Optimal Scheduling for Chemical Processes and its Integration with Design and Control

by

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AUTHOR'S DECLARATION

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Abstract

Optimal scheduling is an active area of research as the economics of many chemical processes is affected to a great extent with the optimality of schedules of their operations. Effective use of resources and their capacities is paramount in order to achieve optimal operations. Manual and heuristics-based approaches used for scheduling have their limitations which inhibit the chemical process industries to achieve economically attractive operations. One such sector is the analytical services industries and success of companies in this sector highly relies on the effective scheduling of operations as large numbers of samples from customers are received, analyzed and reports are generated for each sample. Therefore, it is extremely important to efficiently use all the various resources (labor and machine) for such facilities to remain competitive. This study focuses on the development of an algorithm to schedule operations in an actual large scale analytical services plant using models based on multi-commodity flow (MCF) and integer linear programming (IP) techniques. The proposed scheduling algorithm aims to minimize the total turnaround time of the operations subject to capacity, resource and flow constraints. The basic working principles of the optimization-based algorithm are illustrated with a small representative case study, while its relevance and significance is demonstrated through another case study of a real large scale plant. In the latter case study, the algorithm's results are compared against historical data and results obtained by simulating the current policy implemented in the real plant, i.e., first-come first-served.

Along with scheduling, many chemical processes require the optimization of other aspects that play major part in the process economics, e.g. design and control. An important section of the chemical process industry produces various grades of products (multi-product) and the scheduling of the production of these grades along with optimal design and control play important roles in the economy of the operations. As part of this research study, a new methodology that can address three aspects of the economy of the multiproduct processes together; i.e. simultaneous scheduling, design and control, has been developed. A mixed integer non linear programming (MINLP) optimization framework has been formulated, which aims to simultaneously evaluate optimal design, steady state operating conditions for each grade as a part of design, optimal tuning parameters for the controllers, optimal sequence of production of various grades of product and optimal smooth transitions between the grades. This is achieved via minimization of overall cost of the operation. The proposed methodology takes into account the influence of disturbances in the system by the identification of the critical frequency from the disturbances, which is used to quantify the worst-case variability in the controlled variables via frequency response analysis. The uncertainty in the demands of products has also been addressed by creating critical demand scenarios with different probabilities of occurrence, while the nominal stability of the system has been ensured. Two case studies have been developed as applications of the methodology. The first case study focuses on the comparison of classical semi-sequential approach against the simultaneous methodology developed in this work, while the second case study demonstrates the capability of the methodology in application to a large-scale nonlinear system.

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Nomenclature

List of English symbols

A	Arrhenius constant
A_t	Heat transfer area
AR	Amplitude ratio
$\mathbf{A}_i$	State matrix for grade *i* in state space representation
$\mathbf{B}_i$	Input matrix for grade *i* in state space representation
C_i	Initiator Concentration
C_m	Monomer Concentration
C_b	Butadiene Concentration
C_r	Radical Concentration
C_{br}	Branched Radical Concentration
C_i^{SP}	Set point for specification of grade *i*
$C_i(t)$	Current value of specification variable for grade *i*
Cap_{p_i}	Capacity of a process
CC	Capital Cost
C_A	Concentration of reactant A
$C_{A,F}$	Initial concentration of reactant A
C_B	Concentration of product B

$C_{B_i}^*$	Set point of concentration of product B for grade *i*
C_p	Heat capacity
C_m^{in}	Initial monomer concentration
$\mathbf{c(t)}$	Controllers' states
$\mathbf{C}_i$	Output matrix for grade *i* in state space representation
c_i	Cost associated with the use of resource of a process i
$\mathbf{d}$	Set of optimization variables
$\mathbf{d}_0$	Initial set of optimization variables
$\mathbf{D}_i$	Feedforward matrix for grade *i* in state space representation
d_s	Deadline associated with a job s
e	Error between set point and real value
eig	Eigenvalues
$\mathbf{f}$	Open loop process model
$\mathbf{f}_{closed}$	Closed loop process model
$\mathbf{g}$	Controllers' equations
$\mathbf{G}(z\omega)$	Transfer function in frequency domain
$\mathbf{h}$	Process Constraints
H_0	Heat of reaction
i	Index denoting product grade

I	Number of product grade to be produced
$I^m(\omega)$	Imaginary part of transfer function
j	Index denoting uncertain scenario
k_0	Pre-exponential factor
$k(s)$	Length of the path of a job
k	Index denoting process disturbance
K_{C_1}	Controller gain
l	Index denoting controlled variable
N	Set of samples
n_s	Samples under consideration
ns	Number of critical uncertain scenarios
$NS_{p_i^s}^{t,s}$	New samples entering the system for a job at a process at current time
$N\Delta t$	Total integration time
P	Set of processes
p_i	A process in the system
p_i^s	A process in the path of the job
$p_{k(s)}^s$	Last process in the path of the job
P_L	Penalty for finishing the analysis late
P_N	Penalty for not finishing the analysis within scheduling time horizon

P^j	Probability associated with uncertain critical scenario
$P_{V,i}$	Volume of product grade *i*
$P_{T,i}$	Penalty for transition for grade *i*
$path_s$	Path of a job
q	Outlet flow rate of the reactor
q_F	Inlet flow rate to the reactor
Q_C	Heat duty
q_i	Initiator flow rate
q_m	Monomer flow rate
q_{cw}	Cooling water flow rate
R	Reward for finishing the analysis before the deadline
$R(\omega)$	Real part of transfer function
R	Set of real numbers
$r_t(p_i)$	Resources available for a process at given time
r_A	Rate of reaction of reactant A
OC	Operating cost
S	Set of scheduling variables
s	Sequence of production of grades
SSE	Sum of squared errors

s	Index denoting the job under consideration
S	Set of jobs
t	Time
t_i	Transition time for grade *i*
t_{p_i}	Production time for grade *i*
t_{total}	Total time of operation
T	Temperature in the reactor
T_F	Feed stream temperature
T_j	Jacket temperature
TC	Transition cost
$\mathbf{u}$	Set of manipulated variables
U	Heat transfer coefficient
V	Volume of reactor
V_C	Jacket volume
V_E	Size of equipment
V_i	Size of storage for grade *i*
VC	Variability cost
w_s	Priority number for a job
$\mathbf{w}$	Set of uncertain scenarios

W	Annual Recovery Factor
x(t)	States of the system
$\mathbf{x}_{lin}$	Linearized states of the system
x_m	Monomer conversion
$\chi_{p_i\,p_j}^{t,s}$	Decision variable for the location of samples
y	Process output variables that are in closed-loop (controlled variables)
$y_{p_i}^{t}$	Decision variable for the resources
Z_E	Cost of construction per unit for process equipment
Z_E	Cost of construction per unit for product tanks
Z	Set of integer variables

List of Greek symbols

$\tau(p_i)$	Processing time of a process
τ	Time Constant for PI controller
$\boldsymbol{\varphi}$	Process inputs
$\boldsymbol{\eta}$	Process disturbance
$\boldsymbol{\Omega}$	Process output variables
$\boldsymbol{\theta}$	Process output variables that are not in closed-loop

$\boldsymbol{\kappa}$	Design parameters and operating conditions
$\boldsymbol{\Lambda}$	Controller tuning parameters
$\boldsymbol{\alpha}$	Transition slopes
Φ	Cost function
Φ	Phase angle
$\omega_{c_{k,i}}$	Critical frequency of disturbance *k* affecting grades *i*.
$\varepsilon(t)$	Deviation from set point in transition stage
ξ_p^0	Zeroth moment live polymer moment
ξ_p^1	First moment live polymer moment
ε_r^0	Zeroth moment dead polymer moment
ε_r^1	First moment dead polymer moment
ε_b^0	Zeroth moment butadiene moment
ε_b^0	First moment butadiene polymer moment

List of Abbreviations

CSTR	Continuous Stirred Tank Reactor
FMCG	Fast Moving Consumer Goods
HIPS	High Impact Polystyrene
IP	Integer Programming

MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Nonlinear Programming
MPC	Model Predictive Control
PI	Proportional and Integral (control)
RTN	Resource Task Network
STN	State Task Network

Chapter 1
Introduction

Most of the chemical engineering industries involve highly integrated processes that need to be operated at near optimal conditions to become profitable and studies have been published in order to address various aspects of these industries, e.g., pharmaceutical [1,2], oil and gas [3-5], power generation [6-11]. The success of chemical process industry has always been subjected to the economics of several aspects such as the optimal design of a plant, the development of efficient control schemes that can maintain the dynamic operation of the process within feasible limits and optimal scheduling of the plant's operations. Process scheduling has been an active area of research as a large sector of the chemical process industry highly relies on its optimality in order to achieve near-optimal economic operations. Industries like pharmaceuticals, steelmaking continuous-casting, paint, refinery operations, analytical services, multi-product processes require optimal scheduling in their operations in order to meet demands while reducing the cost and time of operations. Most of such processes are characterized by a complex network of processes, limited resources and capacities, and high level of exposure to deadlines. The limited capacities and resources bottleneck the processes if the schedules for activities are not optimal; thus, the management of resources directly affect the performance of the industry and eventually the process economics. The classical approach for scheduling, i.e., manual approach with dependence on human skills, may become challenging or even prohibitive when attempting to use the capacities and resources in the most optimized pattern. These concerns grow proportionally with the scale of the industry. With ever-increasing demands; it becomes a challenge to schedule operations in the most profitable way. A classical rules-based approach like 'first-come-first-served' also limits the optimum use of design capacities of the processes and thus returns sub-optimal schedules. Following this, development of an optimization-based algorithm that generates the schedules via optimal management of resources and their capacities is paramount.

One of the sections of the chemical process industry that highly relies on the effective scheduling for its success is the analytical services industry. In this sector, several types of analyses are performed by the application of a set of tests based on various analytical techniques for carrying out complete examination of material samples for multiple physical, chemical properties. The analysis of such properties is an important part of the decision-making process of several other companies and, therefore, the efficiency of its operations can have a significant impact in a large number of industries, e.g., life sciences, forensics, petroleum, mining. In this service sector, the inputs to the system are not known in advance and typically have high variability, which makes the task challenging. Along with components common to several scheduling problems, the analytical services industry also has some challenging specific characteristics. One such example is that the processing times of each of the different processes vary significantly from each other and uncertainties may be present in them. In addition, scheduling decisions need to be in the form of location of the samples in the system at any specific point in time and with the large scale size of the industry, a large number of scheduling decisions are required, amplifying the complexity of the problem. Based on the author's knowledge, there is a lack of literature that focuses on the applications of optimal scheduling in the sector of analytical services industry, while the operational characteristics of the analytical services industry are not studied in detail. This constitutes the motivation behind the development of scheduling algorithm for this sector. The scheduling problem can be formulated to achieve specific objectives which may include reducing the overall cost of the operations while meeting the demand, minimizing the use of resources to reduce maintenance and operating costs, and effective management of labor with multiple skills in order to achieve optimal assignments of various tasks.

Apart from addressing the scheduling via optimization as a single aspect in the industries, various other aspects of the chemical processes need to be considered along with scheduling, i.e., design and control. These aspects can be addressed together where combinations of two of these aspects are considered together, e.g., scheduling and design, scheduling and control. In these approaches, optimal parameters are calculated for only two aspects, and therefore, there is no integration of all the aspects of process economics. The solutions obtained through these approaches are limited to only a few aspects. Following this, there is a need to develop an approach where all the aspects are addressed simultaneously by the integration of all three aspects to achieve the optimal scheduling, design and control. This approach is expected to provide more economically attractive results as compared to the classical approach. A section of the chemical process industry that involves scheduling, design and control and strongly needs such integration of theses aspects in order to achieve optimal operations is multi-product processes. These processes produce several grades of products that are specified with certain properties. Multi-product processes operate in two basic modes, i.e. transition between grades and production of the grades. The optimal variables need to be evaluated for equipment design and operating conditions, control parameters, slopes of transition that denote the rate of transition and sequence of production of grades. Most of the chemical processes are often subjected to process disturbances, therefore, an optimal scheduling, design and control obtained without consideration of these process disturbances may fail to comply with the process constraints when it is subjected to these disturbances (e.g., inlet stream's temperature, flowrate and concentration). The resulting instances of infeasibility or constraint violations due to the presence of disturbances will have adverse effects on the process economics. Thus, developing a methodology that takes into account these disturbances is necessary. The process disturbances can be specified in several ways including use of pre-defined function or randomly from a probability distribution. Another challenge that many chemical processes including multi-product processes encounter is parametric uncertainty. The uncertainties are commonly present in several parameters and approaches developed without consideration of these uncertainties, i.e., approaches based on steady state optimization while using a perfect model (model parameters completely known) are not robust and can lead to constraint violation when subjected to these uncertainties. Therefore, the uncertainty in the parameters needs to be addressed at the design stage. Several methods can be found in the literature to address uncertainty which includes multi-scenario approach, stochastic programming and chance-constrained programming. The literature focused on the integration of different aspects of the economics of the multi-product processes is available but there is lack of studies that address the all the three aspects, i.e., scheduling, design and control, under the influence of process disturbances and uncertainty in the parameter. This forms the motivation behind the research conducted to develop a methodology that can address all the aspects discussed above.

1.1 Objectives and Contributions

The research carried out in this thesis develops an application of optimal scheduling in the analytical services industry and a methodology for integration of scheduling with design and control for multi-product processes. The specific objectives of this research are listed below:

1. Development of a basic scheduling algorithm for the improvement of operations in an analytical services facility. An optimization model will be developed using integer programming techniques along with multi-commodity flow. The algorithm will be tested with a small representative case study in order to observe the outcomes of the scheduling algorithm and its potential to improve the turnaround time of operation, i.e., time required to complete the analysis of samples received in the facility.
2. Historical data obtained from the industrial partner will be used to test the performance of the basic scheduling algorithm against the actual operations. This will demonstrate the potential of the scheduling algorithm to improve the actual operations in the facility under the assumptions considered while developing the algorithm.
3. Develop a new methodology to simultaneously address the design, scheduling and control aspects of the multi-product processes under the influence of process disturbances and uncertainty in the process parameters. A mixed integer nonlinear programming (MINLP) optimization formulation will be developed which determines the decision variables related to equipment design, control parameters and optimal schedule for the grades to be produced while maintaining the stability of the system.
4. Performance of the methodology will be compared against semi-sequential approach via application to a simple continuous stirred tank reactor (CSTR) system. The methodology will also be tested with a large scale high impact polystyrene (HIPS) process.

The research work conducted with the objectives mentioned above will make significant contributions to the area of optimal scheduling and its integration with other aspects of process economics. The development of scheduling algorithm for an analytical services facility is a novel application considering the operational characteristics of this sector. Better operations with shorter turnaround time can be achieved via optimal use of resources which eventually can increase the throughput of the operations. The study also brings to the literature the operational characteristics that are less studied and thus developments can be made in this sector of the chemical process industry. Similarly, the methodology developed for the integration of scheduling, design and control for the multi-product processes is a novel approach that integrates all the aspects under the influence of process disturbances and uncertainty in the parameters. Thus, a new contribution will be added to the field of integration of aspects to achieve economically attractive operations. This can be used as reference to further develop/enhance the methodologies in the field of integration of various aspects of chemical processes.

1.2 Structure of the Thesis

The thesis is organized in different chapters as follows:

A detailed literature review is presented in Chapter 2, which outlines the studies available in the open literature that present the various methodologies and approaches developed in the field of optimal scheduling and its integration with other aspects, e.g., design and control. This includes studies that focus on industrial applications of scheduling using several methods. The literature review also focuses on the studies that address the integration of scheduling with design and/or control for various processes, which includes multi-product processes. Chapter 2 also lists several reviews on the optimal scheduling and its integration with the other aspects for chemical processes.

Chapter 3 presents the algorithm developed for optimal scheduling in an analytical services facility owned by the industrial partner. The algorithm is based on an integer programming (IP) problem, which is presented with all the mathematical details along with modeling parameters.

The algorithm has been tested with a small-scale case study in order to depict the working principles of the algorithm along with its advantages and limitations. The second case study focuses on the comparison of actual operations in the facility against the results obtained from the scheduling algorithm, which shows the potential of the scheduling algorithm in achieving better operations, i.e., total time required to complete the analysis of samples has been minimized.

Chapter 4 presents a new methodology that aims to integrate scheduling, design and control of the multi-product processes. The methodology takes into account the influence of process disturbances as well as parameter uncertainty. One of the key features of the approach is the use of ramp functions for smooth transitions between various grades of products considered for production. The nominal stability of the system is also ensured. Two case studies have been developed in order to present the comparison of the simultaneous methodology against the semi-sequential approach and capability of methodology in the application to a large-scale nonlinear system, i.e., high impact polystyrene process.

The conclusions derived from this research are presented in Chapter 5. The Chapter also discusses the possible future path for the research work completed in order to strengthen their applicability.

Chapter 2

Literature Review

Optimal scheduling has been addressed via several studies published in the literature since its impact on the economics of the operations is significant. There have been many studies that present various approaches and techniques to achieve optimal scheduling. These techniques and their applications in various industries and sectors are revised and reported in this chapter. The chapter also discusses the nature of scheduling decisions. The areas in the chemical process industry for which scheduling applications have been developed are also discussed through reviews available in the literature. The works published in the literature that focus on the integration of various aspects of the chemical processes are also discussed. Since the study under the scope of this thesis aims to simultaneously address the scheduling, design and control aspects of multi-product processes, review of the studies that address integration of various aspects have also been reviewed. A review of the studies that focus on multi-product processes is presented along with a discussion on the techniques used in those studies. In addition, the approaches and methodologies that take into account the presence of process disturbances and uncertainty in the parameters are reviewed and presented.

2.1 Optimal scheduling for chemical processes

Scheduling is an important aspect of most of the chemical process industries including manufacturing and services industries. Scheduling can be defined as the assignment of tasks to specified resources under constraints. The main purpose of scheduling is to ensure that resources, equipment, utilities, etc. are ready to execute a task whenever it is assigned to them. Optimal scheduling is often used to achieve economically attractive operation via maximization or minimization of an objective function while assigning tasks to different resources.

A basic scheduling problem can be conceptually formulated as follows:

$$\begin{aligned} &\max \;\; z = f(P, C, S) \\ &s.t. \;\; \text{Process Constraints} \\ &\qquad \text{Resource Constraints} \\ &\qquad \text{Capacity Constraints} \\ &\qquad \text{Demand Constraints} \end{aligned} \tag{2.1}$$

where, z is an objective function representing the profit generated through operations. It is typically a function of market prices of products/services (*P*), cost incurred in operations (*C*) and schedule/sequence of operations (*S*). The optimization problem aims to find a schedule/sequence (*S*) of operations that corresponds to maximum profit, i.e., optimal scheduling decision variables. Note that problem shown in (2.1) can be also be formulated as a minimization problem to reduce, for example, the costs associated with process scheduling. The problem is subject to process constraints that aim to maintain feasibility of the solution in terms of process limitations, e.g., constraints on the operating conditions for the different units considered in process scheduling. Resource and capacity constraints ensure that the generated schedules are practically achievable in terms of design capacities of the resources. Deadlines can also be incorporated in a scheduling problem in the form of demand constraints in order to achieve required demands within due timelines.

