}} \quad \forall j, t \quad (\text{C.38})$$

Integrated demand constraint

$$\sum_t \text{Sales}_{ct} \leq \text{Demand}_c \quad \forall c \quad (\text{C.39})$$

End conditions

$$\text{Coke}_{jNT} \leq \text{Coke}_{\text{calculated}}^{\text{max}} \quad (\text{C.40})$$

$$\text{Coke}_{\text{calculated}}^{\text{max}} = \text{Coke}^{\text{max}} - \text{Nfrs} * \text{Coke}_{\text{accum/period}}^{\text{max}} \quad (\text{C.41})$$

Objective function

The objective function is shown as equation (C.42).

$$\text{Objective function} = \text{Plant Profit} - \text{Penalty}^{\text{Coke}} + \text{profit}^* \quad (\text{C.42})$$

$$\text{Plant Profit} = \text{Value of products} - \text{Cost of feedstocks} - \text{Cost of dilution steam} - \text{Cost of furnace energy} - \text{Cost of compressor energy} + \text{Value of HP and MP steam generated at TLE's} - \text{Cost for furnace decoke.} \quad (\text{C.43})$$

Details of each term in the profit equation are given as follows:

$$\text{Value of products} = \sum_t \sum_c \text{Sales}_{ct} \cdot \text{Cost}_c^{\text{product}} \quad (\text{C.43a})$$

$$\text{Cost of feedstocks} = \sum_t \sum_i F_{it} \cdot \text{Cost}_i^{\text{feed}} \quad (\text{C.43b})$$

$$\text{Cost of dilution steam} = \sum_t \sum_i \sum_j \sum_k \text{PD}_{ijkt} \cdot \rho_{ik}^{\text{S/HC}} \cdot \text{Cost}_{\text{steam}}^{\text{dilution}} \quad (\text{C.43c})$$

$$\text{Cost of furnace energy} = \sum_t \sum_j E_{jt}^{\text{furnace}} \cdot \text{Cost}_{\text{energy}}^{\text{furnace}} \quad (\text{C.43d})$$

$$\text{Cost of compressor energy} = \sum_t E_t^{\text{compressor}} \cdot \text{Cost}_{\text{energy}}^{\text{compressor}} \quad (\text{C.43e})$$

$$\text{Value of HP and MP steam} = \sum_t \sum_i \sum_j F_{ijt}^{\text{HPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{HP}} + \sum_t \sum_i \sum_j F_{ijt}^{\text{MPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{MP}} \quad (\text{C.43f})$$

$$\text{Cost for furnace decoke} = \sum_t \sum_j \delta_{jt}^{\text{decoke}} \cdot \text{Cost}_{\text{energy}}^{\text{decoke}} \quad (\text{C.43g})$$

$$\text{Penalty}^{\text{Coke}} = \frac{\sum_j \text{Coke}_{j\text{NT}}}{\text{Coke}_{\text{max}}} \cdot (\text{Cost}_{\text{decoke}}^{\text{energy}} + \text{Cost}_{\text{decoke}}^{\text{profitloss}}) \quad (\text{C.43h})$$

$$\begin{aligned} \text{profit}^* = & \left(\sum_c \text{Sales}_{ct}^* \cdot \text{Cost}_c^{\text{product}} - \sum_i F_{it}^* \cdot \text{Cost}_i^{\text{feed}} - \sum_i \sum_j \sum_k \text{PD}_{ijkt}^* \cdot \rho_{ik}^{\text{S/HC}} \cdot \text{Cost}_{\text{steam}}^{\text{dilution}} \right. \\ & - \sum_i \sum_j \sum_k \text{PD}_{ijkt}^* \cdot E_{ijk} \cdot \text{Cost}_{\text{energy}}^{\text{furnace}} - \sum_i \sum_j \sum_k \sum_c \left(\frac{\text{PRate}_{ijkct}^*}{\text{MW}_c} \right) \cdot E_{\text{compressor}} \cdot \text{Cost}_{\text{energy}}^{\text{compressor}} \\ & \left. + \sum_i \sum_j F_{ijt}^{\text{HPsteam}^*} \cdot \text{Cost}_{\text{steam}}^{\text{HP}} + \sum_i \sum_j F_{ijt}^{\text{MPsteam}^*} \cdot \text{Cost}_{\text{steam}}^{\text{MP}} \right) \cdot (\Delta t - \Delta t^{\text{decoke}}) \quad (\text{C.43i}) \end{aligned}$$

C.1.2 Fine-grid model

The length of each time period in a fine-grid model is 1 day. Therefore, for a 90 day time horizon, the fine-grid model has 90 time periods. The increase in the number of time periods will increase the number of binary variables in the model. However, many of the binary (decoke) variables in this model are fixed in the two-stage temporal decomposition heuristic. The decoking period of 1 day is equal to the length of each time period in this model. Therefore, there is no production loss in this model during decoking as in coarse grid model.