Following the general formulation presented in problem (2.1), scheduling problems can have various forms that differentiate them from each other. These problems can be categorized in several ways in terms of the representation of the optimization problem as well as the techniques employed to develop these problems. Reviews of process scheduling have been published that discuss the classification of scheduling problems and various techniques used to develop such problems [14, 15]. Figure 2.1 describes the characterization of scheduling problems according to some of the key aspects.

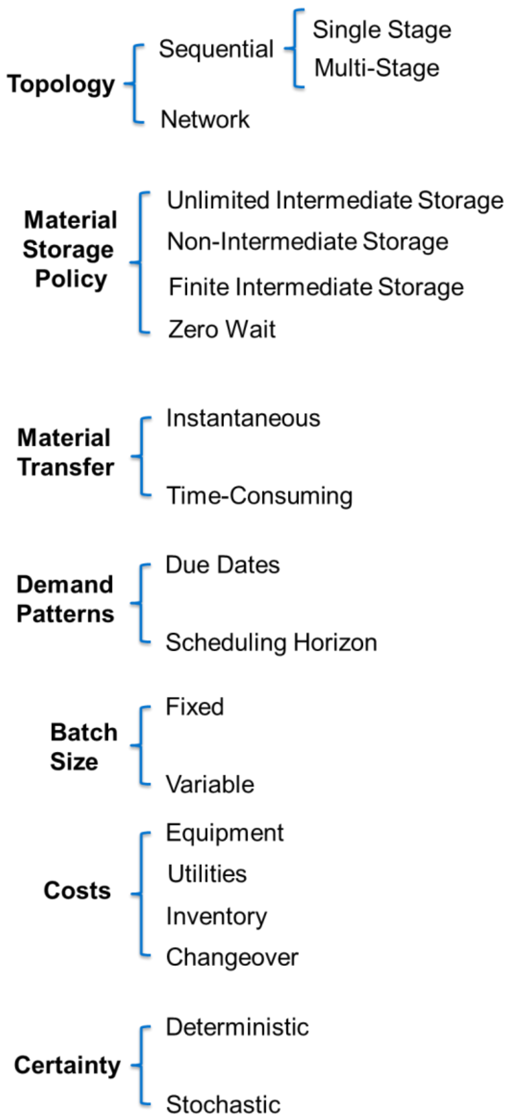

Figure 2.1. Classification of Scheduling Problems

Process layout and its topological implication is one of the main features that affect the scheduling model in terms of model complexity. Many processes are sequential and can be single stage or multi-stage depending upon the units working in parallel. For more complex processes, network process models need to be considered with complex recipes involving interaction of operations. Another important aspect used for the classification of scheduling problems is related to inventory policies, which involve finite and dedicated storage policies. Some cases also include shared tanks and zero-wait, non-intermediate and unlimited storage policies. Material transfer is one of the important aspects; although most cases are characterized by instantaneous transfer, some processes involve time-consuming transfers that also need to be accounted for while developing scheduling models. Another key factor is demand patterns which are typically represented by due dates though time horizons may also be used to consider production completion. Batch sizes must be handled depending upon the processes, fixed or variable. Fixed sizes do not involve mixing or splitting, while variable sizes may involve mixing. The costs associated with equipment, inventory, utilities and changeovers can affect the scheduling model to a great extent. Furthermore, the uncertainty in the parameters is one of the most important characteristics of the processes. Deterministic problems are easier to model as compared to stochastic ones which involve handling uncertainty in the parameters, e.g. production demands.

A few important classifications are based on time representation, different characteristics of scheduling problems and the use of the techniques like integer programming, linear and nonlinear programming. In terms of time representation, the scheduling problems can be divided into discrete time and continuous time representations. A large number of applications in scheduling involve modeling the scheduling problems in discrete-time, in which the time the scheduling horizon is divided into a number of time intervals of uniform duration and the beginning and ending of a task are associated with the boundaries of these time intervals. A good approximation of the actual problem (real continuous time) is limited by the choice of the time interval used for discretization. A smaller interval can achieve better results while increasing the problem's size along with the number variables to be tracked. In order to overcome the limitations of the discrete time approach, continuous time representations of the scheduling problem have been attracting researchers; however modeling using this approach is more challenging task. Events are allowed to take place at any point in the continuous domain of time and therefore the limitation of having inactive event times associated with the discrete time can be eliminated. Thus, the continuous time representations also reduce the problem size and therefore are computationally attractive. However, modeling with this approach can add many complexities as compared to the discrete time approach. For example, handling the variable nature of the timing of the events is difficult, while the resource limitations need complicated definition for constraints increasing the complexity of the problem.

Scheduling problems can be further classified according to their characteristics. Some of these include the processing sequences, the modes of operations and the types of objective functions. In terms of processing sequences, problems can be classified for sequential processes and network represented processes. In the sequential processes, the modeling is based on the fixed processing sequence. Several processing stages can be defined, i.e., single stage or multi-stage, while the processing units are present in the processing stages. For this type of processes, batches are used to represent production and therefore, it is not necessary to consider mass balances explicitly. When there are more complexities in the sequence of processing (i.e., processing sequence is not fixed), the network representation approach is used. The network represented processes are of two main types, state task network (STN) [12] and resource task network (RTN) [13]. In STN representation, two types of nodes are used. The 'state' nodes consist of raw materials, intermediate materials and final products, while the 'task' nodes represent the operations. The representation also involves the arcs connecting the states to tasks, which denote the fraction of states consumed by tasks. The STN can be further extended to RTN representation by describing processing equipment, utilities, storage as resources. These are added to the network as resource nodes. The two representations can be used when the material balance is explicitly required.

Scheduling problems can also be classified according to the operation modes of processing tasks, i.e., batch and continuous. In batch tasks, the material are fed at the start of the task and the products are produced at the end of the task, whereas in the continuous tasks the products are produced throughout the period of the tasks and the processing rates can be constant or remain in a range. The two representations depend upon the operations under consideration and the respective scheduling requirements. Another way of categorizing the scheduling problems is according to the objective function. The objectives can be of several types depending upon the operations. These objectives can include minimizing the make-span, where optimal schedule is generated in order to shorten the overall time of the operation. Another objective can be minimization of earliness or costs, where optimal schedules are searched that correspond to the lowest possible cost, which can be measured by simply the deviations from the deadlines or the costs calculated via various factors of the process economics.

Apart from the characteristics of scheduling problems discussed above, various techniques can be used to develop scheduling problems. Scheduling problems often involve the use of integer programming techniques since the decision taken in these problems involves assignments of tasks to resources, which can be represented by non fractional entities (integers). Most commonly used techniques include linear integer programming (IP), mixed integer linear programming (MILP) and mixed integer nonlinear programming (MINLP). Linear programming

(IP) involves linear objective function as well as linear equality and inequality constraints, while the variables involved in this type of formulations are integers. One of the most commonly used techniques is the mixed integer linear programming (MILP), where linear optimization techniques are used which involves two types of variables. Some of the variables are restricted to be integers or binaries, while others are allowed to be continuous. Mixed integer nonlinear programming (MINLP) techniques have been successfully implemented in several scheduling applications. This technique is similar to the MILP technique, while the objective function and the constraints involved in this formulation can be nonlinear. These problems are much harder to solve as compared to MILP or IP problems.

2.2 Industrial Applications of Optimal Scheduling

Due to its significance for the chemical process industry, several studies that involve industrial applications of scheduling have been reported in the literature. The sectors like pharmaceuticals, oil and gas, paint industry, fast-moving consumer goods, paper and pulp, mining, power plants have been areas of research in terms of optimal scheduling. The industrial applications include work on scheduling in pharmaceutical pipelines involving decisions on scheduling and allocation of resources over development activities in multiple drug-related projects [16]. Case studies from the pharmaceutical sector have been presented that demonstrate the industrial application in that study. Scheduling in the large-scale steelmaking continuous-casting (SCC) process using unit specific event-based continuous time models has been published in the literature [17], where schedule were generated for the casts on machines including allocations, sequencing and timings. Another study presents the application in the same industry using robust optimization and stochastic programming in order to handle uncertainty in the production demands [18]. An industrial application of scheduling in a paint industry has been published which is based on an

MILP formulation and the decisions are made on the scheduling of wide variety of products competing for process equipment [19], whereas an application in the baker's yeast industry for optimal planning and scheduling that can handle variations in production volumes is also available in the literature [20]. Furthermore, another section of the chemical process industry that has several applications in terms of process scheduling with industrial scale is refineries. These studies include several applications for pipelines which include studies that schedule multi-product pipelines that connect the refinery to different distribution centers [21, 22] and work published with the application for hydrogen pipeline network [23]. There also have been studies for the lube oil operations where MILP formulations have been developed in order to schedule different modes of operation for the different processing units [24]. Optimal scheduling application for crude oil operations have been published which address scheduling of loading and unloading of crude oil in intermediate tanks, between port and distillation crude units in a refinery based on a mixed integer formulation [25] and state task network problem [26]. A multi-period optimization model has been presented for optimal scheduling of the hydrogen system within a refinery, where solution is obtained on an iterative method between that of an MILP problem and that of a nonlinear programming (NLP) problem [27]. Scheduling of decoking operation for furnaces have been addressed in the available literature [28-30], where operational modes of the furnaces are scheduled in order to achieve economical operation. Additional studies that discuss applications of scheduling in other sectors are also available. These include fast moving consumer goods (FMCG) industry [31] with the case study that is focused on scheduling for production of ice cream batches. Another MILP formulation has been developed to address scheduling in make and pack continuous plant for assignment decisions with an industrial application in a candy production plant [32]. Application of scheduling for job-shop operation has also been published in the literature which focuses on optimal scheduling of operations via assignments of machines with an objective to minimize the average tardiness [33]. Additional applications of scheduling can be found in the literature for distillation systems presenting swing cut modeling for planning and scheduling [34] and pulp and paper industry with decisions are taken on the paper machine setup pattern and on the production rate of the pulp digester [35]. A study that summarizes the successful industrial applications of scheduling has been published in the literature [36], which involve industries from different sectors, e.g., dairy, petrochemical, paper and pulp, crude blending. Real world scheduling problems have been solved over a long period of time using rolling horizon technique by generating solutions for several smaller problems over small intervals. There are several successful applications that have been published in literature that demonstrate the use of this technique including applications in integration of production planning and scheduling [37, 38], chemical-pharmaceuticals industry [39,40], procurement planning [41], continuous plants [42] and multi-product pipelines [43].

2.3 Optimization of Multi-product processes

Multi-product processes represent an important section of the chemical process industry which involves multiple aspects of process economics, i.e., scheduling, design and control. These processes aim to produce several grades of product specified by the compositions. The process needs to meet the demands and specifications of the required grades. The operation of these processes has two basic modes, i.e., transition and production. For each grade, the required composition of the product grade is achieved in the transition period while required amounts are produced in the production period. The optimization variables can typically include equipment design and operating conditions for each grade, control parameters and sequence of production, i.e., the order in which the grades are produced. A methodology to address these aspects is essential in order to achieve economical operations.

Various aspects of the multi-product processes have been traditionally addressed separately in order to generate optimal design, control and scheduling parameters that will result in most economic operations. Studies addressing the optimal design of multi-purpose /multiproduct processes have been published in the literature [44-46]. These studies show the typical approach considered to achieve optimal design, i.e. optimal equipment sizes and operating conditions are determined via steady-state optimization of plant economics. Another key aspect in multi-product plants is process controllability, which is concerned with the choice and optimal performance of the plant in closed-loop [47-48]. Moreover, optimal process scheduling is a key subject of relevance for various sectors in the chemical process industry including multiproduct plants. In these processes, various grades of the product are produced and scheduling of the production of the different products affect the process economics and therefore it must be addressed in optimal fashion. Scheduling for multi-purpose/multiproduct plants without its integration with any other aspects has been reported in the literature, which includes optimal scheduling of various multiproduct processes [49-51].

The limitation of these approaches is in the fact that the other aspects that affect the process economics are not considered simultaneously, which limits the optimal solution to address only a part of plant economics. Following this, integration of these aspects is necessary in order to address the complete plant economics.

2.4 Methodologies that Integrate Scheduling, Design and Control

The integration of design, scheduling and control for various chemical processes has been reported in various studies published in the literature including multi-product processes.

Consideration of process dynamics performance in the optimal design has been one of the most active research areas, i.e., integration of design and control. The integration of design and control has been addressed in many publications including the optimal design and control of various large-scale processes including bioethanol, extractive distillation, Tennessee Eastman process, sugar cane sulfitation tower, ternary distillation, multi-grade polymerization and styrene polymerization [52-59]. Several methodologies with different features and limitations for integration of design and control have also been proposed in the literature [60-65]. Most of the methodologies developed for the integration of design and control of chemical processes have considered conventional Proportional-Integral (PI) controllers in their analysis, while some of the studies discuss the simultaneous design and control using advanced model-based control techniques such as model predictive control (MPC) [66-71]. Integration of design and control approaches that have taken model parameter uncertainty into account has also been reported [72-77]. The development in the area of integrated design and control has been reviewed [78-82]. Besides the integration of design and control, several studies are also available for the integration of design and scheduling for chemical process systems. In these methodologies, scheduling of the process is incorporated in the design, where scheduling decisions are made along with optimal design in order to achieve economically attractive operations. These works include the publications on simultaneous design and scheduling in plants, multipurpose plants, and multiproduct plants [83-91]. This integration has a limitation since the controllability of the process has not been taken into account and thus it can have adverse effects on the economics of the process. To circumvent this issue, another section of literature focuses on addressing the simultaneous scheduling and control. In this approach, the optimal scheduling and control is achieved with fixed process design and thus achieving less optimal solution considering the complete process economics. The applications include the integration of scheduling and control for plants, polymerization processes, CSTRs, mixed-continuous processes, tubular reactors and multiproduct continuous parallel lines [92-100]. Engell and Harjunkoski have summarized the possible ways of integration of scheduling and control [101] whereas Harjunkoski an co-authors have discussed the practical use of the integration of these two aspects [102].

The different approaches proposed for integration of few of the three aspects for chemical processes have dealt with two aspects of the chemical process simultaneously. For the processes for which depend upon the optimal scheduling of their operations, integration of scheduling, design and optimal control is essential to improve the process economics. There are two main approaches through which the optimization of chemical processes can be addressed taking into account the three aspects described above. The first approach is to address each aspect one-by-one, i.e. sequentially. In the sequential approach, optimal parameters are calculated for different aspects independent of each other, i.e. in sequence and therefore, there is no integration of the aspects. The solutions obtained through this approach are sub-optimal because of the lack of simultaneous consideration of all aspects involved. In the second approach, all the aspects are addressed simultaneously by the integration of all three aspects to achieve the optimal scheduling, design and control. To the author’s knowledge, there is only one study available in the literature that has attempted to integrate design, scheduling and control for multi-product plants. In that study, the decisions were made on design including steady-state operating conditions and equipment sizing, on scheduling including production sequence and on optimal control [103]. The optimal transitions were part of control decisions and were directly obtained from optimization. One of the limitations of that study is that the control decisions did not involve the evaluation of controller tuning parameters as no closed-loop control scheme was implemented, i.e., the control actions were directly obtained from optimization and thus are only valid for the specific conditions used in the problem's formulation. The study also did not consider the effect of process disturbances which is another limitation. Therefore, a methodology that address all the aspects described above simultaneously for multiproduct plants, i.e. design, control and scheduling, is still lacking in the current literature.

The integration of the aspects must take into account the effect of process disturbances, since the optimal solution must comply with process constraints in presence of the disturbances. Many optimization-based approaches for the integration of aspects determine (or specify) the critical realizations in the disturbances that produce the largest deviations in the controlled variables. Several simultaneous methodologies have used time-dependent realizations in the disturbances following certain functions, e.g., a sinusoidal function [104, 105], or a series of step changes [106,107]. Another approach specifies the disturbances as stochastic time-varying perturbations that follow a user-defined probability distribution function [66]. Moreover, the uncertainty in the parameters needs to be handled in order to achieve optimal solutions that are robust to uncertainty in the parameters. The multi-scenario approach is one of the widely used methods to address the uncertainty in the parameters; especially in the cases where the process constraints must be satisfied. Although several methods have been developed to address the uncertainty in parameters, the multi-scenario approach is preferred because it is a widely used technique that has been successfully applied to various problems. Successful applications that use this approach in the optimization of different aspects of the chemical processes have been reported in the literature [8,108]. In this approach, critical scenarios are created for the uncertain parameters where each scenario describes the values of the uncertain parameter. Each scenario is assigned with a pre-defined probability of occurrence. This multi-scenario approach has been successfully applied in previous scheduling studies and therefore will be considered in the present research study to address uncertainty in the parameters during the integration of scheduling, design and control.

2.5 Chapter Summary

The chapter has presented the recent developments published in the literature that are relevant to the research work considered in this thesis. The motivation behind the research work has been discussed through the extent of works available in literature and the scope for development in the area of scheduling. The chapter also discusses the studies published that show the successful implementation of the techniques used in this research in industrial applications, e.g. rolling horizon technique. Moreover, discussion has been included about the integration of various aspects of the chemical process industries, i.e., scheduling, design and control. The development of methodologies within the area of integration of such aspects has been presented, while limitations of developed approaches have also been discussed. Starting from studies that address only one aspect out of scheduling, design and control to the recent studies that integrate two of these aspects and studies that simultaneously address all the aspects have been presented. Review of multi-product processes in terms of integration of these aspects has also been conducted by highlighting the recent studies reported in this area.

Following the literature review presented in this chapter, the application of optimal scheduling in the sector of analytical services industry is presented in the next chapter, which discuses in detail the development and implementation of a scheduling algorithm for a facility in this sector.

Chapter 3

Optimal Scheduling of a Large-scale Scientific Services Facility via Multi-commodity Flow and Optimal Scheduling Algorithm

As discussed in the previous chapter, the application of optimal scheduling in the chemical process industries is an active research field. However, the analytical services sector is a less-studied area, while the operational characteristics of this sector clearly depict the need for a scheduling algorithm in order to optimize performance of the industry. The aim of this work is to develop a basic scheduling algorithm in order to optimally schedule the operations of the facility owned by the industrial partner involved in this project. This chapter is structured as follows. Section 3.1 provides an overview on the typical operations in analytical services industries and presents a flow of the operations and the typical characteristics of this industry. Section 3.2 presents the model description and elements in the workflow of the algorithm. The mathematical formulation proposed in this work is described in detail in that section. Results and discussions are presented in Section 3.3. In this section, a small case study is presented first to illustrate the flow of the algorithm. Then, the effectiveness of this algorithm in developing optimal scheduling strategies for the analytical services sector is demonstrated by using an industrial case study. A comparison between the actual data from operations with simulated actual policy and the results obtained with the use of scheduling algorithm applied to the operational input data is presented. Section 3.4 discusses the summary of the developments and the work in this chapter. The content of this chapter has been published in the Industrial & Engineering Chemistry Research Journal [109].