Constraints

Feed balance constraints

$$F_{it} = \sum_j P_{ijt} \quad \forall i, t \quad (\text{C.44})$$

Disjunctive reactor model constraints

$$\sum_k PD_{ijkt} = P_{ijt} \quad \forall i, j, t \quad (\text{C.45})$$

Production rates

$$PRate_{ijkct} = PD_{ijkt} \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (\text{C.46})$$

$$Prod_{ct} = \sum_i \sum_j \sum_k PRate_{ijkct} \quad \forall c \quad (\text{C.47})$$

$$Sales_{ct} = Prod_{ct} \quad \forall c \quad (\text{C.48})$$

Fraction of flow through disjunctive reactors

$$PD_{ijkt} = x_{ijkt}^d \cdot P_{ij}^{\max} \quad \forall i, j, k, t \quad (\text{C.49})$$

$$\sum_k x_{ijkt}^d \leq 1 \quad \forall i, j, t \quad (C.50)$$

$$x_{ijkt}^d + s_{ijkt}^d = \sigma_{ijkt}^{disj} \quad \forall i, j, k, t \quad (C.51)$$

$$\sum_k \sigma_{ijkt}^{disj} = 1 \quad \forall i, j, t \quad (C.52)$$

$$\sum_k s_{ijkt}^d = \sum_k \sigma_{ijkt}^{disj} - \sum_k x_{ijkt}^d \quad \forall i, j, t \quad (C.53)$$

$$0 \leq s_{ijkt}^d \leq 1 \quad \forall i, j, k, t \quad (C.54)$$

Coking, Tube wall temperature and Decoking

$$Coke_{jt} = Coke_{j,t-1} + \sum_i \sum_k \Delta Coke_{ijk} - \Delta Decoke_{jt} \quad \forall j, t \quad (C.55)$$

$$\Delta Coke_{ijk} = (R_{coke_{ik}} \cdot \sigma_{ijk}^{disj}) \cdot \Delta t \quad \forall i, j, k, t \quad (C.56)$$

$$T_{w_{jt}} = \sum_i \sum_k (T_{w_{ik}}^{clean} \cdot \sigma_{ijk}^{disj}) + T_{w_{jt}}^{const} \cdot Coke_{jt} \quad \forall j, t \quad (C.57)$$

$$0 \leq \Delta Decoke_{jt} \leq M \cdot \delta_{jt}^{decoke} \quad \forall j, t \quad (C.58)$$

$$0 \leq Coke_{jt} \leq Coke_{ij}^{max} \cdot (1 - \delta_{jt}^{decoke}) \quad \forall j, t \quad (C.59)$$

$$P_{ij}^{min} \cdot (1 - \delta_{jt}^{decoke}) \leq P_{ijt} \leq P_{ij}^{max} \cdot (1 - \delta_{jt}^{decoke}) \quad \forall i, j, t \quad (C.60)$$

Decoking single reactor

$$\sum_j \delta_{jt}^{decoke} \leq 1 \quad \forall t \quad (C.61)$$

Threshold limits for decoking

$$\text{Coke}_{jt} \leq \text{Coke}_j^{\max} \quad \forall i, j, t \quad (\text{C.62})$$

$$\text{Tw}_{jt} \leq T_j^{\max} \quad \forall i, j, t \quad (\text{C.63})$$

Energy constraints

$$E_{jt}^{\text{furnace}} = \sum_i \sum_k \text{PD}_{ijkt} \cdot E_{ijk} \quad \forall j, t \quad (\text{C.64})$$

$$E_t^{\text{compressor}} = \sum_i \sum_j \sum_k \sum_c \left(\frac{\text{PRate}_{ijkct}}{\text{MW}_c} \right) * E^{\text{comp}} \quad \forall t \quad (\text{C.65})$$

Steam generated

$$F_{ijt}^{\text{HPsteam}} = P_{ijt} \cdot G^{\text{HPsteam}} \quad \forall i, j, t \quad (\text{C.66})$$

$$F_{ijt}^{\text{MPsteam}} = P_{ijt} \cdot G^{\text{MPsteam}} \quad \forall i, j, t \quad (\text{C.67})$$

Tightening constraints

$$\sum_{t'=t}^{t+\eta} \delta_{jt'}^{\text{decoke}} \leq 1 \quad \forall j, t \quad (\text{C.68})$$

$$\sum_t \delta_{jt}^{\text{decoke}} \leq \beta \quad \forall j \quad (\text{C.69})$$

$$\sum_{t=1}^{t+\gamma} \delta_{jt}^{\text{decoke}} \leq 0 \quad \forall j \quad (\text{C.70})$$

$$\text{Coke}_{jt-1} \geq \text{Coke}_{\text{allowed}}^{\text{decoke}} \cdot \delta_{jt}^{\text{decoke}} \quad \forall j, t \quad (\text{C.71})$$

Integrated demand constraint

$$\sum_t \text{Sales}_{ct} \leq \text{Demand}_c \quad \forall c \quad (\text{C.72})$$

End conditions

$$\text{Coke}_{\text{jNT}} \leq \text{Coke}_{\text{calculated}}^{\text{max}} \quad (\text{C.73})$$

$$\text{Coke}_{\text{calculated}}^{\text{max}} = \text{Coke}^{\text{max}} - \text{Nfrs} * \text{Coke}_{\text{accum/period}}^{\text{max}} \quad (\text{C.74})$$

Objective function

The objective function is shown as equation (C.75).

$$\text{Objective function} = \text{Plant Profit} - \text{Penalty}^{\text{Coke}} \quad (\text{C.75})$$

$$\begin{aligned} \text{Plant Profit} = & \text{Value of products} - \text{Cost of feedstocks} - \text{Cost of dilution} \quad (\text{C.76}) \\ & \text{steam} - \text{Cost of furnace energy} - \text{Cost of compressor energy} + \text{Value of} \\ & \text{HP and MP steam generated at TLE's} - \text{Cost for furnace decoke.} \end{aligned}$$