3.1 Description of Operations in Analytical Services Industry

In this section, the focus is on describing the operations that will be considered for scheduling. The plant considered receives a large number of testing samples from different clients with their own set of analysis requirements, which are performed through various tests. Before the tests are performed, the samples undergo various pre-processing steps (i.e., preparation and chemical processing of the samples). Once the tests have been completed, the results are analyzed and are sent to the customers with reports describing the properties analyzed.

Before describing the typical workflow in the analytical services industry, below we summarize and define explicitly all the required terms used. These definitions will be relevant when presenting the optimization model in Section 3.2.

1. *Samples*- Samples are the basic unit in the analytical service industry. A sample is a smallest testing entity provided by the customer to go through a set of analyses that are required to know the properties of the samples.

2. *Process*- A process is an activity performed in the plant. This can be a test, a pre-process or a post-process activity that needs to be completed in order to complete the analysis.

3. *Resources*- The resources are the means of execution of the process. A resource is for example a machine that performs a particular activity. Every resource is entitled to a limited capacity.

4. *Job*- Samples going through the same analysis need to go through same set of processes in the system. A job is a group of samples that require the same analysis and belong to the same customer.

5. *Path*- The term path is assigned to each of the jobs. A path is a sequence of processes that a group of samples must go through. Given a particular analysis requested, the path that the samples must follow is pre-determined; therefore all samples in a specific job must go through a particular set of processes according to the path associated to that job.

6. *Turnaround time* – The 'turnaround time' of a sample is the time passed from the time when that sample arrived to the time where all the tests are completed and the results on that sample are ready to be sent to the customer. This includes the time required to carry out every single process involved in the path of the job.

7. *Schedule*- A schedule is the framework describing the execution of processes for various samples at various points in time. It provides the time of execution of each process for each sample.

The definitions described above are associated to various sections of the analytical services industry. The sections of the industry are described in what follows and can be represented as shown in Figure 3.1.

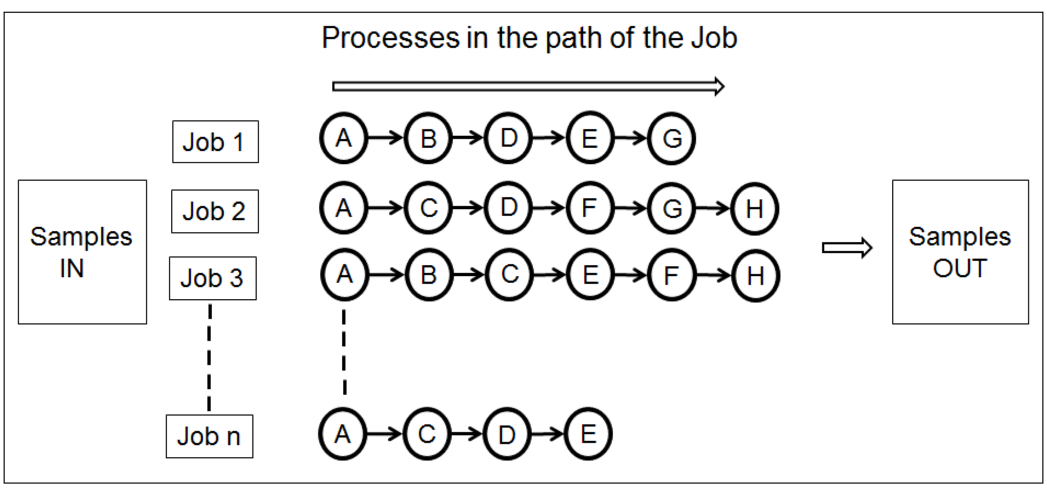

Figure 3.1. Overview of operations in Analytical Services Industry

Phase 1: Receive testing samples from various customers – this is a planning activity in preparation for analyses requested by customers, where the samples are made ready for the analysis and are assigned to go through specific processes, i.e. path, required to complete the analysis. This includes various sub-activities such as collecting, sorting samples as well as grouping them according to the analyses requested. This can be represented by the block 'Samples IN' in Figure 3.1.

Phase 2: Sample Analysis- the samples are examined with different testing techniques by using the various instruments referred to as resources. This stage also includes the processing required before conducting the tests, which may involve chemical processes carried out on samples so that they can be detected with certain properties with the instruments. The network of the processes is complex and is divided into a number of departments. There is high interaction between the departments because a department may receive samples from and send samples to various other departments simultaneously. The samples are processed in different numbers of processes depending upon the analysis requested, but the sequence of processes is pre-determined based on the type of analysis required. The use of resources to conduct the activities depends on the quantity of samples to be treated in a particular process, time required and available capacity of resources. The major portion of the samples' turnaround time of operation involves time spent in the analysis; therefore the effective scheduling of activities in this region becomes critically important. As shown in Figure 3.1, the processes carried out between blocks 'Samples IN' and 'Samples OUT' represent the sample analysis phase.

Phase 3: results and closure of analysis- This is the final phase of the operation where reports are generated detailing the results obtained from the analyses. All successful analyses are closed and that encompasses the final step in the scheduling process. Re-analyses are performed if the results are not up to the standards. This is the last stage of the workflow and is represented by block ‘Samples OUT’ in Figure 3.1.

As shown in Figure 3.1, for example, all the samples grouped in Job 1 have to go through processes in the specific order A, B, D, E and G, which is termed as the ‘path’ that must be followed to complete the analysis. The facility considered in the presented work receives around 14,000-15,000 samples every week, which are grouped in about 400-500 jobs on average.

3.2 Description of the Model

In this section, the modeling of scheduling problem under consideration is presented; defining the appropriate mathematical notation and discussing a few simplifying assumptions that have been made to make the problem tractable.

Consider that a set N of samples have been received and need to be analyzed for different properties, while P is the set of processes in the system with p_i being the i^{th} process. Samples are grouped together into a set S of ‘jobs’ according to the analysis required, thus samples requiring the same analysis can be grouped together as a ‘job’. This set of jobs and the number of samples in each job is part of the input data to the scheduling algorithm. The jobs that are considered for scheduling can have various statuses, which represent the process where the samples are at a particular point in time. Thus, the new jobs can have status as ‘start of the first process’, while other jobs that have finished some processes required for analysis would have appropriate statuses depending on the process the job is undergoing or has completed. A job can also have multiple statuses depending on the processes that different groups of samples within a job are at, i.e., different groups of samples within a job can be undergoing different processes. Each job s in S has n_s number of samples in it and goes through a specific path, denoted by $path_s$.

Each path represents a fixed sequence of processes, where each process p_i^s is an element of the path. For example, lets consider a facility that has 6 different processes A, B,C, D, E, F. A $path_1$ represents the path for job 1 that may correspond to processes A, B, F while $path_2$ represents the path for job 2 that may include processes A, C, D, F. Formally, $path_s$ will correspond to $k(s)$ number of processes p_1^s, p_2^s, ..., $p_{k(s)}^s$, representing the first, second,…, last process 'in the path' of the job s, while $k(s)$ representing the length of the path, i.e., number of processes involved in the analysis of job s. Thus in the example stated above, for $path_1$ (path for s =1), the first process in the path would be A $(p_1^1 = A)$, the second would be B $(p_2^1 = B)$ and the last would be F $(p_{k(1)}^1 = F)$ and $k(1) = 3$. This sequence of processes depends on the analysis required and the analysis completes once the last process in the path has been completed.

From here onwards, to simplify notation, the indices for the job in terms of processes have been excluded, for example – in the context of job s, p_i is the same as p_i^s if the discussion is specifically limited to job s.

Each process p_i in the system requires a processing time $\tau(p_i)$ to complete and there are $r_t(p_i)$ resources available for that process at time t. The resources can be machines or personnel performing the activity required to complete the process. Every unit of resource available for process p_i has a fixed capacity Cap_{p_i}, which corresponds to the number of samples that the resource can analyze per processing time. Every job s present in the network is associated with a priority weight w_s and a deadline d_s. The priority weight is a user-defined parameter that determines a preference to each job so that the turnaround time for jobs with higher priority weight will be given more importance by the scheduling algorithm. A deadline is the maximum allowed time that a job can take to complete the analysis. All the samples with their analyses finishing before the deadline are entitled to a ‘reward’ R whereas analyses that finish after the deadline are penalized with a ‘penalty for finishing late’ (P_L).

The scheduling problem has been modeled as a multi-commodity flow (network flow with multiple flow demands) process where the processes correspond to the nodes in the model. Time discretization is considered where system is tracked at finite time intervals, while the scheduling time horizon is provided as an input to the model. The samples that could not finish the analysis within the scheduling time horizon are penalized with 'penalty for not finishing' (P_N). The location of the samples at the end of the scheduling time horizon represents the starting point for the next scheduling time horizon (i.e., rolling horizon). The path dictates the flow through nodes and the capacity constraints limit the flow across nodes. The scheduling problem was formulated as an integer linear program. The integer linear program (IP) problem was solved using the software IBM ILOG CPLEX ver. 12.5.

3.2.1 Mathematical Framework

Let $\chi_{p_i\, p_{i+1}}^{t,s}$ be the decision variable that represents the number of samples from job s that start process p_i in the path for the job s at time t and therefore would be ready to start process p_{i+1} at time $t + \tau(p_i)$. In some cases, samples may need to wait at a certain process for some amount of time, e.g., if the resource has no capacity left to process more samples at time t. Accordingly, $\chi_{p_i, p_i}^{t,s}$ is an integer decision variable that denotes the number of samples in job s waiting at process p_i in the path from time t to $t+1$. The decision variable ($\chi^{t,s}_{p_i, p_i}$ or $\chi^{t,s}_{p_i\ p_{i+1}}$) describes the location of the group of samples in the path of the job and is defined such that there does not exist a variable that represents the samples moving backward in the path, i.e. samples going from process p_i to p_{i-1}. This has been achieved by forcing such variables to be zero. Moreover, $y^{t}_{p_i}$ is an integer decision variable that specifies the number of resources used by process p_i starting at time t. Similarly, $NS^{t,s}_{p_i}$ is an integer parameter for job s that represents number of new samples in job s that enter the system to start process p_i in the path of the job at time t. These samples can be considered as fresh samples. These can be samples newly entering into the system, i.e. ready to start the first process in the path of the job or from backlog jobs, for which partial analysis has been previously completed. The samples from the backlog jobs are the samples that enter the system at a process except the first process in their path, i.e. they have completed some processes before being considered for the scheduling.

The decision variables $\chi^{t,s}_{p_i\ p_{i+1}}$ and $\chi^{t,s}_{p_i, p_i}$ for a job s and the parameter $NS^{t,s}_{p_i}$ can be represented with the flow network as shown in Figure 3.2. These decision variables along with $NS^{t,s}_{p_i}$ can be interpreted as flows in the network of nodes. Each node in Figure 3.2 represents the process at each time unit. With time on horizontal axis and processes on vertical axis, the χ decision variables and $NS^{t,s}_{p_i}$ constitute the flow in terms of number of samples in the flow network.

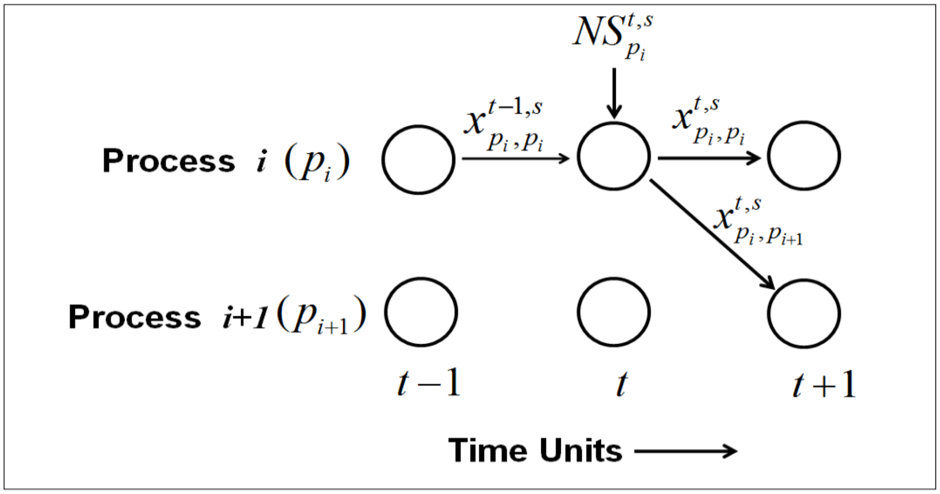

Figure 3.2. Flow network of processes as nodes at each time unit

3.2.2 Objective Function

The expression for the objective function to be minimized for the optimal scheduling of the operations in the analytical services sector has been defined as follows:

$$OF = \sum_{s\in S, t-d_s\le 0} tx_{p_{k-1},p_k}^{t-\tau(p_{k-1}),s} w_s R + \sum_{s\in S, t-d_s>0} tx_{p_{k-1},p_k}^{t-\tau(p_{k-1}),s} w_s P_L +$$

$$\sum_{s\in S, i<k, t>T-\tau(p_i)} tx_{p_i,p_{i+1}}^{t,s} w_s + \sum_{s\in S, i<k, t>T-\tau(p_i)} tx_{p_i,p_i}^{t,s} w_s) P_N + \sum_{t,p_i} c_i y_{p_i}^t \qquad (3.1)$$

A job s finishes at time t if it arrives at time t at its final process p_k, which is an artificial (dummy) process created to represent the end of the analysis or equivalently when it starts process p_{k-1} in the path of the job s at time $t-\tau(p_{k-1})$. That is, $\tau(p_{k-1})$ is the processing time of the final 'actual' process whereas the processing time of the artificial process p_k is zero as no actual work is performed for it. Large part of the objective function is based on the minimization of the samples' turnaround time that have not finished their analysis completely (that are anywhere but at the last process in the network).

The first term on the right-hand-side in the objective function (OF) in (3.1) determines the product of time t and the number of samples that start the second last process p_{k-1} (last actual process); thus, this term aims to account for the total amount of work left before finishing the analysis as well as the time required for it, i.e., this term considers the total turnaround time of the analysis. This term accounts for the samples that have completed the analysis before the deadline associated with the job $(t \le d_s)$ and therefore, is entitled to a reward (R), which minimizes the objective function. The value of reward (R) has to be less than 1 so that it can reduce the weight on the objective function. The priority number w_s prioritizes the analysis for different jobs. The values assigned for different jobs are relative.

The second term is similar to the first term but represents the samples that finish their analysis after deadline $(t > d_s)$. Hence, the reward (R) weight is replaced by a penalty weight for finishing late (P_L) so as to add weight to the objective function. The value of the penalty can be a reasonably higher number that must be greater than the unity so that it adds sufficient weight to the objective function.

The third and fourth summation terms on the left-hand-side in (3.1) correspond to the number of samples that cannot complete their analysis within the scheduling time horizon (i.e. final time unit T). These terms are added with the penalty for not finishing within the scheduling time horizon (P_N). The terms aim to minimize the number of samples that cannot finish within scheduling time horizon. The penalty P_N can be assigned a very high value as not finishing the analysis is the least desired outcome of the schedule. As it will be shown in the case studies presented in section 3.3, the reward, penalty for finishing late and penalty for not finishing within the scheduling time horizon have been assigned the values: $R = 0.1, P_L = 30, P_N = 100$. These values were chosen experimentally so as to achieve required effects of the parameters on the objective function shown in (3.1). The values are suitable for the case studies discussed in this paper. While similar values can be used for other instances of the problem, it is recommended to perform a fine-tuning of the parameter values based on the quality of the final solution obtained via experiments.

The last term in the expression is the summation of resources used multiplied by the cost of using a resource c_i for a process p_i, which accounts for the expenditure on the use of resources. This makes the operation economical. For the presented work, all the weights corresponding to the costs of the resources have been set as 1 in order to simplify the problem $(i.e., c_i = 1, \forall i)$, while the weights corresponding to the actual costs of the resources could be included in the expression to minimize the cost associated with the use of various resources.

3.2.3 Flow Constraints

Flow constraints can be interpreted as the measure to balance the input and output flow of the processes and the entire system. These constraints ensure that the total amount of samples from job s waiting at a process p_i at time t from a previous time unit $t-1$ and that from time $t-\tau(p_{i-1})$ is equal to the amount leaving it after time t or waiting at the process after time t. Thus for each job s, time $2 \le t \le T$ such that $t-\tau(p_{i-1}) > 0$, and for every $2 \le i \le k(s)-1$:

$$x_{p_{i-1},p_i}^{t-\tau(p_{i-1}),s} + x_{p_i,p_i}^{t-1,s} + NS_{p_i}^{t,s} = x_{p_i,p_{i+1}}^{t,s} + x_{p_i,p_i}^{t,s} \tag{3.2}$$

For all jobs s and all time units $2 \le t \le T$:

$$x_{p_1,p_1}^{t-1,s} + NS_{p_1}^{t,s} = x_{p_1,p_1}^{t,s} + x_{p_1,p_2}^{t,s} \tag{3.3}$$

For all jobs s and all time units $2 \le t \le T$ such that $t - \tau(p_{k-1}) > 0$, the flow constraint for the last process is:

$$x_{p_k,p_k}^{t-1,s} + x_{p_{k-1},p_k}^{t-\tau(p_{k-1}),s} + NS_{p_k}^{t,s} = x_{p_k,p_k}^{t,s} \tag{3.4}$$

For all jobs s and time unit 1, i.e., constraint when time unit is set to 1, samples waiting at time unit 1 are the new samples entering the system from previous run or as fresh samples:

$$x_{p_i,p_i}^{1,s} = NS_{p_i}^{1,s} \tag{3.5}$$

It is assumed that all the processes start only after time unit 1. This effectively means that time starts at $t = 2$. All the samples wait at the respective locations at time unit 1, i.e.,

$$x_{p_i,p_{i+1}}^{1,s} = 0 \text{ for all } s \in S \text{, for } 1 \le i < k. \tag{3.6}$$

3.2.4 Capacity and Resource Constraints

The capacity constraints ensure that the number of samples in job s leaving a process p_i (i.e. the samples completing the process p_i) at time t is not more than the total capacity of the machine. Thus, for every process p_i and all times t:

$$\sum_{s \in S,\, p_i \ne p_j} x_{p_i,p_j}^{t,s} \le y_{p_i}^{t} Cap_{p_i} \tag{3.7}$$

Constraint (3.7) has been developed under the assumption that all the resources for a process have the same capacity. The assumption is based on the characteristics of the analytical services industry problem addressed in this study, i.e. the resources have similar capacities. However, the constraint can be generalized in order to account for different capacities for different resource of a process as follows.