Details of each term in the profit equation are given as follows:

$$\text{Value of products/ Income} = \sum_t \sum_c \text{Sales}_{ct} \cdot \text{Cost}_c^{\text{product}} \quad (\text{C.76a})$$

$$\text{Cost of feedstocks} = \sum_t \sum_i F_{it} \cdot \text{Cost}_i^{\text{feed}} \quad (\text{C.76b})$$

$$\text{Cost of dilution steam} = \sum_t \sum_i \sum_j \sum_k \text{PD}_{ijkt} \cdot \rho_{ik}^{\text{S/HC}} \cdot \text{Cost}_{\text{steam}}^{\text{dilution}} \quad (\text{C.76c})$$

$$\text{Cost of furnace energy} = \sum_t \sum_j E_{jt}^{\text{furnace}} \cdot \text{Cost}_{\text{energy}}^{\text{furnace}} \quad (\text{C.76d})$$

$$\text{Cost of compressor energy} = \sum_t E_t^{\text{compressor}} \cdot \text{Cost}_{\text{energy}}^{\text{compressor}} \quad (\text{C.76e})$$

$$\text{Value of HP and MP steam} = \sum_t \sum_i \sum_j F_{ijt}^{\text{HPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{HP}} + \sum_t \sum_i \sum_j F_{ijt}^{\text{MPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{MP}} \quad (\text{C.76f})$$

$$\text{Cost for furnace decoke} = \sum_t \sum_j \delta_{jt}^{\text{decoke}} \cdot \text{Cost}_{\text{energy}}^{\text{decoke}} \quad (\text{C.76g})$$

$$\text{Penalty}^{\text{Coke}} = \frac{\sum_j \text{Coke}_{j\text{NT}}}{\text{Coke}_{\text{max}}} \cdot (\text{Cost}_{\text{decoke}}^{\text{energy}} + \text{Cost}_{\text{decoke}}^{\text{profitloss}}) \quad (\text{C.76h})$$

C.2 Multiple feedstock scenarios

Ethane, Propane and Naphtha are the feedstocks used in these scenarios. Only ethane is recycled back for subsequent cracking. The time horizon of 90 days is chosen for all the scenarios. A complete set of constraints and objective function for coarse-grid and fine-grid models used to solve the multiple feedstock scenarios are presented here.

C.2.1 Coarse-grid model

The length of each time period in a coarse-grid model is 3 days. Therefore, for a 90 day time horizon, the coarse-grid model has 30 time periods. The time required for decoking is considered to be 1 day. Therefore, to model a 1-day decoke in a 3-day time period, additional set of constraints were added to accommodate decoking of multiple reactors and production for the remaining two days as discussed in Section 4.4.2. The constraints and the objective function of the coarse-grid model are presented as follows.

Constraints

Feedstock allocation

$$W_{ij=1t} = (1 - \delta_{j=1t}^{\text{decoke}}) \quad i = \text{ethane}, \forall t \quad (\text{C.77})$$

(Reactor 1 is allocated to crack ethane)

$$\sum_i W_{ijt} \leq (1 - \delta_{jt}^{\text{decoke}}) \quad \forall j, t \quad (\text{C.78})$$

$$W_{ijt} + \sum_{i' \neq i} W_{i'jt-1} \leq 1 \quad \forall i, j, t \quad (\text{C.79})$$

$$W_{ijt-1} - W_{ijt} \leq \delta_{jt}^{\text{decoke}} \quad \forall i, j, t = 2..NT \quad (\text{C.80})$$

$$P_{ij}^{\min} \cdot W_{ijt} \leq P_{ijt} \leq P_{ij}^{\max} \cdot W_{ijt} \quad \forall i, j, t \quad (\text{C.81})$$

Feed balance constraints

$$F_{it} + FRcy_{it} = \sum_j P_{ijt} \quad \forall i, t \quad (C.82)$$

Disjunctive reactor model constraints

$$\sum_k PD_{ijkt} = P_{ijt} \quad \forall i, j, t \quad (C.83)$$

Production rates

$$PRate_{ijkct} = PD_{ijkt} \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (C.84)$$

$$Prod_{ct} = \sum_i \sum_j \sum_k PRate_{ijkct} \quad \forall c \quad (C.85)$$

$$Sales_{ct} = Prod_{ct} \quad \forall c \quad (C.86)$$

Recycle Inventory constraints

$$frcy_{it} = \sum_j \sum_k PD_{ijkt} \cdot X_{ikc} \quad i = \text{ethane} \quad \forall t \quad (C.87)$$

$$Rcy_Inv_{it} = Rcy_Inv_{it-1} + frcy_{it} - FRcy_{it} \quad i = \text{ethane} \quad \forall t \quad (C.88)$$

$$FRcy_{it} = 0 \quad i \neq \text{ethane}, \forall t \quad (C.89)$$

Fraction of flow through disjunctive reactors

$$PD_{ijkt} = x_{ijkt}^d \cdot P_{ij}^{\max} \quad \forall i, j, k, t \quad (C.90)$$

$$\sum_k x_{ijkt}^d \leq 1 \quad \forall i, j, t \quad (C.91)$$

$$X_{ijkt}^d + S_{ijkt}^d = \sigma_{ijkt}^{disj} \quad \forall i, j, k, t \quad (C.92)$$

$$\sum_k \sigma_{ijkt}^{disj} \leq W_{ijt} \quad \forall i, j, t \quad (C.93)$$

$$\sum_k S_{ijkt}^d = \sum_k \sigma_{ijkt}^{disj} - \sum_k X_{ijkt}^d \quad \forall i, j, t \quad (C.94)$$

$$0 \leq S_{ijkt}^d \leq X_{ijkt}^d + \delta_{jt}^{decoke} \quad \forall i, j, k, t \quad (C.95)$$

$$0 \leq s_{ijkt}^d \leq W_{ijt} \quad \forall i, j, k, t \quad (C.96)$$

Coking, Tube wall temperature and Decoking

$$Coke_{jt} = Coke_{j,t-1} + \sum_i \sum_k \Delta Coke_{ijkt} + Coke_{jt-1}^* - \Delta Decoke_{jt} \quad \forall j, t \quad (C.97)$$

$$\Delta Coke_{ijkt} = (Rcoke_{ik} \cdot \sigma_{ijkt}^{disj}) \cdot \Delta t \quad \forall i, j, k, t \quad (C.98)$$