Let $y^{t}_{p_i,l}$ be a binary decision variable defined as follows:

$$y^{t}_{p_i,l} = \begin{cases} 1 & l^{th} \text{ resourceof process } p_i \text{ is turned ON} \\ 0 & \text{otherwise} \end{cases} \quad (3.8)$$

The capacity constraint to account for different capacities can therefore be written as follows:

$$\sum_{s\in S, p_i \neq p_j} x^{t,s}_{p_i,p_j} \leq \sum_{l=1}^{r_t(p_i)} y^{t}_{p_i,l} Cap_{p_i,l} \quad (3.9)$$

where $Cap_{p_i,l}$ is the capacity of l^{th} resource of process p_i, while $r_t(p_i)$ is number of resources available for process p_i at time unit t.

Consider a process p_i with processing time $\tau(p_i)$. All the resources that started to be used after time $t-\tau(p_i)$ would remain in use at time t as the process would still be running. Thus, the following expression sums up all such resources of p_i that remain in use simultaneously at time t and makes sure that the sum is no more than the total number of resources available. Thus, for each process p_i in the system and time t:

$$\sum_{t'=t-\tau(p_i)+1}^{t} y^{t'}_{p_i} \leq r_t(p_i) \quad (3.10)$$

Based on these developments, the conceptual problem can be mathematically formulated as follows:

$$
\begin{aligned}
&\min \sum_{s\in S, t-d_s\le 0} tx_{p_{k-1},p_k}^{t-\tau(p_{k-1}),s} w_s R + \sum_{s\in S, t-d_s>0} tx_{p_{k-1},p_k}^{t-\tau(p_{k-1}),s} w_s P_L + \\
&\sum_{s\in S, i<k, t>T-\tau(p_k)} tx_{p_i,p_{i+1}}^{t,s} w_s + \sum_{s\in S, i<k, t>T-\tau(p_k)} tx_{p_i,p_i}^{t,s} w_s) P_N + \sum_{t,p_i} c_i y_{p_i}^t \\
&s.t. \\
&\forall (2\le t\le T : t-\tau(p_{i-1})>0, s\in S, 2\le i\le k-1): \\
&x_{p_{i-1},p_i}^{t-\tau(p_{i-1}),s} + x_{p_i,p_i}^{t-1,s} + NS_{p_i}^{t,s} = x_{p_i,p_{i+1}}^{t,s} + x_{p_i,p_i}^{t,s} \\
&\forall (2\le t\le T, s\in S): \\
&x_{p_1,p_1}^{t-1,s} + NS_{p_1}^{1,s} = x_{p_1,p_1}^{t,s} + x_{p_1,p_2}^{t,s} \\
&\forall (t : 2\le t\le T : t-\tau(p_{k-1})>0, s\in S): \\
&x_{p_k,p_k}^{t-1,s} + x_{p_{k-1},p_k}^{t-\tau(p_{k-1}),s} + NS_{p_k}^{t,s} = x_{p_k,p_k}^{t,s} \\
&\forall (s\in S): \\
&x_{p_i,p_i}^{1,s} = NS_{p_i}^{1,s} \\
&\forall (s\in S, 2\le i\le k): \\
&x_{p_i,p_{i+1}}^{1,s} = 0 \\
&\forall (t): \\
&\sum_{s\in S, p_j\ne p_i} x_{p_i,p_j}^{t,s} \le y_{p_i}^t Cap_{p_i} \\
&\forall (p_i\in P, t): \\
&\sum_{t'=t-\tau(p_i)+1}^{t} y_{p_i}^{t'} \le r_t(p_i)
\end{aligned}
\tag{3.11}
$$

Given that a feasible solution exists, the model outputs the location of groups of samples belonging to the jobs at each time interval ($\chi_{p_i,p_j}^{t,s}$) and the number of machines that should be used/turned ON ($y_{p_i}^{t}$) to implement the schedule. As mentioned above, the rolling horizon technique is used to connect the end of the current run to the start of the next run, where the status of groups of samples in the jobs at the end of the current run are used as an input at the start of next run and the finite time horizon is shifted forward. Thus, the jobs for which the analysis has not been completed in the current scheduling run are considered for the next from their final location in the current run as the horizon rolls forward. The brief steps in the scheduling algorithm are presented in Figure 3.3.

Remarks

Some assumptions/limitations are considered in this optimization framework to simplify the operational characteristics and some modeling aspects. These are described as follows:

(1) Processing times for the processes are known in advance (deterministic) – average times are considered.

(2) Availability of resources is known a priori. This is based on the fact that the resources in the analytical services industry are mostly machines and therefore the number of resources remains constant most of the time, while the unavailability of resources due to maintenance activities can usually be known before the start of scheduling horizon. No break downs of resources are taken into account. All resources for a process have the same characteristics, i.e. capacities. The assumption is based on the characteristics of the resources used in the analytical services problem under consideration. Most of the resources have similar capacities, while the specific information of each resource in the analytical services facility considered in this study was not

available for confidentiality. Thus, the average capacities have been used for all resources of a process.

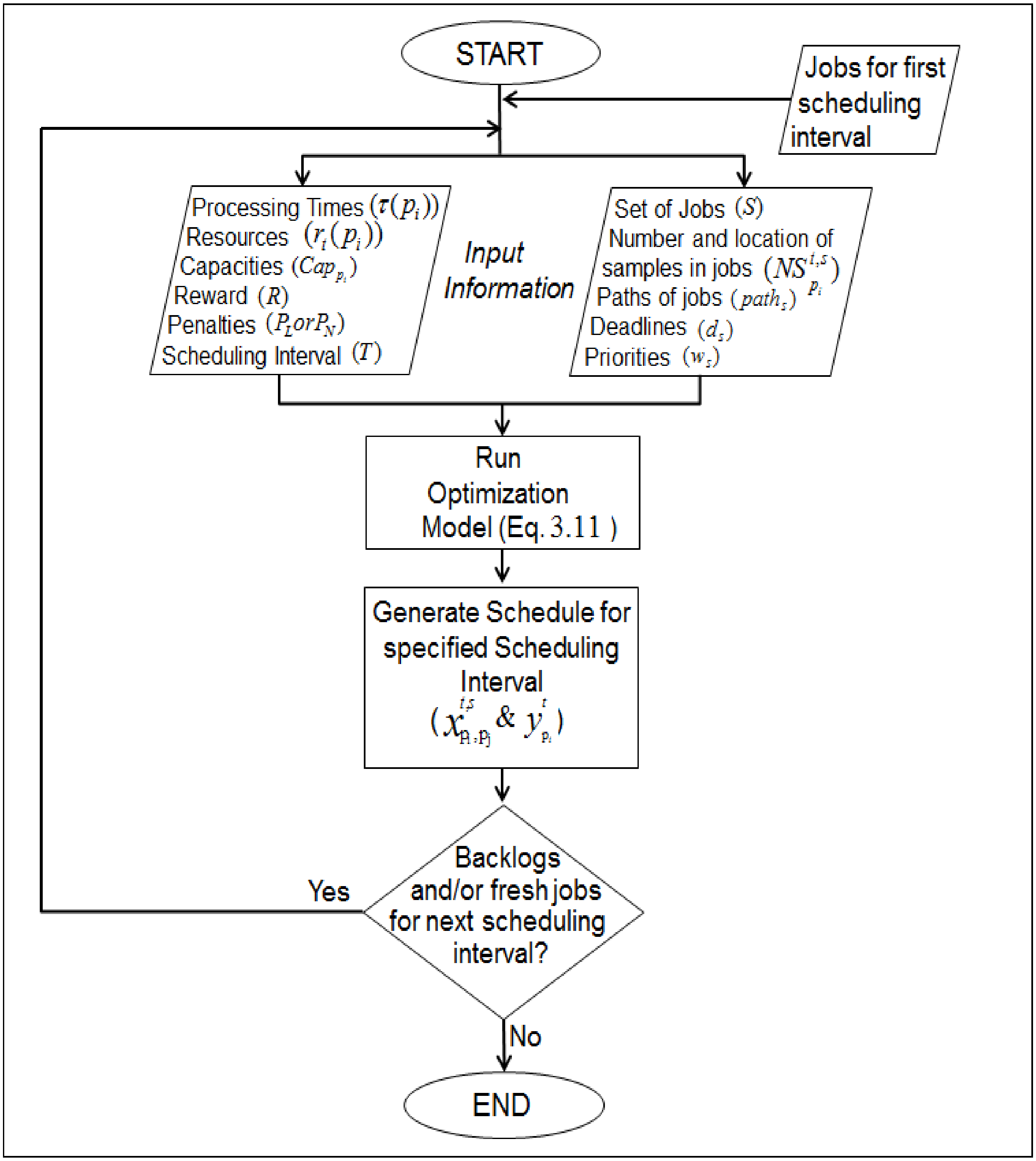

Figure 3.3. Summary of the scheduling algorithm

(3) The re-analysis of samples where sample may have to go through all or some processes in the path is not considered.

(4) Time is discretized into a finite set of time intervals, keeping track of the system at each interval. This is because the system under consideration behaves in a discrete form with input, processes involved and output being independent blocks in the system as shown in Figure 3.1. Thus, the system can be viewed as a set of batches and therefore tracking at specific intervals is suitable. To limit the problem size, time intervals of one hour were considered as this size of the interval tracks the system appropriately considering the changes occurring in the system per time. Also, processing times and the capacities can be easily modified according to the time interval of one hour, i.e. the values are adjusted as multiples of one hour to match with the time interval chosen. Finer discretization implies a more accurate representation of time, but will result in a higher number of variables/constraints involved in the problem.

(5) The optimization is considered to generate schedules over a finite time horizon. If the desired total scheduling time exceeds the finite time horizon considered, the rolling horizon technique is used to connect the current run to the next run of the algorithm. In this technique, the final status of the samples/jobs at the end of the current run of the algorithm is used as the input in the next run, where the respective finite time horizon would be shifted forward. Though there is possibility of achieving sub-optimal solutions with shorter rolling horizon, the technique is used to limit the problem size with number of variables to track.

(6) The samples from different jobs can be combined together for a process; therefore there is no issue of contamination of samples. The samples can be tracked as a group and not individually.

The assumptions/limitations stated above will be addressed in the future work associated with the presented study.

3.3 Results and Discussions

Two case studies have been considered in the present analysis. The first case study illustrates how the schedules were obtained from the optimization formulation presented in 3.2.1 and has been used mostly to demonstrate the capability of the algorithm. The second case study demonstrates the potential of the present scheduling algorithm via comparison of the model's performance against the actual operation of a plant in the analytical services sector. The key difference between the case studies is the size of the problem. Actual plant data (real values for capacities, processing times, resources) was used in case study 2, while case study 1 was developed to describe the working principles of the algorithm via creating an example of smaller size than the actual plant with arbitrary values for capacities, resources and processing times. All the simulations were run using a machine with the configuration: Win 8,i3,@2.40GHz, RAM-8GB.

Case Study 1

For this case study, an illustrative example consisting of 8 processes occurring in an analytical services facility is considered. The model is used to generate a schedule for 5 jobs (i.e., $s = 5$) which contain 100 samples in total (i.e., $n = 100$). Three scenarios have been developed to evaluate the scheduling model's performance under the effect of a few model parameters. All the jobs have been assumed to have a common deadline (d_s) of 30 hours.

Scenario 1 – Standard capacities and priorities

This scenario is a basic illustrative example of the schedule obtained via the optimization formulation shown in equation (3.11). The information related to the jobs considered for scheduling is provided in Table 3.1. The scheduling time horizon has been set to 24 hours, while the capacities, processing times and resources considered for this scenario are reported in Table 3.2.

The results obtained as the output of the model are represented in the form of the Gantt charts. Figure 3.4 presents the results for *Scenario 1*.

As shown in Figure 3.4, the latest turnaround time obtained for this scenario is 12 hours, though the scheduling time horizon was set to 24 hours. The model makes various combinations of samples from various jobs so that the capacity of all resources for each process can be used optimally. An example of such combination can be seen at time unit 2 at process 1, where 30 samples from Job 1 are combined with 9 samples from Job 2 so that the maximum capacity of 39 for process 1 can be used. All such combinations eventually minimize the overall turnaround time. As shown in Figure 3.3, if the scheduling time horizon is set to 10 hours, this would return the schedule only until 10 time units in the Gantt chart and then the samples that could not complete the analysis would be considered for the next scheduling time horizon as backlogs jobs. This procedure is repeated until all the samples considered in the analysis reach process p_k .

Scenario 2 – Effect of Reduced capacities

This scenario has been generated to analyze the effect of capacities on the schedule generated as well as the overall turnaround time. In this scenario capacities per resource of all the processes (p_i) are reduced to approximately 10% of the values shown in Table 3.2, while all other details remain the same as in *Scenario 1*. The new capacities are listed in Table 3.3. As shown in the table, capacity of process 5 has been kept same as in *Scenario 1*, as the capacity per resource is relatively small.

Table 3.1. Job Details for Case Study 1, Scenario 1

Job Number (s)	Path to follow (processes to be completed) ($path_s$)	Number of samples in the job (n)	Priorities (w_s)
1	1,2,3,4,8	30	1
2	1,2,3,5,8	20	1
3	1,2,3,4,6,8	20	1
4	1,2,3,4,8	20	1
5	1,2,3,7,8	10	1

Table 3.2. Data for Processes for Case Study 1, Scenario 1

Process Number (p_i)	Process time (in hours) $\tau(p_i)$	Resources (number of machines) $r_t(p_i)$	Capacity (per resource, per process time) (Cap_{p_i})	Total Capacity of all Resources
1	1	3	13	39
2	1	3	13	39
3	1	3	160	480
4	4	3	84	252
5	1	3	6	18
6	1	3	34	102
7	2	3	20	60
8	1	3	40	120

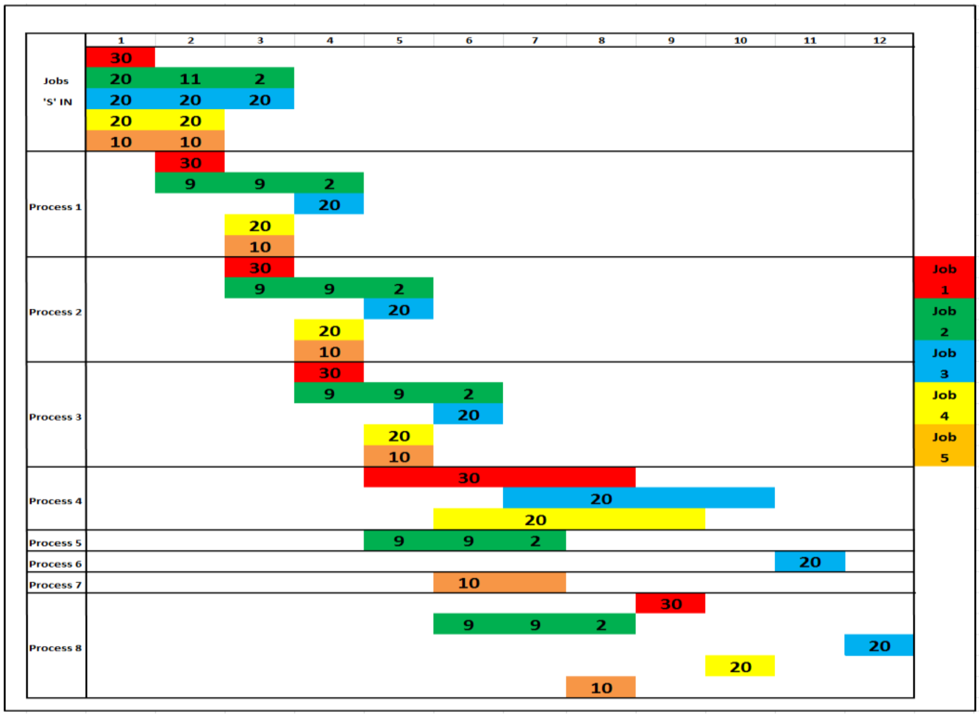

Figure 3.4. Schedule for the case study 1, Scenario 1

Since the capacities have been reduced, the scheduling time horizon has been changed to 30 hours with same priorities $(w_s = 1)$ for all the jobs. The latest turnaround time obtained for *Scenario 2* increased to 25, while the schedule for each job also changed and can be tracked in Figure 3.5. Thus, a reduction of 90% in capacity resulted in increase of turnaround time by 13 hours as compared to *Scenario 1*. Most of the samples wait for longer time as there is no enough capacity to process all the samples that queue up to complete the process. This can be seen in the Figure 3.5, where samples have to wait to start *Process 1* as it represents the first bottleneck in the network with total capacity of 6 samples. Thus, the effect of capacities on the schedule and the turnaround time is verified with the present scenario.

Table 3.3. Reduced Capacities for Case Study 1, Scenario 2

Process Number (p_i)	Capacity (per resource, per process time) (Cap_{p_i})	Total Capacity of all Resources
1	2	6
2	2	6
3	16	48
4	8	24
5	6	18
6	3	9
7	2	6

Scenario 3 – Effect of Priorities

This scenario depicts the influence that the priorities of the jobs have on the schedule generated. To analyze this effect, job 4 has been set to a higher priority $(w_4 = 2)$ while all others have default priority $(w_s = 1)$. All the other input data is same as *Scenario 2*. Job 4 was chosen to have maximum priority since it was the job finishing latest in *Scenario 2*. The new schedule was expected to have shorter turnaround time for job 4 and this was confirmed through the results obtained.

As shown in Figure 3.6, the schedule generated for this scenario shows that all the processes required for job 4 are completed faster than the other jobs, i.e. job 4's analyses are completed in 13 hours, while the total turnaround time is 26, which is greater than *Scenario 2* by an hour (4%). Thus, the change in priorities affects the schedule, while the total turnaround time of operations increased for *Scenario 3*.

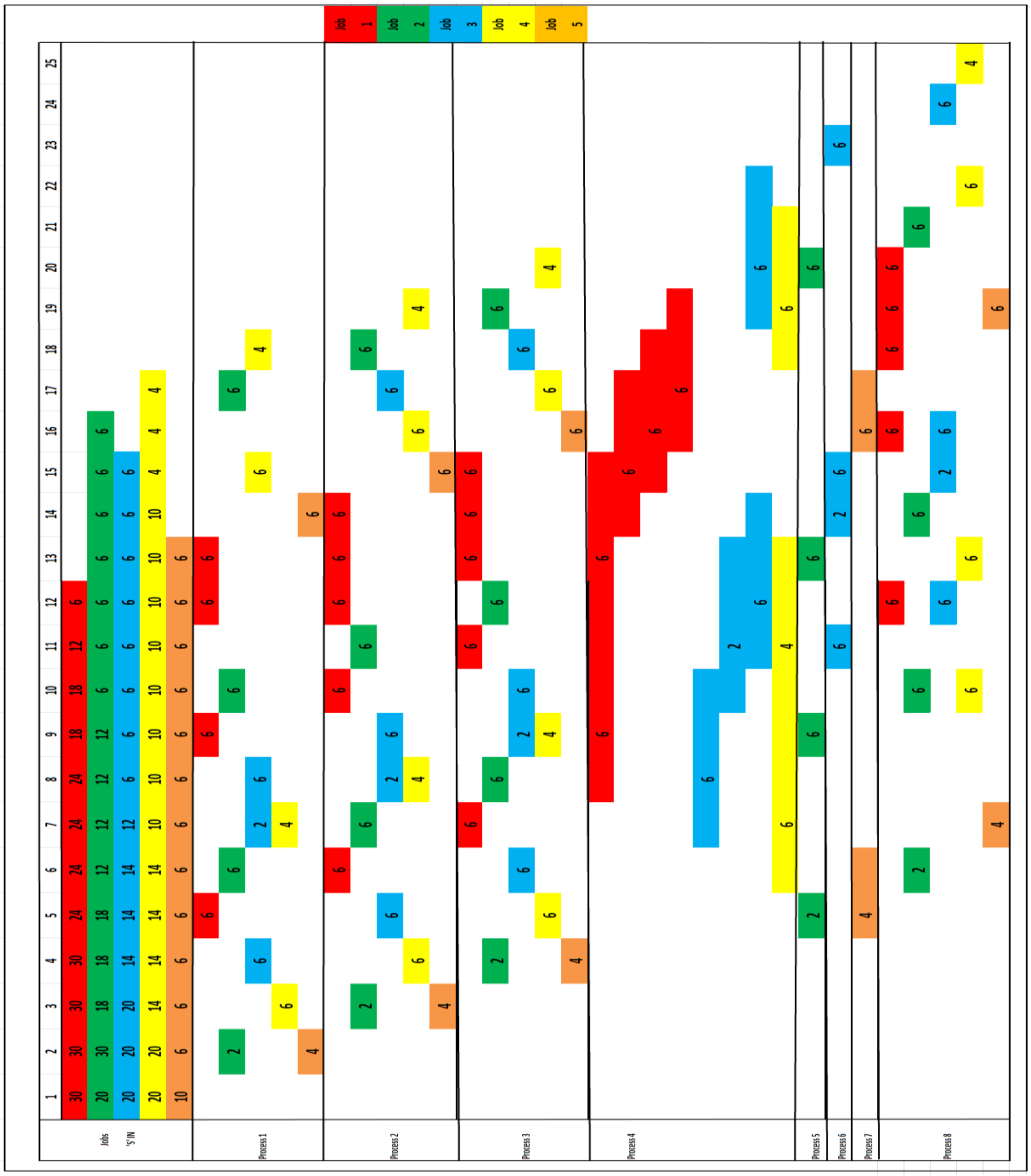

Figure 3.5. Schedule for Case Study-1, Scenario 2

In *Scenario 1*, the number of decision variables involved in the solution for the location of the samples $x^{t,s}_{p_i, p_j}$ is 624, while there were 96 decisions taken on the resources to be used, represented by $y^{t}_{p_i}$. The *Scenario 2* involved 1300 $x^{t,s}_{p_i, p_j}$ decision variables in the solution for location of samples as the number of time units required is more, while it goes up to 1352 in *Scenario 3* with increase in total turnaround time. The number of decision variables involved in the solution for resources, $y_{p_i}^{t}$, were 200 for *Scenario 2*, while this number goes up to 208 for *Scenario 3*. The CPU time required to generate the schedules for these scenarios is 50 seconds on average.

Case Study 2

This case study has been developed to demonstrate the potential benefits of using an optimization-based scheduling algorithm for operations management in an actual analytical services facility. Here, the turnaround time obtained via the optimization model developed in this study is compared against actual turnaround time in the plant. There are 38 processes, each characterized by specific processing time, capacities and set of resources. All the values for capacities, resources are obtained from the actual operation, while averaged processing times were used in the analysis. In order to mimic the characteristics of operation in the actual plant, and be able to make a comparison between actual data and results obtained by the present analysis, the proposed scheduling model assumed that operations were limited to a shift of 8 hours each day, 5 days a week. This was achieved through additional constraints which restrict turning ON the resources after the 8th hour of the shift each day and all the time on 2 days of the week (weekend). Therefore, the resources can be started only for 8 hours of shift in a day. Thus, even if the model runs for a period of 24 hours, it effectively schedules operation over the period of 8 hours, while a ‘day’ refers to a shift of eight hours for this case study in further discussion. The time interval considered in the optimization model was set to 1 hr.

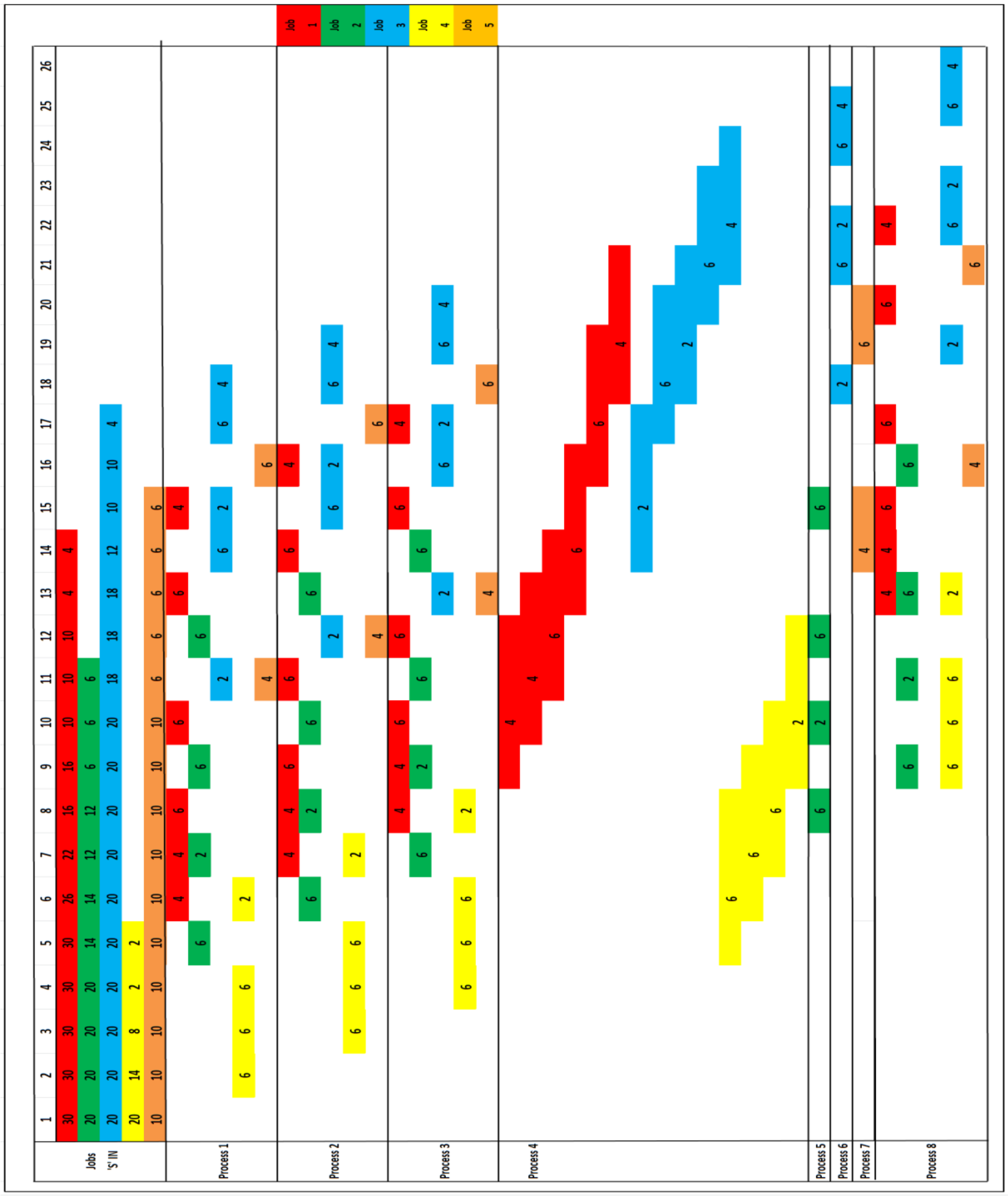

Figure 3.6. Schedule with reduced capacities and priority on Job 4

The number of jobs considered for scheduling was 408 $(s = 408)$, which contains about 14,941 samples in total $(n = 14941)$; this represents the operation of a week in the actual plant. A rolling horizon technique has been used and schedules are obtained day by day. Samples in jobs entering the system as 'new entities' (i.e. starting first process in the analysis) in a day are not known in advance. Thus, only the samples present at the start of the scheduling horizon and the samples entering in the system after start of the horizon by finishing a process (i.e. backlogs) are considered for scheduling. The samples entering the system as 'new entities' during the scheduling horizon will be considered in the next scheduling horizon. To ensure that a fair comparison can be made, the model has been run to schedule the operations starting from 10 days before the start of the week under consideration and stopped after all the samples have finished the analysis. This has been done to create the load of samples similar to the actual load in the facility before, over and after the week chosen for the comparison. Because of this, the resources are occupied partially to fully before start of the week chosen for comparison, which is similar to the actual operations. For the presented case study all the jobs have been assigned the default priority $(w_s = 1)$ and a common deadline of 336 hours $(d_s = 14 days)$. The input information consisting of number of resources, capacities and average processing times have been obtained from the facility owned by the industrial partner along with the historical data of jobs and samples and for confidentiality reasons, these values have not been reported in the presented work.

Two approaches have been considered in the present analysis and the results obtained from each of them are compared against the actual operations.

Approach 1- Optimal Scheduling: The scheduling time horizon is set to 24 hours, though the effective schedule of operations is over shift of 8 hours as discussed above. After obtaining the schedule for the day, the algorithm is re-run for the next day for the next 24 hours. As shown in Figure 3.3, this procedure continues up until all samples received in the week considered have completed the analysis required.

Approach 2- Simulated Actual Policy: The current scheduling policy used in actual operations (i.e. first-come first-serve) has been simulated using the present scheduling model. The rationale behind this approach is that there are several simplifications that the model makes (for instance using average processing times), which may be the reason for any performance improvement as compared to actual operations. Because the same strategy as in the actual operations is used in this approach, any improvement in the performance should be due to the simplifying assumptions. This allows the identification of what share of performance improvement of *Approach 1* was obtained due to simplifying assumptions and what share due to better scheduling.

The results obtained from the two approaches have been compared with the historical data obtained from the facility for the period before, after and including the one week under consideration as presented in Table 3.4. This has been done to analyze the performance of the model during that week. The Table 3.4 shows the comparison of actual operations against the optimal scheduling and simulated policy approach. This Table also presents a comparison between the optimal scheduling against simulated policy approach. This comparison in particular shows the improvement achieved solely due to optimization.

As shown in Table 3.4, the results show that the turnaround time with the optimal scheduling (*Approach 1*) is 67.5 % less than of the actual operations, which demonstrates the effect of optimization based scheduling under the modeling assumptions, while the approach with the simulated actual policy (*Approach 2*) also shows the improvement in the turnaround time by 50% as compared to the actual operations.

Table 3.4. Results for Case Study 2

	Optimal Scheduling (*Approach 1*)	Scheduling using simulated actual policy (*Approach 2*)	Actual operations in the facility
Period	A week's operation		
Latest finishing (turnaround) time	32.5 % of actual time	Around 50% of actual time	Actual turnaround time
Deadlines violated	0 jobs, 0 samples	Around 12 % jobs	Around 16 % jobs
Avg. no of jobs finished per day	39.5% > Actual Average	12.1% > Actual Average	Actual average
Standard deviation in jobs finished per day	7%< Actual (less variability)	46% < Actual (less variability)	Actual standard deviation

The results also show that no samples violated the deadline with the optimal scheduling *(Approach 1).* There are about 12% jobs that violated the deadline with simulated first-come first serve policy *(Approach 2),* while in actual operations 16% of the jobs in the specific week violated the deadline. The number of jobs analyzed per day is also higher in *Approach 1* as compared to actual operations and the simulated first-come first serve approach (*Approach 2*). In terms of comparison between optimal scheduling and simulated policy approach, 17.5% more improvement is achieved in the turnaround time in optimal scheduling approach, whereas the number of jobs finished per day is also greater by 27.4 in optimal scheduling approach. Table 3.4 also shows the values for standard deviation in the number of jobs analyzed per day. It is clear that with the scheduling algorithm *(Approach 1),* the variability in the jobs analyzed per day is slightly reduced, even though the variability for the first-come first serve policy *(Approach 2)* is even less. This is an unintended, but positive outcome for the optimization-based scheduling since no explicit enforcement of reduced variability is considered in the model. This can be seen in Figure 3.7(a), where the graphs are plotted for number of jobs finishing the analysis per day and daily average for actual plant, simulated policy and optimal scheduling approach (*Approach 1*), while Figure 3.7(b) shows the trend of number jobs entering the process per day. The graphs shown in Figure 3.7 are over 29 days of the month, which includes the week considered for comparison (days 11-15), the span before the week and after it as late as the deadline of the analysis for the jobs considered. In addition, the model allows the identification of processes with active capacity constraints. These processes may potentially represent bottlenecks in the operations, so identifying these bottlenecks allow the recommendation of corrective measures to reduce their impact on operations management.

The number of decision variables related to location of samples ($\chi_{p_i, p_j}^{t,s}$) varies each days since it depends upon the number of jobs received on the day. The average number of decision variables involved in the solution each day (i.e. per run of the scheduling model) is 8256 with a maximum of 10480. The number of decision variables related to use of resources ($y_{p_i}^{t}$) involved in the solution every day remains unchanged throughout the case study and is equal to 304. Furthermore, the optimality gap achieved for each solution was 0%. These figures provide an idea of the size of the scheduling problem in the analytical services industry that has been considered in the present study. The size of the problem is extensive in terms of number of decision variables involved in the solution while the problem becomes challenging with different operational characteristics. The CPU time required to generate schedules each day (an eight hour shift) is 130 seconds on an average depending on the number of samples under consideration for scheduling.

3.4 Summary of the Chapter

This Chapter has presented the details of the application of the optimal scheduling in an analytical services facility. This includes the overview of the operations in this industry which can be used to describe the scope for optimal scheduling and need of the scheduling algorithm. The mathematical model based on integer programming (IP) has been presented in detail. The model involves the objective function that focuses on minimization of turnaround time of operation and various constraints including flow constraints, capacity constraints and resources constraints.

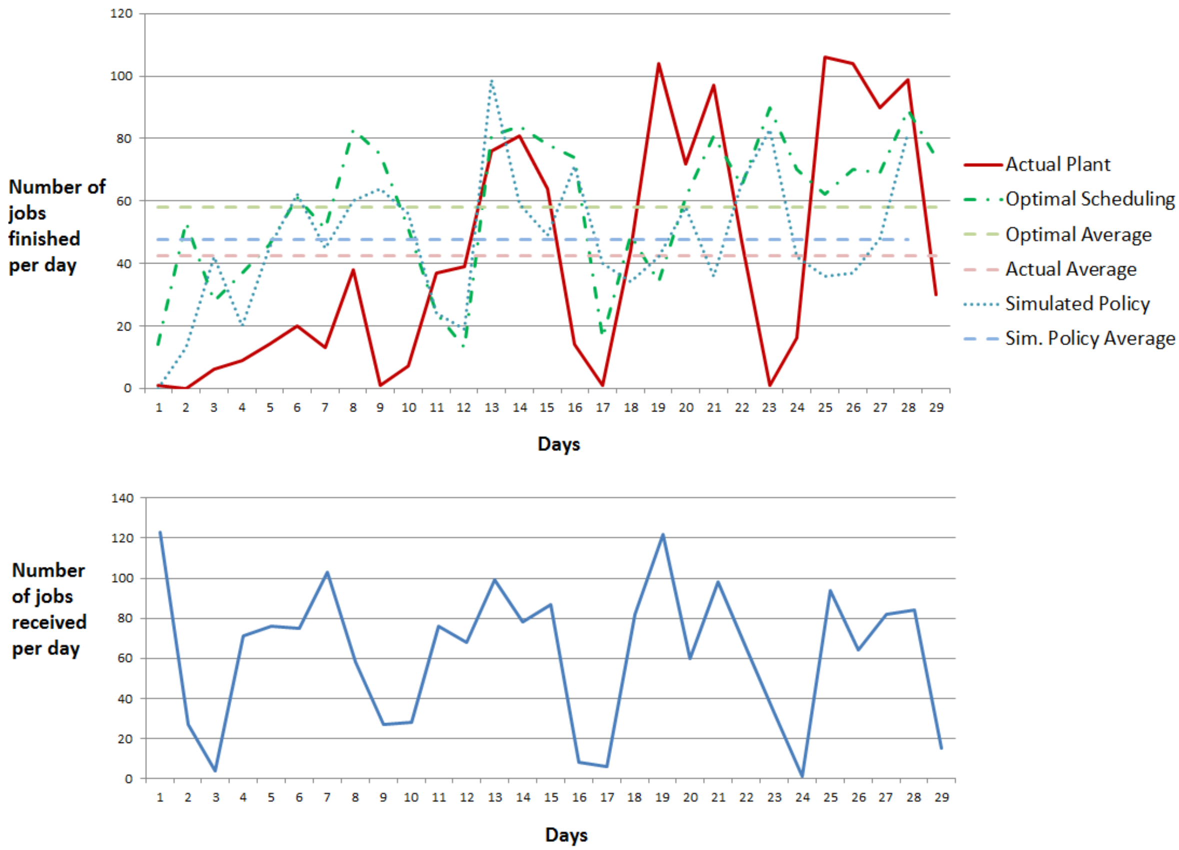

Figure 3.7. (a) Comparison of number of jobs finished per day; (b) Number of jobs entering the system.

The aim of applying flow constraints is to maintain the balance of the samples across processes, while capacity and resource constraints make sure that the numbers of samples processed do not exceed the design capacities of the resources. The case studies depict the advantages of optimal scheduling. The first case study also describes the basic working principles of the algorithm and effect of various parameters used in the optimization model.

A second case study has been presented in this chapter in order to demonstrate the potential of the algorithm to achieve operation that require lesser time than the actual operations in the facility. The results show that the scheduling algorithm can be used to improve the turnaround time of operations, while variability in the number of samples analyzed per day has been reduced.

The industrial application discussed in this chapter focuses on optimal scheduling; however, other aspects of chemical process industry also play important roles in process economics. Thus, scheduling needs to be addressed simultaneously with other aspects of the chemical processes, i.e., design and control. In the next chapter, a methodology is presented in detail along with its application to two case studies.