$$Tw_{jt} = \sum_i \sum_k (Tw_{ik}^{clean} \cdot \sigma_{ijkt}^{disj}) + Tw^{const} \cdot Coke_{jt} \quad \forall j, t \quad (C.99)$$

$$Coke_{jt}^* = Rcoke^* \cdot (\Delta t - \Delta t^{decoke}) \quad \forall j, t \quad (C.100)$$

$$Tw_{jt}^* = Tw^{const} \cdot Coke_{jt}^* \quad \forall j, t \quad (C.101)$$

$$0 \leq \Delta Decoke_{jt} \leq M \cdot \delta_{jt}^{decoke} \quad \forall j, t \quad (C.102)$$

$$0 \leq Coke_{jt} \leq Coke_{ij}^{max} \cdot (1 - \delta_{jt}^{decoke}) \quad \forall j, t \quad (C.103)$$

$$P_{ij}^{min} \cdot (1 - \delta_{jt}^{decoke}) \leq P_{ijt} \leq P_{ij}^{max} \cdot (1 - \delta_{jt}^{decoke}) \quad \forall i, j, t \quad (C.104)$$

Threshold limits for decoking

$$\text{Coke}_{jt} \leq \text{Coke}_j^{\max} \quad \forall i, j, t \quad (\text{C.105})$$

$$\text{Tw}_{jt} \leq T_j^{\max} \quad \forall i, j, t \quad (\text{C.106})$$

Decoking multiple reactors

$$\sum_j \delta_{jt}^{\text{decoke}} \leq \tau \quad \forall t \quad (\text{C.107})$$

$$\tau = \frac{\Delta t}{\Delta t^{\text{decoke}}}$$

Accommodate lost production due to coarse time grid

$$P_{ij}^{\min} \cdot \delta_{jt}^{\text{decoke}} \leq P_{ijt}^* \leq P_{ij}^{\max} \cdot \delta_{jt}^{\text{decoke}} \quad \forall i, j, t \quad (\text{C.108})$$

$$P_{ij}^{\min} \cdot W_{ijt} \leq P_{ijt}^* \leq P_{ij}^{\max} \cdot W_{ijt} \quad \forall i, j, t \quad (\text{C.109})$$

$$F_{it}^* = \sum_j P_{ijt}^* \quad \forall i, t \quad (\text{C.110})$$

$$\sum_k PD_{ijk}^* = P_{ijt}^* \quad \forall i, j, t \quad (\text{C.111})$$

$$\text{PRate}_{ijkct}^* = PD_{ijk}^* \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (\text{C.112})$$

$$\text{Pr od}_{ct}^* = \sum_i \sum_j \sum_k \text{PRate}_{ijkct}^* \quad \forall c, t \quad (\text{C.113})$$

$$\text{Sales}_{ct}^* = \text{Pr od}_{ct}^* \quad \forall c, t \quad (\text{C.114})$$

$$\text{Pr od}_{ct} = \text{Pr od}_{ct}^* + \text{Pr od}_{ct}^* \cdot (\Delta t - \Delta t^{\text{decoke}}) \quad \forall c, t \quad (\text{C.114a})$$

$$0 \leq PD_{ijkt}^* \leq P_{ij}^{\max} \cdot \sigma_{ijkt}^{\text{disj}^*} \quad \forall c \quad (\text{C.114a})$$

$$\sum_k \sigma_{ijkt}^{\text{disj}^*} \leq \delta_{jt}^{\text{decoke}} \quad \forall i, j, t \quad (\text{C.115})$$

Energy constraints

$$E_{jt}^{\text{furnace}} = \sum_i \sum_k PD_{ijkt} \cdot E_{ijk} \quad \forall j, t \quad (\text{C.116})$$

$$E_t^{\text{compressor}} = \sum_i \sum_j \sum_k \sum_c \left(\frac{\text{PRate}_{ijkct}}{\text{MW}_c} \right) * E^{\text{comp}} \quad \forall t \quad (\text{C.117})$$

Steam generated

$$F_{ijt}^{\text{HPsteam}} = P_{ijt} \cdot G^{\text{HPsteam}} \quad \forall i, j, t \quad (\text{C.118})$$

$$F_{ijt}^{\text{MPsteam}} = P_{ijt} \cdot G^{\text{MPsteam}} \quad \forall i, j, t \quad (\text{C.119})$$

Tightening constraints

$$\sum_{t'=t}^{t+\eta} \delta_{jt'}^{\text{decoke}} \leq 1 \quad \forall j, t \quad (\text{C.120})$$

$$\sum_t \delta_{jt}^{\text{decoke}} \leq \beta \quad \forall j \quad (\text{C.121})$$

$$\sum_{t=1}^{t+\gamma} \delta_{jt}^{\text{decoke}} \leq 0 \quad \forall j \quad (\text{C.122})$$

$$\text{Coke}_{jt-1} \geq \text{Coke}_{\text{allowed}}^{\text{decoke}} \cdot \delta_{jt}^{\text{decoke}} \quad \forall j, t \quad (\text{C.123})$$

Integrated demand constraint

$$\sum_t \text{Sales}_{ct} \leq \text{Demand}_c \quad \forall c \quad (\text{C.124})$$

End conditions

$$\text{Coke}_{jNT} \leq \text{Coke}_{\text{calculated}}^{\text{max}} \quad (\text{C.125})$$

$$\text{Coke}_{\text{calculated}}^{\text{max}} = \text{Coke}^{\text{max}} - \text{Nfirs} * \text{Coke}_{\text{accum/period}}^{\text{max}} \quad (\text{C.126})$$

Objective function

The objective function is shown as equation (C.127).

$$\text{Objective function} = \text{Plant Profit} - \text{Penalty}^{\text{Coke}} - \text{Penalty}^{\text{Rey-Inv}} + \text{profit}^* \quad (\text{C.127})$$

$$\begin{aligned} \text{Plant Profit} = & \text{Value of products} - \text{Cost of feedstocks} - \text{Cost of dilution} \quad (\text{C.128}) \\ & \text{steam} - \text{Cost of furnace energy} - \text{Cost of compressor energy} + \text{Value of HP} \\ & \text{and MP steam generated at TLE's} - \text{Cost for furnace decoke.} \end{aligned}$$

Details of each term in the profit equation are given as follows:

$$\text{Value of products/ Income} = \sum_t \sum_c \text{Sales}_{ct} \cdot \text{Cost}_c^{\text{product}} \quad (\text{C.128a})$$

$$\text{Cost of feedstocks} = \sum_t \sum_i F_{it} \cdot \text{Cost}_i^{\text{feed}} \quad (\text{C.128b})$$

$$\text{Cost of dilution steam} = \sum_t \sum_i \sum_j \sum_k \text{PD}_{ijkt} \cdot \rho_{ik}^{\text{S/HC}} \cdot \text{Cost}_{\text{steam}}^{\text{dilution}} \quad (\text{C.128c})$$

$$\text{Cost of furnace energy} = \sum_t \sum_j E_{jt}^{\text{furnace}} \cdot \text{Cost}_{\text{energy}}^{\text{furnace}} \quad (\text{C.128d})$$

$$\text{Cost of compressor energy} = \sum_t E_t^{\text{compressor}} \cdot \text{Cost}_{\text{energy}}^{\text{compressor}} \quad (\text{C.128e})$$

$$\text{Value of HP and MP steam} = \sum_t \sum_i \sum_j F_{ijt}^{\text{HPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{HP}} + \sum_t \sum_i \sum_j F_{ijt}^{\text{MPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{MP}} \quad (\text{C.128f})$$

$$\text{Cost for furnace decoke} = \sum_t \sum_j \delta_{jt}^{\text{decoke}} \cdot \text{Cost}_{\text{energy}}^{\text{decoke}} \quad (\text{C.128g})$$

$$\text{Penalty}^{\text{Rcy_Inv}} = \lambda \cdot \sum_t \sum_i \text{Rcy_Inv}_{it} \quad (\text{C.128h})$$

$$\text{Penalty}^{\text{Coke}} = \frac{\sum_j \text{Coke}_{j\text{NT}}}{\text{Coke}_{\text{max}}} \cdot (\text{Cost}_{\text{decoke}}^{\text{energy}} + \text{Cost}_{\text{decoke}}^{\text{profitloss}}) \quad (\text{C.128i})$$

$$\begin{aligned} \text{profit}^* = & \left(\sum_c \text{Sales}_{ct}^* \cdot \text{Cost}_c^{\text{product}} - \sum_i F_{it}^* \cdot \text{Cost}_i^{\text{feed}} - \sum_i \sum_j \sum_k \text{PD}_{ijkt}^* \cdot \rho_{ik}^{\text{S/HC}} \cdot \text{Cost}_{\text{steam}}^{\text{dilution}} \right. \\ & - \sum_i \sum_j \sum_k \text{PD}_{ijkt}^* \cdot E_{ijk} \cdot \text{Cost}_{\text{energy}}^{\text{furnace}} - \sum_i \sum_j \sum_k \sum_c \left(\frac{\text{PRate}_{ijkct}^*}{\text{MW}_c} \right) \cdot E_{\text{compressor}} \cdot \text{Cost}_{\text{energy}}^{\text{compressor}} \\ & \left. + \sum_i \sum_j F_{ijt}^{\text{HPsteam}^*} \cdot \text{Cost}_{\text{steam}}^{\text{HP}} + \sum_i \sum_j F_{ijt}^{\text{MPsteam}^*} \cdot \text{Cost}_{\text{steam}}^{\text{MP}} \right) \cdot (\Delta t - \Delta t^{\text{decoke}}) \end{aligned} \quad (\text{C.128j})$$

C.2.2 Fine-grid model

The length of each time period in a fine-grid model is 1 day. Therefore, for a 90 day time horizon, the fine-grid model has 90 time periods. The increase in the number of time periods will increase the number of binary variables in the model. However, many of the binary (decoke) variables in this model are fixed in the two-stage temporal decomposition heuristic.

Constraints

Feedstock allocation

$$W_{ij=1t} = (1 - \delta_{j=1t}^{\text{decoke}}) \quad i = \text{ethane}, \forall t \quad (\text{C.129})$$

(Reactor 1 is allocated to crack ethane)

$$\sum_i W_{ijt} \leq (1 - \delta_{jt}^{\text{decoke}}) \quad \forall j, t \quad (\text{C.130})$$

$$W_{ijt} + \sum_{i' \neq i} W_{i'jt-1} \leq 1 \quad \forall i, j, t \quad (\text{C.131})$$

$$W_{ijt-1} - W_{ijt} \leq \delta_{jt}^{\text{decoke}} \quad \forall i, j, t = 2..NT \quad (\text{C.132})$$

$$P_{ij}^{\min} \cdot W_{ijt} \leq P_{ijt} \leq P_{ij}^{\max} \cdot W_{ijt} \quad \forall i, j, t \quad (\text{C.133})$$

Feed balance constraints

$$F_{it} + \text{FRcy}_{it} = \sum_j P_{ijt} \quad \forall i, t \quad (\text{C.134})$$