Chapter 4
Integration of Scheduling, Design and Control of Multi-Product Chemical Processes under Uncertainty

An industrial application discussed in the previous chapter demonstrated the benefits of implementing optimal scheduling in the chemical processes. However, in order to achieve optimal operations in chemical processes, other aspects of process economics need to be addressed in integration with scheduling. Design and control are two important aspects which play important roles in the process economics of any chemical system. Multi-product processes represent a section of the chemical process industry that involve all the three aspects and require simultaneous optimization of those aspects. Despite the developments in the field of integration of scheduling, design and control, studies that account for all three aspects are limited. This chapter presents a methodology developed in order to simultaneously address scheduling, design and control for multi-product processes under the influence of process disturbances and uncertainty in the parameters. The organization of this paper is as follows: Section 4.1 presents the problem statement in terms of multi-product processes along with description of the operation, while Section 4.2 presents the mathematical formulation proposed in this work for the integration of scheduling, design and control of multiproduct processes. Section 4.3 presents the case studies developed to implement the methodology on a CSTR system and a large scale HIPS process. The results are discussed on each of the subsections of the case studies.

4.1 Problem Statement

Consider a multiproduct plant which produces various grades of the product. Each grade has a particular specification and a demand to meet. As shown in Figure 4.1, the operation consists of production and transition periods for each grade i. During the transition period of a grade i, the required specification of the grade is reached and then the production stage of the grade starts. The production stage is continued until the required demand is met at the required grade specification. Once the required production of the grade i is achieved, transition to grade $i+1$ begins and eventually the production is achieved for that grade. The procedure is repeated until all the required product grades (I) are produced to meet the product demands. The present study assumes that, once the production wheel is completed, it is immediately and indefinitely repeated. Also, each grade is produced only once in the complete production cycle.

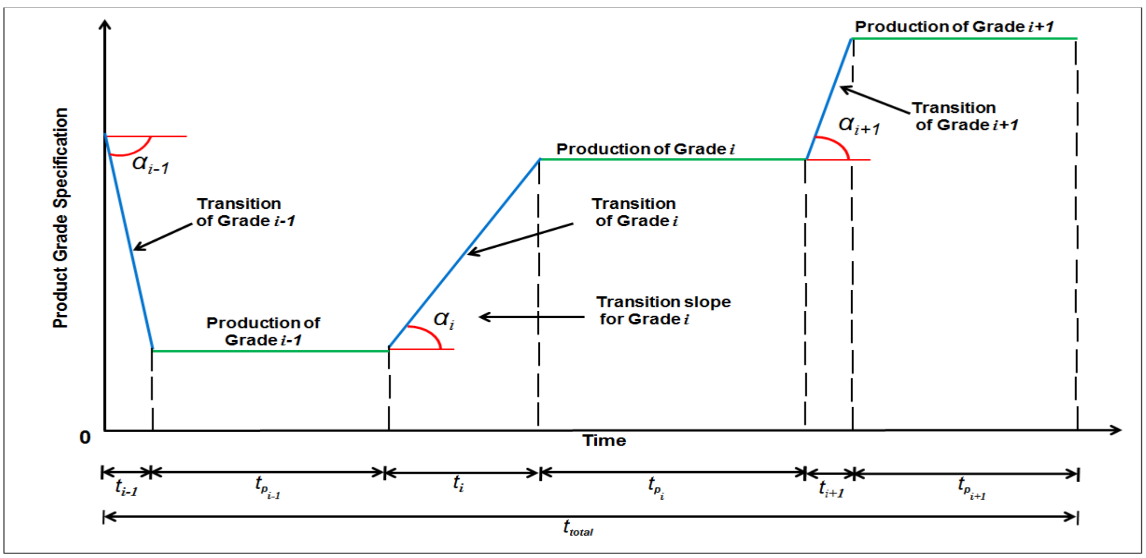

Figure 4.1. Various product grades in a multiproduct process

As shown in Figure 4.1, t_i and t_{p_i} represent the transition and production times of grade i, while t_{total} is the time required to complete productions and transitions for all product grades.

All the transitions are assumed to occur following a ramp function to achieve the set point related to specification of the grades. The slope of the ramp (α_i) denotes the transition rate for the i^{th} grade and is part of the optimization variables considered in the presented analysis. Once the transition of grade is completed and the required composition is achieved, the production period starts; the product is assumed to be stored in a product (storage) tank.

The product tank starts filling only after the required specification is achieved, i.e. only within the production period, and stops when both the required composition (grade) and demand are achieved. The complete operation is assumed to occur under the influence of critical realizations in the process disturbances, which are assumed to follow an oscillatory behavior, and uncertainty in the system's parameters, e.g., production demands.

In the problem under consideration the given are (a) the actual dynamic nonlinear process model describing the behavior of a multiproduct process, (b) the process model parameters (e.g., molar flow rate of the feed), (c) the control scheme, (d) the required specifications and demands of the grades to be produced, (e) the disturbance specification, assumed to be a sinusoidal signal with given amplitude and critical frequency, (f) uncertainty specification in terms of critical scenarios and their probabilities for uncertain parameter, and (g) process constraints to be satisfied during operation. The problem to be formulated aims to determine- (a) the optimal equipment design and steady state operating conditions for each grade, (b) the optimal tuning parameters for the control scheme, (c) optimal transition slopes for each grade and (d) optimal sequence of production.

4.2 Methodology for Integration of Scheduling, Design and Control

This section presents the details of the methodology developed for integration of scheduling, design and control. The description of the features considered in the methodology is presented next along with the mathematical description of the optimization formulation.

4.2.1 Parameter Uncertainty

The methodology presented in this work explicitly accounts for uncertainty in the process parameters, e.g., uncertainty in the demand of products. To account for this condition, the critical uncertain scenarios in the parameters are assumed to be discretized and need to be specified *a priori*, i.e.,

$$\mathbf{w} = [\mathbf{w}^1, \mathbf{w}^2, ..., \mathbf{w}^z, ...\mathbf{w}^{ns}] \tag{4.1}$$

where '*ns*' denotes the number of critical scenarios to be considered in the analysis; each uncertain scenario $\mathbf{w}^z$ has been assigned with a probability of occurrence P^z .

4.2.2 Process Disturbances

In the presented study, each k^{th} process disturbance is specified as follows:

$$\boldsymbol{\eta}_k(t) = \boldsymbol{\eta}_{k_{nom}} + \boldsymbol{\eta}_{k_m} \sin(\omega_{c_{k,i}} t) \tag{4.2}$$

where $\boldsymbol{\eta}_{k_{nom}}$ is the nominal operating value of the process disturbance and $\boldsymbol{\eta}_{k_m}$ is the amplitude of the k^{th} process disturbance, which is chosen depending upon the process dynamics, whereas $\omega_{c_{k,i}}$ represents the critical frequency evaluated for each grade i that generates maximum variability in the controlled variables due to critical realizations in the k^{th} disturbance. The critical parameter $\omega_{c_{k,i}}$ is not known *a priori* and will be calculated internally. This is a new feature introduced by the present approach. The response in the l^{th} controlled variable as a result of a sinusoidal process disturbance input is as follows:

$$\mathbf{y}_l(t) = \mathbf{y}_{l_{nom}} + \mathbf{y}_{l_m} \sin(\omega_{c_{k,i}} t + \Phi) \tag{4.3}$$

where $\mathbf{y}_{l_{nom}}$ is the nominal operating value of the process disturbance, $\mathbf{y}_{l_m}$ is the amplitude of the controlled variable and Φ is the phase angle by which the l^{th} controlled output is delayed. The largest (worst-case) variability in the controlled variable due to k^{th} disturbance is determined by the frequency of the sine function, i.e. $\omega_{c_{k,i}}$. In this work, this critical frequency $\omega_{c_{k,i}}$ is identified from the linearization of the actual nonlinear closed-loop process model ($\mathbf{f}_{closed}$) around the steady-state operating conditions specified for the production of grade i. The identification of the critical frequency from the actual closed-loop nonlinear process model ($\mathbf{f}_{closed}$) requires the solution of an intensive optimization formulation, which needs to appear as a constraint in the overall integration of scheduling, design and control formulation. Therefore, this formulation can become prohibitive for large-scale applications. Thus, the approximation in terms of linearized process model along with frequency response analysis has been used in this work for the identification of the critical frequency ($\omega_{c_{k,i}}$).

Based on the above, the critical frequency $\omega_{c_{k,i}}$ is obtained from the linearized closed-loop process model via frequency response analysis as follows.

The closed-loop process model ($\mathbf{f}_{closed}$) is linearized around a steady state operating condition for each product grade i specified as part of decision variables ($\mathbf{d}$) as follows:

$$\begin{aligned} \dot{\mathbf{x}}_{lin} &= \mathbf{A}_i\mathbf{x} + \mathbf{B}_i\boldsymbol{\varphi} \\ \boldsymbol{\Omega}_{lin} &= \mathbf{C}_i\mathbf{x} + \mathbf{D}_i\boldsymbol{\varphi}, \ \forall i = 1 \ldots I \end{aligned} \tag{4.4}$$

where $\mathbf{x}_{lin}$ is the vector of states of the linearized closed-loop process model, $\boldsymbol{\varphi}$ is an input vector which includes the disturbances affecting the process, while $\boldsymbol{\Omega}_{lin}$ represent the output vector that includes controlled variables calculated from the linearized closed-loop process model. The matrices $\mathbf{A}_i$, $\mathbf{B}_i$, $\mathbf{C}_i$, $\mathbf{D}_i$ are the state matrices of the linearized closed-loop process model. The closed-loop state-space model is identified at each single function evaluation of the optimization formulation for each grade i using the values specified for the optimization variables at each optimization step. The non-linear closed loop process model can be linearized analytically, e.g., using Taylor's series expansion, or from systems identification methods using the traditional least-squares technique.

The linearized closed-loop model (4.4) can further be represented in the frequency domain for each pair of k^{th} process disturbance and l^{th} controlled variable as follows:

$$\mathbf{G}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k}(j\omega) = \mathbf{C}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k}(j\omega\mathbf{I}_{\mathbf{y}_l-\boldsymbol{\eta}_k} - \mathbf{A}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k})^{-1}\mathbf{B}_{\mathbf{i},\mathbf{y}_l-\boldsymbol{\eta}_k} \tag{4.5}$$

where j is imaginary number ($j = \sqrt{-1}$), while ω denotes the frequency domain. $\mathbf{G}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k}(j\omega)$ represents the transfer function between the k^{th} process disturbance and the l^{th} controlled variable. The matrices shown in (4.5) represent the dynamics between the k^{th} process disturbance and the l^{th} controlled variable and are subsets of the matrices shown in (4.4), i.e., $\mathbf{A}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k} \in \mathbf{A}_i, \mathbf{B}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k} \in \mathbf{B}_i, \mathbf{C}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k} \in \mathbf{C}_i$.

$\mathbf{G}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k}(j\omega)$ can be further decomposed as follows:

$$\mathbf{G}_{i,\mathbf{y}_l-\boldsymbol{\eta}_k}(j\omega) = R_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega) + jI^m_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega) \tag{4.6}$$

where $R_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega)$ and $I^m_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega)$ are the real and imaginary parts of the transfer function and are functions of the frequency ω. The amplitude ratio representing the variability in $\mathbf{y}_l$ due to changes in $\boldsymbol{\eta}_k$ can be expressed as follows:

$$AR_{\mathbf{y}_l-\boldsymbol{\eta}_k} = \sqrt{R_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega)^2 + I^m_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega)^2} \tag{4.7}$$

From frequency response analysis, the maximum amplitude ratio, which corresponds to the maximum variability expected in $\mathbf{y}_l$ due to $\boldsymbol{\eta}_k$, is achieved at the critical frequency $\omega_{c_{k,i}}$. Following equation (4.7), the maximum amplitude ratio can be expressed as follows:

$$AR^{\max}_{\mathbf{y}_l-\boldsymbol{\eta}_k} = \sqrt{R_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega_{c_{k,i}})^2 + I^m_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega_{c_{k,i}})^2} \tag{4.8}$$

The maximum amplitude ratio is pictorially represented in Figure 4.2 via Bode plot. Since the amplitude ratio corresponding to the critical frequency is maximum, the disturbance generates the worst case variability in the controlled variable at this frequency. Note that for the cases where there is no clear maximum frequency (e.g. first order system), i.e. a range of frequencies correspond to maximum amplitude ratio in a bode plot, a numerical approximation must be made by selecting as critical frequency the highest or smallest frequency value that generates the maximum variability in the controlled variable.

Following equation (4.2), the critical frequency for each process disturbance *k* is specified for each grade *i* and for each critical scenario *z* as shown in (4.1) from the following equation:

$$\boldsymbol{\eta}^{z}(t) = \boldsymbol{\eta}^{z}_{k_{nom}} + \boldsymbol{\eta}^{z}_{k_m} \sin(\omega^{z}_{c_{k,i}} t) \qquad (4.9)$$

That is, the process disturbances are specified for each grade i using the critical frequency ($\omega_{c_{k,i}}$) that generates the maximum variability in the controlled variables at each critical realization *z* in the uncertain parameters **w**.

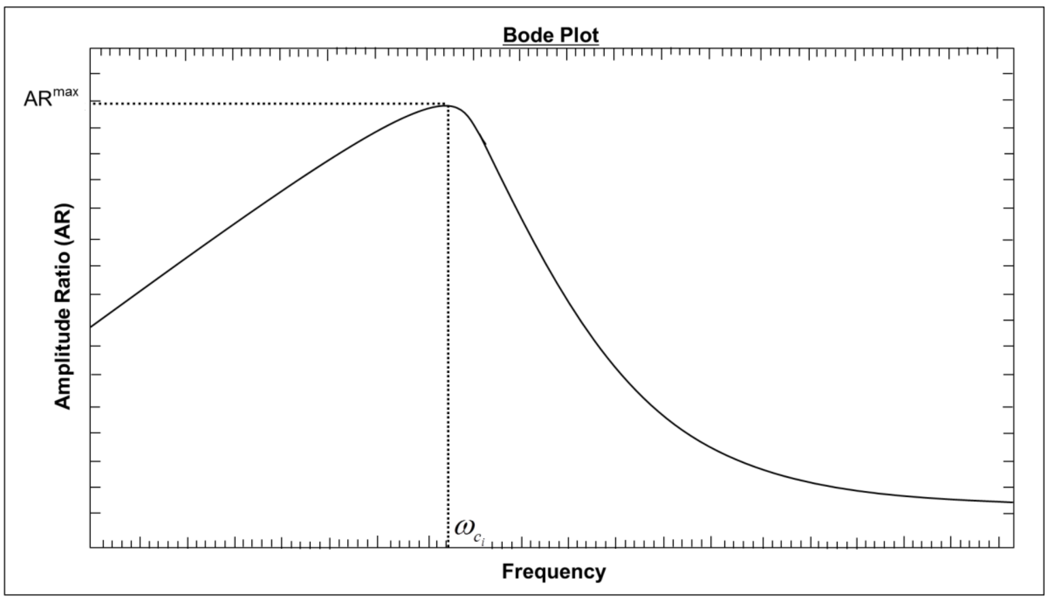

Figure 4.2. Bode Plot- Frequency Response Analysis

For the cases where multiple disturbances are simultaneously acting on the controlled variables, the critical frequency at which the disturbances generate the maximum variability in a controlled variable is the frequency that produces the maximum total amplitude ratio. The total amplitude ratio is the sum of individual amplitude ratios for the disturbances.

Therefore, equation (4.8) can be modified for multiple disturbances as follows:

$$AR^{\max}_{\mathbf{y}_l-\boldsymbol{\eta}} = \sum_{k=1}^{K} \sqrt{R_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega_{c,i})^2 + I^{m}_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega_{c,i})^2} \tag{4.10}$$

where, K represents number of process disturbances acting simultaneously on l^{th} controlled variable, while $\omega_{c,i}$ represents the common critical frequency for the simultaneously acting disturbances.

Using these disturbances' critical frequency specifications, the worst-case variability is computed in the controlled variables through simulation of the closed loop nonlinear process model $\mathbf{f}_{closed}$ of the system for transition and production for all the grades. As mentioned above, the approach relies on the linear approximation of the non-linear closed loop process model in order to identify the critical frequency for the process disturbances. Thus, the maximum (worst-case) variability in the controlled variables is the result of the linear approximation, which limits the approach from considering the true maximum variability of the non-linear behavior. This particular aspect of the methodology will be examined using one of the case studies presented in this work.

4.2.3 Nominal Closed-loop Stability

Once a linear closed-loop model representation of the actual nonlinear closed-loop system is available, it can be used to evaluate the system's nominal stability under disturbances and uncertainty in the model parameters. The stability check can be conceptually formulated for each grade i and each critical scenario z of the uncertain parameter as follows:

$$eig(\mathbf{A}_i^z(\mathbf{x}_{lin})|_{\mathbf{d}}) < \mathbf{0}, \forall i = 1 \ldots I \tag{4.11}$$

where '*eig*' denotes the eigenvalues of linearized state matrices $\mathbf{A}_i^z$ at the operating point specified for grade *i*. Note that the $\mathbf{A}_i^z$ state space matrices include all the inputs and outputs considered in the linear state-space representation shown in (4.4) and they must be identified at each optimization step, i.e., around the set of values specified for the methodology's optimization variables **d**. Constraint (4.11) will therefore be added to the methodology's optimization formulation to enforce nominal stability for the different operating points that need to be achieved by the system to produce the required grades.

4.2.4 Cost Function

The cost function Φ considered in the presented methodology includes the capital cost, operating cost, variability cost and transition costs. The annualized capital costs (CC) refers to the fixed costs/capital investments associated with the process equipment and units in the process and is given by the following equation:

$$CC = f(V_E, W_E, Z_E) + \sum_{i=1}^{I} f(V_i, W_P, Z_P) \tag{4.12}$$

where V_E is the size of the process equipment and W_E is the annual capital recovery factor per unit size of equipment; V_i represents the size of the storage tank used to store product grade i whereas W_P is the annual capital recovery factor per unit size of that product storage tank. Z_E and Z_P denote the per unit capital costs associated with the equipment and product tanks. The volume of the product tank is considered to be a measure of the variability in the product grade specification, i.e., with higher product variability due to disturbances and model parameter uncertainty, more off-specification product is produced which leads to larger volumes of the product tanks thus affecting the plant's economy.

The operating cost OC represents the expenditure associated with production in terms of consumption of utilities; this cost can be calculated from the per unit rates for utilities. The variability cost VC aims to measure the effect of time-varying disturbances and model parameter uncertainty during the production stage, i.e., product variability.