Disjunctive reactor model constraints

$$\sum_k PD_{ijkt} = P_{ijt} \quad \forall i, j, t \quad (\text{C.135})$$

Production rates

$$\text{PRate}_{ijkct} = \text{PD}_{ijkt} \cdot X_{ijkc} \quad \forall i, j, k, c, t \quad (\text{C.136})$$

$$\text{Prod}_{ct} = \sum_i \sum_j \sum_k \text{PRate}_{ijkct} \quad \forall c \quad (\text{C.137})$$

$$\text{Sales}_{ct} = \text{Prod}_{ct} \quad \forall c \quad (\text{C.138})$$

Recycle Inventory constraints

$$\text{frcy}_{it} = \sum_j \sum_k \text{PD}_{ijkt} \cdot X_{ikc} \quad i = \text{ethane} \quad \forall t \quad (\text{C.139})$$

$$\text{Rcy_Inv}_{it} = \text{Rcy_Inv}_{it-1} + \text{frcy}_{it} - \text{FRcy}_{it} \quad i = \text{ethane} \quad \forall t \quad (\text{C.140})$$

$$\text{FRcy}_{it} = 0 \quad i \neq \text{ethane}, \forall t \quad (\text{C.141})$$

Fraction of flow through disjunctive reactors

$$\text{PD}_{ijkt} = x_{ijkt}^d \cdot P_{ij}^{\text{max}} \quad \forall i, j, k, t \quad (\text{C.142})$$

$$\sum_k x_{ijkt}^d \leq 1 \quad \forall i, j, t \quad (\text{C.143})$$

$$x_{ijkt}^d + s_{ijkt}^d = \sigma_{ijkt}^{\text{disj}} \quad \forall i, j, k, t \quad (\text{C.144})$$

$$\sum_k \sigma_{ijkt}^{\text{disj}} \leq W_{ijt} \quad \forall i, j, t \quad (\text{C.145})$$

$$\sum_k s_{ijkt}^d = \sum_k \sigma_{ijkt}^{\text{disj}} - \sum_k x_{ijkt}^d \quad \forall i, j, t \quad (\text{C.146})$$

$$0 \leq s_{ijkt}^d \leq x_{ijkt}^d + \delta_{jt}^{\text{decoke}} \quad \forall i, j, k, t \quad (\text{C.147})$$

$$0 \leq s_{ijkt}^d \leq W_{ijt} \quad \forall i, j, k, t \quad (\text{C.148})$$

Coking, Tube wall temperature and Decoking

$$\text{Coke}_{jt} = \text{Coke}_{j,t-1} + \sum_i \sum_k \Delta \text{Coke}_{ijkt} - \Delta \text{Decoke}_{jt} \quad \forall j, t \quad (\text{C.149})$$

$$\Delta \text{Coke}_{ijkt} = (\text{Rcokes}_{ik} \cdot \sigma_{ijkt}^{\text{disj}}) \cdot \Delta t \quad \forall i, j, k, t \quad (\text{C.150})$$

$$\text{Tw}_{jt} = \sum_i \sum_k (\text{Tw}_{ik}^{\text{clean}} \cdot \sigma_{ijkt}^{\text{disj}}) + \text{Tw}^{\text{const}} \cdot \text{Coke}_{jt} \quad \forall j, t \quad (\text{C.151})$$

$$0 \leq \Delta \text{Decoke}_{jt} \leq M \cdot \delta_{jt}^{\text{decoke}} \quad \forall j, t \quad (\text{C.152})$$

$$0 \leq \text{Coke}_{jt} \leq \text{Coke}_{ij}^{\text{max}} \cdot (1 - \delta_{jt}^{\text{decoke}}) \quad \forall j, t \quad (\text{C.153})$$

$$P_{ij}^{\text{min}} \cdot (1 - \delta_{jt}^{\text{decoke}}) \leq P_{ijt} \leq P_{ij}^{\text{max}} \cdot (1 - \delta_{jt}^{\text{decoke}}) \quad \forall i, j, t \quad (\text{C.154})$$

Decoking single reactor

$$\sum_j \delta_{jt}^{\text{decoke}} \leq 1 \quad \forall t \quad (\text{C.155})$$

Threshold limits for decoking

$$\text{Coke}_{jt} \leq \text{Coke}_j^{\text{max}} \quad \forall i, j, t \quad (\text{C.156})$$

$$\text{Tw}_{jt} \leq T_j^{\text{max}} \quad \forall i, j, t \quad (\text{C.157})$$

Energy constraints

$$E_{jt}^{\text{furnace}} = \sum_i \sum_k \text{PD}_{ijkt} \cdot E_{ijk} \quad \forall j, t \quad (\text{C.158})$$

$$E_t^{\text{compressor}} = \sum_i \sum_j \sum_k \sum_c \left(\frac{\text{PRate}_{ijkct}}{\text{MW}_c} \right) * E^{\text{comp}} \quad \forall t \quad (\text{C.159})$$

Steam generated

$$F_{ijt}^{\text{HPsteam}} = P_{ijt} \cdot G^{\text{HPsteam}} \quad \forall i, j, t \quad (\text{C.160})$$

$$F_{ijt}^{\text{MPsteam}} = P_{ijt} \cdot G^{\text{MPsteam}} \quad \forall i, j, t \quad (\text{C.161})$$

Tightening constraints

$$\sum_{t'=t}^{t+\eta} \delta_{jt'}^{\text{decoke}} \leq 1 \quad \forall j, t \quad (\text{C.162})$$

$$\sum_t \delta_{jt}^{\text{decoke}} \leq \beta \quad \forall j \quad (\text{C.163})$$

$$\sum_{t=1}^{t+\gamma} \delta_{jt}^{\text{decoke}} \leq 0 \quad \forall j \quad (\text{C.164})$$

$$\text{Coke}_{jt-1} \geq \text{Coke}_{\text{allowed}}^{\text{decoke}} \cdot \delta_{jt}^{\text{decoke}} \quad \forall j, t \quad (\text{C.165})$$