As shown in Figure 4.3(a), the minimum and maximum values around the set point for specification of a grade i can be used to calculate the variability cost as follows:

$$VC = \sum_{i=1}^{I} t_{p_i} ((MaxC_i(t) - C_i^{SP}) + (C_i^{SP} - MinC_i(t)))P_{V,i} / t_{total} \quad (4.13)$$

where t_{p_i} is the production time required for grade i, t_{total} is the total time of production cycle, C_i^{SP} denotes the specification for product grade i, while $MaxC_i(t)$ and $MinC_i(t)$ are the maximum and minimum values associated with the specification at any time t within the production time interval for the grade i, i.e., t_{pi}. Both $MaxC_i(t)$ and $MinC_i(t)$ are obtained from simulations of the non-linear closed loop process model $\mathbf{f}_{closed}$ for the production stages of grade i. The term $P_{V,i}$ is a user-defined penalty cost associated with product variability of grade i per unit time. Furthermore, the transition cost TC represents the cost associated with the waste production during the transition from one grade to another, which is off-specification.

The deviations ($\varepsilon(t)$) between the set-point associated with the grade specification (C_i^{SP}) and the actual grade at time t ($C_i(t)$) are shown in Figure 4.3(b), which are used to calculate the transition cost. The deviations $\varepsilon(t)$ are evaluated at discrete time intervals over transition period t_i. The time is discretized in N intervals and sum of squared errors is evaluated as follows:

$$SSE_i = \sum_{n=0}^{N} \varepsilon(n\Delta t)^2, \ \forall t = 0, \Delta t, 2\Delta t, 3\Delta t....n\Delta t...N\Delta t \tag{4.14}$$

where, Δt is the sampling time at which deviations are evaluated, while $N\Delta t$ represents the total integration time, i.e. transition period t_i.

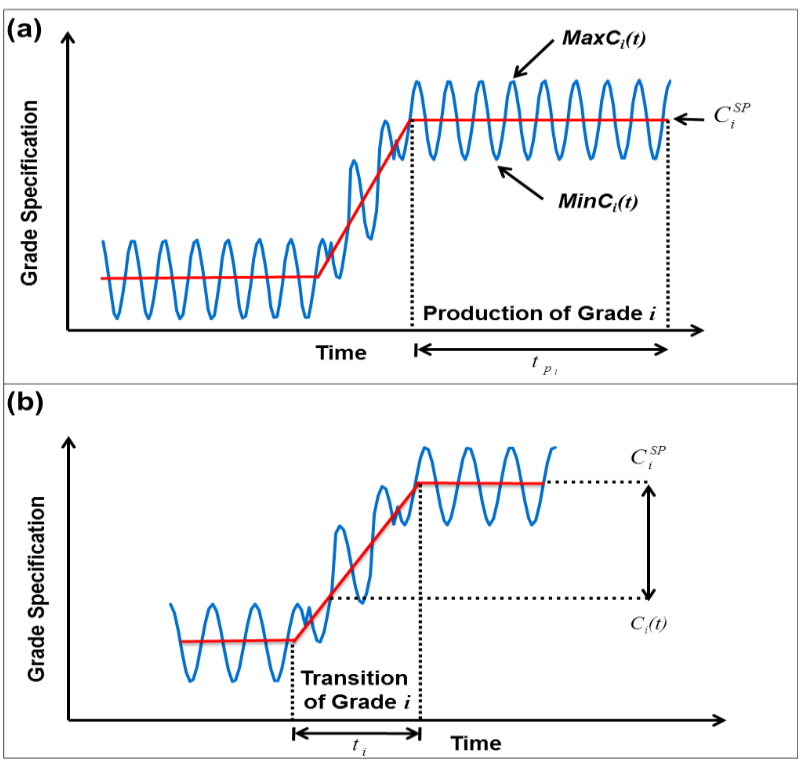

Figure 4.3. (a) Variability cost (b) transition cost

Accordingly, the transition cost can be estimated as follows:

$$TC = \sum_{i=1}^{I} P_{T,i} t_i SSE_i / t_{total} \tag{4.15}$$

where t_i is the transition time for the grade i and $P_{T,i}$ is the user-defined penalty during the transition stage from grade *i-1* to grade *i*, which is the cost associated with the production of the off-specification product of grade *i* per unit time.

4.2.5 Optimization Formulation

Following the developments in the previous sub-sections, an MINLP optimization formulation to address the simultaneous design, scheduling and control can be formulated for multiproduct process that produces *I* number of grades of product under the influence of process disturbances ($\boldsymbol{\eta}$) and model parameter uncertainty (**w**):

$$\begin{aligned}
&\min_{\mathbf{d}=[\boldsymbol{\kappa},\boldsymbol{\Lambda},\mathbf{S}]} \Phi = \sum_{z=1}^{ns} P^z (CC + OC + VC + TC) \\
&\text{s.t.} \\
&\quad \mathbf{f}(\mathbf{x}^z(t), \dot{\mathbf{x}}^z(t), \mathbf{u}^z(t), \boldsymbol{\eta}^z(t), \mathbf{y}^z(t), \boldsymbol{\theta}^z(t), \boldsymbol{\kappa}, \mathbf{w}^z(t)) = 0, z = 1..ns \\
&\quad \mathbf{g}(\mathbf{x}^z(t), \dot{\mathbf{x}}^z(t), \mathbf{c}^z(t), \dot{\mathbf{c}}^z(t), \mathbf{u}^z(t), \mathbf{y}^z(t), \mathbf{w}^z(t), \boldsymbol{\Lambda}) = 0, \ z = 1..ns \\
&\quad \mathbf{h}(\mathbf{x}^z(t), \mathbf{u}^z(t), \boldsymbol{\eta}^z(t), \mathbf{y}^z(t), \boldsymbol{\theta}^z(t), \boldsymbol{\kappa}, \boldsymbol{\Lambda}, \mathbf{S}, \mathbf{w}^z(t)) = 0, \ z = 1..ns \\
&\quad \dot{\mathbf{x}}^z_{lin} = \mathbf{A}^z_i \mathbf{x} + \mathbf{B}^z_i \boldsymbol{\varphi} \\
&\quad \boldsymbol{\Omega}^z_{lin} = \mathbf{C}^z_i \mathbf{x} + \mathbf{D}^z_i \boldsymbol{\varphi}, \ i = 1...I, z = 1..ns \\
&\quad \text{eig}(\mathbf{A}^z_i (\mathbf{x}_{lin})_{\mathbf{d}}) < 0, \forall i = 1....n, z = 1..ns \\
&\quad \boldsymbol{\eta}^z_k(t) = \boldsymbol{\eta}^z_{k_{nom}} + \boldsymbol{\eta}^z_{k_m} \sin(\boldsymbol{\omega}^z_{\mathbf{c}_{k,i}} t), i = 1....n, z = 1..ns, \forall k \\
&\quad \mathbf{d}^l \le \mathbf{d} \le \mathbf{d}^u
\end{aligned} \tag{4.16}$$

where the decision variables (**d**) consist of process design variables $\boldsymbol{\kappa}$, tuning parameters for the control scheme considered $\boldsymbol{\Lambda}$ and the scheduling parameters **S**. The design variables ($\boldsymbol{\kappa}$)

consist of fixed/equipment design parameters and nominal operating conditions for each grade *i*, i.e.

($\overline{\mathbf{u_i}}$ and $\overline{\mathbf{y_i}}$), while the scheduling parameters ($\mathbf{s}$) involve the optimal sequence of production $\mathbf{s}$, which is a set of integer variables, i.e. $\mathbf{s} \in \mathbf{Z}^{I\mathrm{x}1}$, and the set of transition slopes for each grade *i*, $\boldsymbol{\alpha} \in \mathbf{R}^{I\mathrm{x}1}$. The remaining variables used in (4.16) are listed in the notation section.

The optimization formulation shown in (4.16) involves the use of linearized closed-loop model, frequency response analysis, nominal stability check via eigenvalues and dynamic simulations of the actual process model in closed-loop under critical realizations in the disturbances and for each uncertain (discrete) scenario considered in the analysis. Given, an initial set of values in the decision variables $\mathbf{d}_0$, an nonlinear process model ($\mathbf{f}$), closed-loop control scheme ($\mathbf{g}$), nominal values ($\boldsymbol{\eta}_{nom}$) and amplitudes ($\boldsymbol{\eta}_m$) for disturbances, product grade specifications (C_i^{SP}) and demands (V_{p_i}) and critical scenarios for uncertain parameters ($\mathbf{w}$), the following steps are followed at each optimization step to evaluate the cost function and constraints included in problem (4.16):

(1) For each grade *i*, the linearized closed loop model of the system is identified for each critical realization in uncertain parameters by linearization of nonlinear closed-loop model $\mathbf{f}_{closed}$ at the nominal operating steady state conditions specified by decision variables $\mathbf{d}$. The linearized closed-loop model will be used to identify the critical frequencies in the process disturbances that are expected to generate the largest variability in the production stage of grade *i*, i.e., $\omega_{c_{k,i}}$.

(2) For each grade *i*, the critical frequency ($\omega_{c_{k,i}}$) is identified from the linearized model for each critical realization in uncertain parameters via frequency response analysis as described by equations (4.2)-(4.9). The disturbances are specified using the critical frequency and model parameter uncertainty scenarios as shown in (4.9).

(3) For each grade *i* and each critical realization in the uncertain parameter w^z, a stability check is performed for the nominal stability of the system via evaluation of the eigenvalues as shown in (4.11).

(4) For each critical scenario in the uncertainty in the parameters, the transition and production for all the grades is achieved through simulation of the closed loop nonlinear process model $\mathbf{f}_{closed}$ of the system. This is achieved under the influence of critical realizations in the disturbances using ($\omega_{c_{k,i}}$) and that were identified from step 2 for each grade *i*.

(5) The simulation results from the previous step are then used to evaluate the process constraints and each of the cost function terms described above. If an optimization criterion is met, the optimization algorithm stops, else it leaves the workflow and the steps are repeated with new set of decision variables, i.e. go back to step 1.

Remarks

The methodology presented in this work integrates the design, scheduling and control aspects of the multi-product plants under the influence of process disturbances and uncertainty in the parameters. These aspects are novel features for the optimal design of multi-product plants.

The process disturbances ($\boldsymbol{\eta}$) are specified as sinusoidal functions at critical frequency obtained from the linearized closed-loop process model. This variability may not be the true worst-case since the responses for controlled variables are linearized. While the actual critical frequency that generates the worst-case variability in the controlled variables can be obtained from a formal dynamic feasibility analysis test [64,77,80], this test needs to be performed for each grade *i* and at each optimization step thus increasing the computational costs and may even become prohibitive if the problem under analysis is relatively large. The approach proposed here is expected to provide reasonabley accurate results since the critical frequency is identified under feedback control. As such, it is expected that the control actions will aim to maintain the system around a nominal operating point (i.e., the product grade's set-point) thus making the linear closed-loop approximation valid. Tests need to be performed to evaluate this approximation. Furthermore, the approach of computing critical frequency corresponding to worst case variability can be assumed when there is no prior information available for the anticipated range of frequencies of the disturbances. For the cases where this information is available *a priori*, the anticipated range of frequencies for the disturbances can be used to design the controller instead of critical frequency in order to attenuate most of the typical anticipated disturbances at a given (pre-specified) frequency range. This can provide more realistic (less conservative) designs for the controller. Accordingly, equation (4.8) can be modified to represent this range of frequencies that correspond to anticipated disturbances as follows:

$$AR^{\max}_{\mathbf{y}_l-\boldsymbol{\eta}_k} = \sqrt{R_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega_{c_{k,i}})^2 + I^m_{\mathbf{y}_l-\boldsymbol{\eta}_k}(\omega_{c_{k,i}})^2}\ ,\ \omega_l \le \omega_{c_{k,i}} \le \omega_u \qquad (4.17)$$

where, ω_l and ω_l are lower and upper bounds on the frequencies which represent the anticipated range of frequencies for the process disturbances that have been pre-specified *a priori*.

Moreover, the process flow-sheet of the multi-product process has been assumed to remain the same throughout the calculations in the presented methodology. The control scheme has also been assumed to be fixed. This leads the methodology to be able to compute the process scheduling, design and control parameters only for the fixed flow sheet and control structures. To make the methodology robust to the changes in the flow-sheet and control schemes, advanced approaches need to be considered which result in higher computational costs. The application of such highly demanding approaches to the methodology of integration of scheduling, design and control is considered part of the future work in this study. In terms of product grades, the production of all the grades has been assumed to be consumed/sold before the production begins, i.e. availability of storage tanks has been assumed to be constant. All grades are produced only once in the complete operation cycle.

4.3 Results and Discussions

This section describes the two case studies developed for the application of the methodology described in this study. The two applications demonstrate the effect of simultaneous consideration of the three aspects on the overall cost of operation, i.e. design, control and scheduling. The results presented for these case studies were obtained using MATLAB software on system with a Win Server 2012, Intel® Core i7-3770 CPU 340GHz, 8 GB RAM.

4.3.1 Case Study 1: Non-isothermal CSTR

The methodology discussed in the previous section was applied to a non-isothermal CSTR system with an irreversible reaction which is assumed to produce 3 grades of the product. Figure 4.4 shows the CSTR system pictorially with a reactor, control system and product tanks for the three grades to be produced which are to be filled one by one. However, the sequence of filling the tanks, i.e. the production of grades, is part of the decision variables. The case study has been developed to simultaneously determine the optimal design, control and scheduling parameters for the CSTR system under consideration, compare the results against the semi-sequential approach, i.e., optimal design and control followed by optimal scheduling, and evaluate the methodology's capability to handle uncertainty in grade demands.

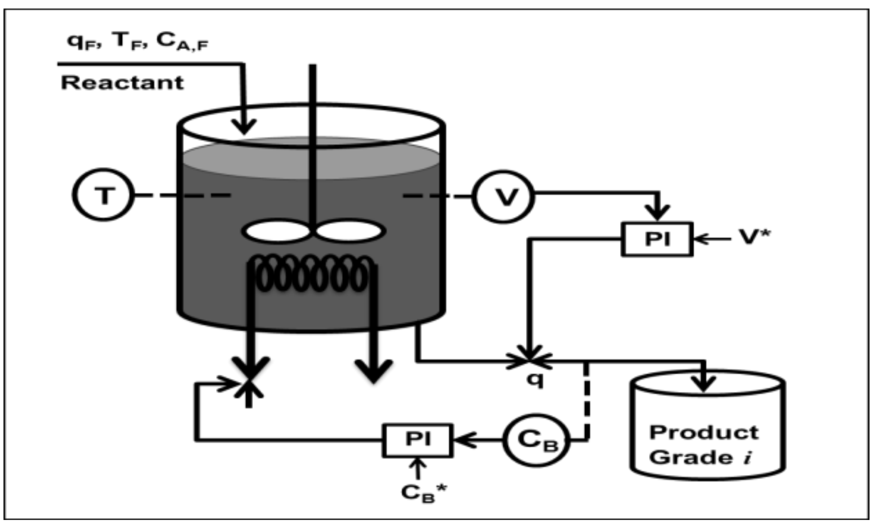

Figure 4.4. Non-isothermal CSTR system

Mathematical Model

An irreversible exothermic reaction $A \rightarrow B$ occurs in the CSTR for the production of product *B* from reactant *A*. The reaction has been assumed to follow first-order dynamics and the reaction rate is given by the Arrhenius law as follows:

$$r_A = k_0 C_A \exp(-\frac{E}{RT}) \tag{4.18}$$

where C_A (mol/L) is the concentration of reactant *A* inside the reactor at any time t, k_0 is the pre-exponential factor (7.2 X 10^{-10}), *E* is the activation energy (83145 J/mol) and *R* is the gas constant (8.3144 J/mol K). The CSTR system is equipped with a cooling jacket in order to maintain the temperature inside the reactor (*T*). The concentration of reactant *A* in the inlet stream $(C_{A,F})$ has been assumed to remain constant during the operation $(C_{A,F} = 2 \text{ mol/lit})$.

The mechanistic dynamic model that describes the non-isothermal CSTR system is given as follows:

$$\frac{dV}{dt} = q_F - q \tag{4.19}$$

$$\frac{dT}{dt} = \frac{q_F (T_F - T)}{V} + \frac{(H_0 k_0 \exp(\frac{-E}{RT})(C_{A,F} - C_B)}{\rho C_p} - Q_C (C_B^* - C_B) \tag{4.20}$$

$$\frac{dC_B}{dt} = k_0 \exp(-\frac{E}{RT})(C_{A,F} - C_B) - \frac{C_B q_F}{V} \tag{4.21}$$

$$q = 10 u_2 \sqrt{V} \tag{4.22}$$

$$Q_C = 48.1909\, u_1 \tag{4.23}$$

where the volume of the reactor (V), the temperature inside the reactor (T), and the product concentration (C_B) are the states and outputs of the system. As shown in (4.22) and (4.23), the outlet flow-rate of the reactor q is used to control the volume (V) or level in the reactor, while the heat flow to the system (Q_C) has been used as a handle to control the amount of heat transferred to the CSTR system, respectively. There are two manipulated variables available in the system, i.e., u_1 and u_2 $(\mathbf{u} = [u_1, u_2])$. The two manipulated variables are used to control the volume of the reactor (V) and the product concentration (C_B), respectively. The density of the fluid is ρ (1 X 10^3 g/L), C_p is the fluid's heat capacity (0.239 J/g K), while H_0 is the heat of reaction (4.78 X 10^4 J/mol).

Two PI controllers have been used to regulate this process. K_{C_1} and K_{C_2} represent the two controller gains whereas τ_1 and τ_2 are the time integral time constants for the two controllers, i.e. tuning parameters $(\mathbf{\Lambda} = [K_{C_1}, K_{C_2}, \tau_1, \tau_2])$. The errors e_1 and e_2 for the two controllers at any time t represent the difference between the set-points $(V^*$ and $C_B^*)$ and the controlled variables' values at time t, i.e. V(t) and C_B (t). The aim of the irreversible reaction is to produce required grades of product B. Each grade is characterized with specification in terms of product concentration $(C_{B_i}^*)$ and a demand in terms of product volume (V_{p_i}). As shown in Figure 4.4, the system consists of a reaction vessel and a dedicated product tank for each grade of product.

The dynamics of the product tank for grade i of product B can be represented by the following equation:

$$\frac{dV_{P_i}}{dt} = q \tag{4.24}$$

The product tank for a particular grade starts filling as soon as required product specification of a grade is achieved, i.e. production period for grade *i* starts. The time at which the condition is satisfied gives the transition time required for the grade *i*, i.e. t_i. The product tank continues filling until the required product demand is achieved and specification has been maintained. The product tank is then instantaneously changed to the product tank for the next required grade of the product. The time at which this happens is the production time of the grade *i*.

The following operational constraint has been applied in order to impose limits on the temperature of the CSTR:

$$430 \leq T(t) \leq 500 \tag{4.25}$$

Process Disturbances

Following the disturbance description shown in (4.2), the process disturbances T_F and q_F are defined as follows:

$$\begin{aligned} T_F(t) &= 450 + 10\sin(\omega_{c_{T_F,i}} t) \\ q_F(t) &= 200 + 10\sin(\omega_{c_{q_F,i}} t) \end{aligned} \tag{4.26}$$

For each grade *i*, the critical frequencies ($\omega_{c_{T_F,i}}, \omega_{c_{q_F,i}}$) used to generate the disturbances are obtained from the frequency response analysis of linearized closed-loop process model at operating conditions for each grade *i* specified by the decision variables **d**.