Integrated demand constraint

$$\sum_t \text{Sales}_{ct} \leq \text{Demand}_c \quad \forall c \quad (\text{C.166})$$

End conditions

$$\text{Coke}_{jNT} \leq \text{Coke}_{\text{calculated}}^{\text{max}} \quad (\text{C.167})$$

$$\text{Coke}_{\text{calculated}}^{\text{max}} = \text{Coke}^{\text{max}} - \text{Nfrs} * \text{Coke}_{\text{accum/period}}^{\text{max}} \quad (\text{C.168})$$

Objective function

The objective function is shown as equation (C.169).

$$\text{Objective function} = \text{Plant Profit} - \text{Penalty}^{\text{Coke}} - \text{Penalty}^{\text{Recy_Inv}} + \text{profit}^* \quad (\text{C.169})$$

$$\begin{aligned} \text{Plant Profit} = & \text{Value of products} - \text{Cost of feedstocks} - \text{Cost of dilution} \\ & \text{steam} - \text{Cost of furnace energy} - \text{Cost of compressor energy} + \text{Value of HP} \\ & \text{and MP steam generated at TLE's} - \text{Cost for furnace decoke.} \end{aligned} \quad (\text{C.170})$$

Details of each term in the profit equation are given as follows:

$$\text{Value of products/ Income} = \sum_t \sum_c \text{Sales}_{ct} \cdot \text{Cost}_c^{\text{product}} \quad (\text{C.170a})$$

$$\text{Cost of feedstocks} = \sum_t \sum_i F_{it} \cdot \text{Cost}_i^{\text{feed}} \quad (\text{C.170b})$$

$$\text{Cost of dilution steam} = \sum_t \sum_i \sum_j \sum_k \text{PD}_{ijkt} \cdot \rho_{ik}^{\text{S/HC}} \cdot \text{Cost}_{\text{steam}}^{\text{dilution}} \quad (\text{C.170c})$$

$$\text{Cost of furnace energy} = \sum_t \sum_j E_{jt}^{\text{furnace}} \cdot \text{Cost}_{\text{energy}}^{\text{furnace}} \quad (\text{C.170d})$$

$$\text{Cost of compressor energy} = \sum_t E_t^{\text{compressor}} \cdot \text{Cost}_{\text{energy}}^{\text{compressor}} \quad (\text{C.170e})$$

$$\text{Value of HP and MP steam} = \sum_t \sum_i \sum_j F_{ijt}^{\text{HPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{HP}} + \sum_t \sum_i \sum_j F_{ijt}^{\text{MPsteam}} \cdot \text{Cost}_{\text{steam}}^{\text{MP}} \quad (\text{C.170f})$$

$$\text{Cost for furnace decoke} = \sum_t \sum_j \delta_{jt}^{\text{decoke}} \cdot \text{Cost}_{\text{energy}}^{\text{decoke}} \quad (\text{C.170g})$$

$$\text{Penalty}^{\text{Rcy_Inv}} = \lambda \cdot \sum_t \sum_i \text{Rcy_Inv}_{it} \quad (\text{C.170h})$$

$$\text{Penalty}^{\text{Coke}} = \frac{\sum_j \text{Coke}_{j\text{NT}}}{\text{Coke}_{\text{max}}} \cdot (\text{Cost}_{\text{decoke}}^{\text{energy}} + \text{Cost}_{\text{decoke}}^{\text{profitloss}}) \quad (\text{C.170i})$$

Appendix D

**Optimization under uncertainty: A brief review of the
state-of-the-art**

Multi-period optimization under uncertainty: State-of-the-art review of tools		
Predictive approaches (Open loop)	Advantages	Disadvantages
Deterministic optimization methods (Kallrath 2002, Floudas et al., 2004, Grossmann, 2005 and Mendez et al., 2006)	<ul style="list-style-type: none"> ▪ Is the basis for mathematical formulation of general SSC problems ▪ First and necessary step for problem formulation ▪ Issues of modeling uncertainties are usually embedded onto these models using various robust optimization techniques 	<ul style="list-style-type: none"> ▪ Open loop solution. Cannot update the solution at later stages in the event of occurrence of disturbances. ▪ Uncertainty is not explicitly modeled ▪ Problem size of the MILP dictates the computational complexity ▪ Not ideal for online implementation
Robust optimization technology (Second Order Conic Programs (SOCP)) (Ben Tal and Nemirovski, 2000, Lin and Floudas, 2004)	<ul style="list-style-type: none"> ▪ Can explicitly model the uncertainty in the model parameters and the exogenous inputs (i.e. measured and unmeasured disturbances) ▪ Convex problem. Robust solutions ▪ Can handle continuous and integer variables ▪ Problems with continuous variables can be solved easily in a reasonable amount of time to global optimality 	<ul style="list-style-type: none"> ▪ Open loop solution. ▪ Solution obtained based on predicted uncertain parameters. Cannot update the solution upon realization of uncertainty. ▪ Problem size dictates the computational complexity when considering integer variables. ▪ Not ideal for online implementation.

<p>Probabilistic or chance constraint (Birge and Louveaux, 1997, Warren, 2004, Sen and Hilge 1999)</p>	<ul style="list-style-type: none"> ▪ Addresses the uncertainty in a probabilistic manner ▪ Confidence level can be used as a tuning parameter to adjust the system near constraints 	<ul style="list-style-type: none"> ▪ Open loop solution. Solution obtained based on predicted exogenous inputs. ▪ Can become computationally intractable if standard distributions (e.g. normal) are not used to define uncertainty. ▪ Probabilistic constraints should be well formulated. Their deterministic counterpart could be non-convex. ▪ Not ideal for online implementation
<p>Parametric programming (Pistikopoulos et al., 2002, Sakizlis et al., 2004, Li et al., 2006 and Ryu et al., 2004).</p>	<ul style="list-style-type: none"> ▪ General framework to parameterize the solution (i.e solution as a function of model parameters) by solving the optimization problem only once. ▪ Then use the same solution for various realizations of uncertain parameters ▪ Small problems can be solved in a reasonable amount of time 	<ul style="list-style-type: none"> ▪ Open loop solution. Cannot readjust the solution upon realization of uncertainty ▪ Computationally intensive to obtain the basis or parametric solution for large problems ▪ Not ideal for online implementation

Reactive approaches (Closed loop)	Advantages	Disadvantages
Nominal MPC framework (Qin and Badgwell, 1996, 2003, Marlin, 2000)	<ul style="list-style-type: none"> ▪ Stability, performance and robust constraint handling is achieved by heuristically tuning the parameters and providing appropriate safety margins ▪ Feedback information available at every execution time. Rolling horizon approach, can compensate stochastic disturbances ▪ Computationally efficient. Ideal for online application 	<ul style="list-style-type: none"> ▪ Does not use an explicit model of uncertainty. ▪ Could be more conservative due to the oversized safety margins ▪ Handles only continuous variables
Robust MPC framework (Warren, 2004, Bemporad and Morari, 1999, Van Hessem, 2004)	<ul style="list-style-type: none"> ▪ Explicitly considers uncertainty due to plant/model mismatch and exogenous variables (measured, unmeasured disturbances) ▪ Closed loop prediction of future behaviour ▪ Guarantees stability, feasibility and performance (Robust solutions) ▪ Certain formulations are computationally efficient. Ideal for online application 	<ul style="list-style-type: none"> ▪ Could be computationally intensive depending on the size of the problem. ▪ Handles only continuous variables.
Stochastic programming (SP) with recourse (van der Vlerk, 2004, Sen and Hilge 1999)	<p><u>Two stage and multistage SP</u></p> <ul style="list-style-type: none"> ▪ Models closed loop uncertainty using recourse ▪ Two stage SP approximation in computationally tractable. ▪ Ideal for online application 	<ul style="list-style-type: none"> ▪ Two stage SP doesn't handle future uncertainty appropriately ▪ Multistage SP is computationally intensive (intractable for a large number of stages or time steps). ▪ Handles only continuous variables

<p>MPC for supply chain management (Wang et al., 2003, Rivera et al., 2004, Seferlis and Giannelos, 2004)</p>	<ul style="list-style-type: none"> ▪ Uses heuristics to select the model parameters that guarantee performance and robustness ▪ Rolling horizon approach, can compensate stochastic disturbances ▪ Ideal for online implementation 	<ul style="list-style-type: none"> ▪ Deterministic controller model, i.e., included in back-off calculations ▪ Uses simple heuristics to back off from infeasibilities ▪ Can handle only continuous variables
<p>MPC for control of hybrid systems (Bemporad and Morari, 1999, Pistikopoulos et al., 2002, Sakizlis et al., 2004)</p>	<ul style="list-style-type: none"> ▪ Can handle continuous and integer variables ▪ Rolling horizon approach, can compensate disturbances ▪ MILP or MIQP is solved at each execution time. Ideal for online application (if MILP can be solved within each execution period) ▪ Uses parametric programming to obtain robust solutions 	<ul style="list-style-type: none"> ▪ Uncertainty is not explicitly modelled for the nominal case. ▪ Size of MILP or MIQP could dictate the computational complexity. ▪ Also, obtaining a parametric solution could be computationally intensive for large problems.
<p>MPC for supply chain optimization (Mestan et al., 2006, Perea-Lopez et al., 2004)</p>	<ul style="list-style-type: none"> ▪ Can handle continuous and integer variables (solves a MILP at each execution time) ▪ Rolling horizon approach to react against disturbances (varying demand) ▪ Ideal for online implementation (if MILP can be solved within each execution period) 	<ul style="list-style-type: none"> ▪ Uncertainty is not explicitly modelled. ▪ Similar to nominal MPC but with integer variables. ▪ Can be computationally intensive depending on the size of MILP

<p>Simulation based optimization (Honkomp et al., 1999 and Jung et al., 2004)</p>	<ul style="list-style-type: none"> ▪ Can handle continuous and integer variables ▪ Two simulation plant models (deterministic and stochastic models) are used to assess the performance and validate the robustness of the solution. ▪ Reactive solution update if the solution is found infeasible or below the specified tolerance limits by re-optimization. 	<ul style="list-style-type: none"> ▪ Only deterministic optimizer is used. So, the solutions could become infeasible due to uncertainty. ▪ Only the solution in the future stages is adjusted to account for infeasibility ▪ Could be computationally intensive depending on the number of re-optimizations.
<p>Stochastic integer programming (SIP) with recourse (Sand and Engell, 2004, Shultz 2003 and Grossmann et al 2003)</p>	<p><u>Multistage SIP</u></p> <ul style="list-style-type: none"> ▪ Can handle continuous and integer variables. ▪ Multistage SIP models the closed loop uncertainty appropriately (using recourse). ▪ An approximate solution framework has been proposed Grossmann (2003) using the idea of solving several two stage SIP's within a shrinking horizon. 	<ul style="list-style-type: none"> ▪ Multistage SIP is computationally intensive (intractable for large stages or time steps). ▪ Cannot be used for online application unless approximation strategies are used.
	<p><u>Two stage SIP</u></p> <ul style="list-style-type: none"> ▪ Can handle continuous and integer variables. ▪ Models closed loop uncertainty ▪ Computationally tractable for moderate problem sizes. Ideal for online application. 	<ul style="list-style-type: none"> ▪ Two stage SP doesn't handle future uncertainty appropriately ▪ Can be computationally intractable for large problems