Cost Function

The annualized capital cost of the CSTR system associated with the volume of the reactor and the volume of the product grade tanks can be formulated as follows:

$$CC = 1000(0.1)V + \sum_{i=1}^{I} 1000(0.1)V_{p_i} \tag{4.27}$$

where V is the volume for the reactor whereas V_{p_i} is the volume of product tank for grade *i*. To simplify the analysis, all costs associate with the equipment have been assigned the same value. Following (4.12), $W = 0.1/yr$, $Z = \$1000$, $W_P = 0.1/yr$ and $Z_P = \$1000$.

Moreover, the variability cost can be calculated by modifying (4.13) as follows:

$$VC = \sum_{i=1}^{I} t_{p_i}((MaxC_{B_i}(t) - C^*_{B_i}) + (C^*_{B_i} - MinC_{B_i}(t)))10/t_{total} \tag{4.28}$$

where, $C^*_{B_i}$ is the product grade specification, $C_{B_i}(t)$ is the value at time t for the product concentration, while the penalty for variability has been assigned the value of $10/(mol/lit)-min.

The operating cost can be calculated as follows:

$$OC = \sum_{i=1}^{I} t_{p_i}(10(\overline{Q_{c_i}}))/t_{total} \tag{4.29}$$

where, $\overline{Q_{c_i}}$ is the steady state value for heat duty at production of each grade *i*, while 10 is the per unit cost of heat per unit time.

Furthermore, the transition cost can be calculated from (4.15) as follows, i.e.,

$$TC = \sum_{i=1}^{I} 10 t_i SSE_i / t_{total} \tag{4.30}$$

where SSE_i is the sum of squared errors during the transition period of the grade i as shown in (4.14). The penalty for waste production has been assigned the value of $\$10/(\text{mol/lit})^2$ - min.

Following the developments above, the optimization formulation has been solved for the CSTR system. The decision variables to be evaluated include volume of the reactor and steady state operating conditions for each grade $(\boldsymbol{\kappa} = [V, \overline{u_{1i}}, \overline{u_{2i}}])$, tuning parameters for the two PI controllers $(\boldsymbol{\Lambda} = [K_{C_1}, K_{C_2}, \tau_1, \tau_2])$, slopes for transition of each grade, i.e., $\alpha_1, \alpha_2, \alpha_3$, and the optimal sequence of production ($\mathbf{s}$).

Scenario 1

This scenario has been developed to compare the results obtained via the present simultaneous approach and a semi-sequential approach. In the semi-sequential approach, the following procedure was considered: in the first step, decision variables related to process design and control (i.e. integration of design and control) are evaluated first and then, in the second step, the scheduling decision variables are determined while the design and control variables obtained in step 1 remain fixed in the calculations. The specifications and the demands of the required product grades considered for the problem addressed for this scenario are reported in Table 4.1. The methodology has been used to obtain results for the CSTR system to integrate the scheduling, design and control aspects of the system. For each single function evaluation, values for the decision variables are selected by the optimization algorithm. These decision variables are further used to calculate for each grade *i*, steady-state operating conditions ($\overline{u_{1i}}, \overline{u_{2i}}$, T_i) by solving the process model (**f**) at steady state. For each grade *i*, the steady-state operating conditions are then used to identify a linear closed-loop model of the system as shown in (4.4). The resulting linear model is further used to identify the critical frequency ($\omega_{c_{k,i}}$) for each grade *i* for each process disturbance (T_F, q_F) as described by equations (4.7)-(4.12), which is used to specify the process disturbances as shown in (4.2). The closed-loop process model described by equations 4.18-4.24 is simulated for each critical scenario for uncertainty in product demand. The results from this simulation are then used to evaluate the process constraints and cost function shown in (4.16). This procedure is repeated until an optimization criterion is met.

The results obtained from the implementation of the two approaches are reported in Table 4.1 (Results). The decision variables obtained from each approach vary significantly from each other and there is approximately 20% improvement in the overall cost with the simultaneous approach as compared to the semi-sequential approach. The maximum improvement can be seen in the transition costs (~60%). The volume of the reactor (*V*), which is a design decision variable, is almost 8% less in the simultaneous approach than that obtained in semi-sequential approach, while tuning parameters for the two controller are also significantly different, which indicates that different process performance may be obtained from the two solution methods.

Table 4.1. Grade specifications, demands and results for scenario 1, case study CSTR

Grade Specifications and Demands		
Grade	**Product Concentration (mol/lit)**	**Demand (lit)**
1	1.7023	3,000
2	1.830	3,000
3	1.950	3,000
Results		
Decision Variables and Costs	**Simultaneous Approach**	**Semi-Sequential Approach**
Design: V (L)	80.6828	87.416
Control: $K_{C_1}, K_{C_2}, \tau_1, \tau_2$	-13.634, -0.002, 7.40, 8.77	- 5.425, -0.0016, 2.235, 9.314
Scheduling: **s** (sequence of grades) $\alpha_1, \alpha_2, \alpha_3$ (transition slopes)	2-1-3 0.0872, -0.0803, 0.006	2-1-3 0.0131, -0.0281, 0.0011
Capital Cost ($/yr)	15,715.53	18,844.25
Operating Cost ($/yr)	1,021.1	1,699.1
Variability Cost ($/yr)	131.616	318.66
Transition Cost ($/yr)	153.18	382.39
Total Cost ($/yr)	17,021.43	21,244.4

The slopes obtained for the transition between the grades of the product are observed to be more aggressive in the simultaneous approach as compared to the semi-sequential approach, which provide the basis for the improvement in the transition cost. The transition and production of various grades are depicted in Figure 4.5(a). The variability in the concentration is the result of process disturbances oscillating at critical frequency, which has a different value for each grade obtained via frequency response analysis of linearized process model at the different operating conditions specified by **d**. The process constraint on temperature has been satisfied throughout the operation of the entire production cycle as shown in Figure 4.5(b). Thus, the results obtained via two approaches show that the simultaneous methodology generates more economical solution as compared to the semi-sequential approach.

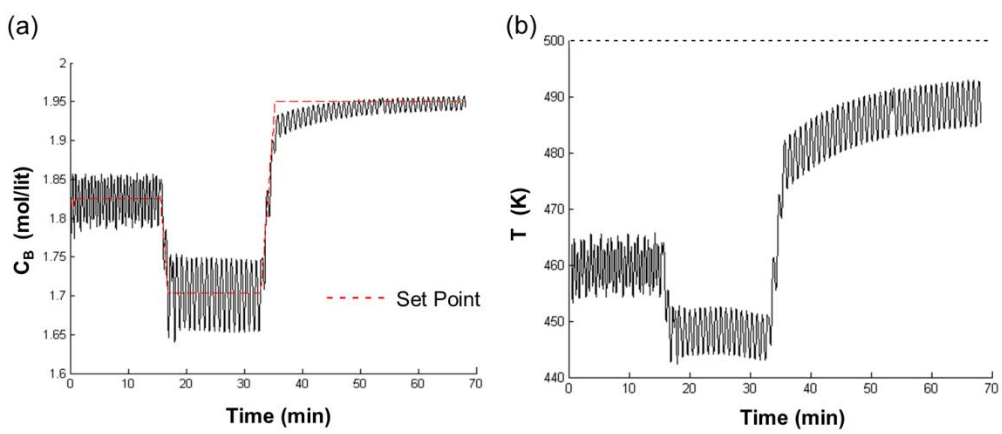

Figure 4.5. CSTR case study, scenario 1 (a) transition and production of product grade (b) temperature profile

Scenario 2

This second scenario has been developed to evaluate the capability of the methodology developed in this study to handle uncertainty in the parameters. As shown in the methodology's formulation in (4.16), a multi-scenario approach has been used for this purpose; critical scenarios have been created with a specific demand for each grade of the product. Each scenario has been assigned the probability of occurrence of the scenario. As shown in Table 4.2, four demand scenarios have been created with first scenario with uniform production demands, i.e., 3,000 lit of each grade having the highest probability of occurrence. The other three scenarios consist of maximum and minimum of the demands for each grade of the product.

The optimization formulation presented in (4.16) has been modified for this scenario and the results obtained are also shown in Table 4.2 (Results). As shown in this table, the optimal volume of the reactor is 75.655 lit, while the optimal sequence of production is determined to be 2-1-3, which is same as in Scenario 1, i.e. without uncertainty in demands.

The Figure 4.6 depicts the trends for transition and production of the grades in four critical scenarios for uncertainty in demands, where optimal smooth transitions between grades is the result of optimal transition slopes computed by the optimization formulation. This is achieved while maintaining the dynamic operability of this process under their corresponding constraints.

In terms of computational costs, the computational time required to complete a single evaluation of the optimization formulation for Scenario 1 was 40 seconds on average, while the solution was obtained in 2.5 hours. For Scenario 2, the single evaluation of the optimization formulation required 60 seconds on average, while the solution was obtained in 3 hours.

Table 4.2. Demands and Probabilities of Scenarios, CSTR

Demand Scenario	**Demands of Product Grades (1,2,3)(L)**	**Probability**
1	3,000, 3,000, 3,000	0.4
2	5,000, 2,000, 1,000	0.3
3	2,000, 5,000, 1,000	0.2
4	1,000, 5,000, 2,000	0.1
Results		
Decision Variables and Costs	**Values**	
Design: V (L)	75.655	
Control: $K_{C_1}, K_{C_2}, \tau_1, \tau_2$	-16.4633, -0.073, 3.6428, 10.0432	
Scheduling: **s** (sequence of grades) $\alpha_1, \alpha_2, \alpha_3$ (transition slopes)	2-1-3 0.0507, -0.510, 0.00265	
Total Cost ($/yr)	17,2059.9	

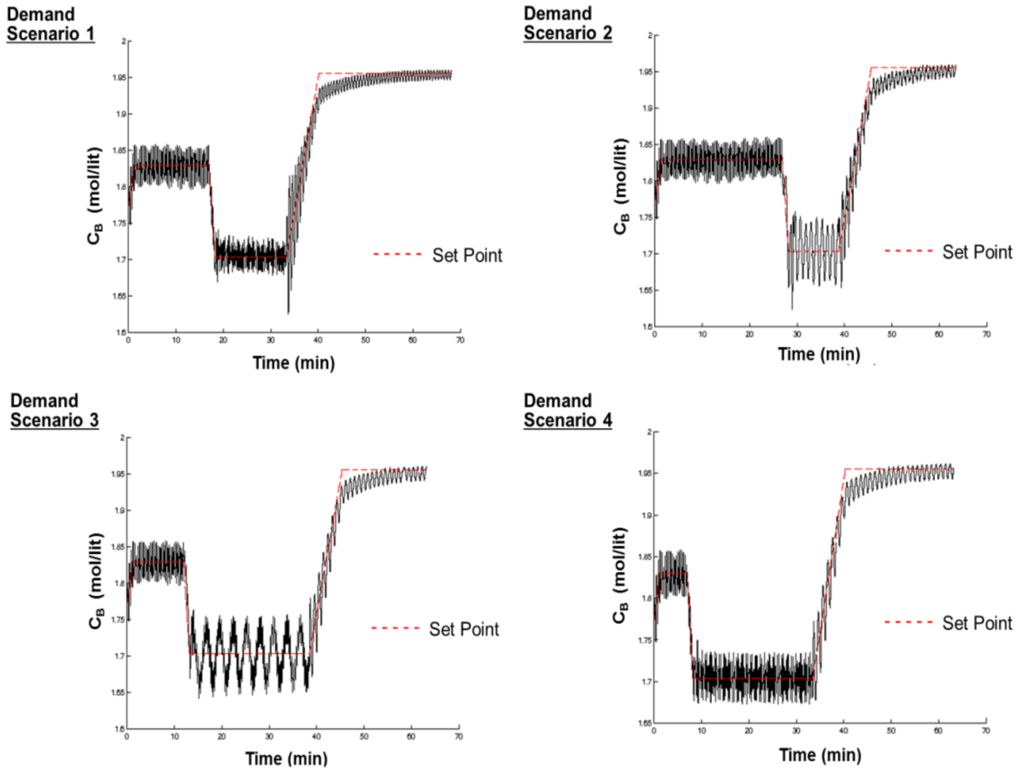

Figure 4.6. CSTR case study, scenario 2, transition and production of product grades

4.3.2 Case Study 2: HIPS Polymerization Reactor

The second case study has been developed with the goal of demonstrating the capability of the methodology to be applied to a large-scale problem with a strongly nonlinear behavior. The case study focusses on integration of scheduling, design and control aspects for the high impact polystyrene (HIPS) process characterized by the parameters and the mathematical model [57]. The process is operated by the continuous stirred tank reactor with highly non-linear reaction mechanism. The results are obtained for the critical uncertain scenarios developed for the varying product demands.

Mathematical Model

Initiator Concentration:

$$\frac{dC_i}{dt} = \frac{q_i C_i^{in} - q_m C_i}{V} - K_d C_i \tag{4.31}$$

Monomer Concentration:

$$\frac{dC_m}{dt} = \frac{q_m (C_m^{in} - C_m)}{V} - K_P C_m (\varepsilon_r^0 + \varepsilon_b^0) \tag{4.32}$$

Butadiene Concentration:

$$\frac{dC_b}{dt} = \frac{q_m (C_b^{in} - C_b)}{V} - C_b (K_{i2} C_r + K_{fs} \varepsilon_r^0 + K_{fb} \varepsilon_b^0) \tag{4.33}$$

Radicals Concentration:

$$\frac{dC_r}{dt} = \frac{-q_m}{V} C_r + 2 e_f K_d C_i - C_r (K_{i1} C_m + K_{i2} C_b) \tag{4.34}$$

Branched radicals concentration:

$$\frac{dC_{br}}{dt} = \frac{-q_m}{V} C_{br} + C_b (K_{i2} C_r + K_{fb} (\varepsilon_r^0 + \varepsilon_b^0)) - C_{br} (K_{i3} C_m + K_t (\varepsilon_r^0 + \varepsilon_b^0 + C_{br})) \tag{4.35}$$

Reactor temperature:

$$\frac{dT}{dt} = \frac{q_m}{V} (T^{in} - T) + \frac{\Delta H_r K_p C_m (\varepsilon_r^0 + \varepsilon_b^0)}{\rho_{st} C_{ps}} - \frac{UA(T - T_j)}{\rho_{st} C_{ps} V} \tag{4.36}$$

Jacket Temperature:

$$\frac{dT_j}{dt} = \frac{q_{cw}}{V_c} (T_j^{in} - T_j) + \frac{UA(T - T_j)}{\rho_{st} C_{ps} V_c} \tag{4.37}$$

Zeroth moment live polymer:

$$\frac{d\xi_p^0}{dt} = \frac{-q_m}{V}\xi_p^0 + \frac{K_t}{2}(\varepsilon_r^0)^2 + (K_{fs}C_m + K_{fb}C_b)\varepsilon_r^0 \quad (4.38)$$

First moment live polymer:

$$\frac{d\xi_p^1}{dt} = \frac{-q_m}{V}\xi_p^1 + K_t\varepsilon_r^1\varepsilon_r^0 + (K_{fs}C_m + K_{fb}C_b)\varepsilon_r^1 \quad (4.39)$$

Zeroth moment dead polymer:

$$\begin{aligned}\frac{d\varepsilon_r^0}{dt} &= \frac{-q_m}{V}\varepsilon_r^0 + 2K_{i0}C_m^3 + 2K_{i1}C_rC_m + C_mK_{fs}(\varepsilon_r^0 + \varepsilon_b^0) \\ &-(K_pC_m + K_t(\varepsilon_r^0 + \varepsilon_b^0 + C_{br}) + C_mK_{fs} + C_bK_{fb})\varepsilon_r^0 + K_pC_m\varepsilon_r^0\end{aligned} \quad (4.40)$$

First moment dead polymer:

$$\frac{d\varepsilon_r^1}{dt} = \frac{-q_m}{V}\varepsilon_r^1 - (K_pC_m + K_t(\varepsilon_r^0 + \varepsilon_b^0 + C_{br}) + C_mK_{fs} + C_bK_{fb})\varepsilon_r^0 + K_pC_m(\varepsilon_r^0 + \varepsilon_r^0) \quad (4.41)$$

Zeroth moment butadiene:

$$\frac{d\varepsilon_b^0}{dt} = \frac{-q_m}{V}\varepsilon_b^0 + 2K_{i3}C_{br}C_m - (K_pC_m + K_t(\varepsilon_r^0 + \varepsilon_b^0 + C_{br}) + C_mK_{fs} + C_bK_{fb})\varepsilon_b^0 + K_pC_m\varepsilon_b^0 \quad (4.42)$$

Number molecular weight distribution:

$$M_w = \frac{\xi_p^1 + \varepsilon_r^1}{\xi_p^0 + \varepsilon_r^0} \quad (4.43)$$

where C_i, C_m, C_b, C_r, C_{br}, T *and* T_j are the initiator concentration, monomer concentration, butadiene concentration, radicals concentration, branched radical concentration, reactor temperature and jacket temperature, respectively. The live polymer moments are denoted by ξ_p^0 and ξ_p^1, with first being zeroth moment, while the latter is first moment. Similarly, ε_r^0 and

ε_r^1 are zeroth and first dead polymer moments, while ε_b^0 and ε_b^0 are zeroth and first butadiene moments.

The terms q_i, q_m and q_{cw} represent the initiator, monomer and cooling water flow rates, respectively. V is the reactor volume, V_C is the jacket volume, while ρ is the density, C_p is the specific heat and ΔH_r is the heat of reaction. Initiator efficiency is denoted by e_f, M_w is the number average molecular weight, *U* is the global heat transfer coefficient, *A* is the heat transfer area, *K* is the Arrhenius kinetic rate constant. The superscripts d, p, i0, i1, i2, i3, fs, fb, t on the reaction rates represent the different free radical reactions steps. The superscript 'in' stands for feed stream conditions, while 'cw' refers to cooling water properties. The symbol's' in the subscripts denotes styrene properties. The parameters are listed in Table 4.3.

Control Scheme:

Two PI controllers have been implemented with the aim of controlling monomer conversion x_m and reactor temperature T. The manipulated variables used in order to control these variables are monomer flow rate q_m and cooling water flow rate q_{cw}, respectively. K_{C_1} and K_{C_2} represent the two controller gains, τ_1 and τ_2 are the time integral time constants for the two controllers, i.e. tuning parameters $(\mathbf{\Lambda} = [K_{C_1}, K_{C_2}, \tau_1, \tau_2])$. The errors e_1 and e_2 for the two controllers at any time t represent the difference between the set-points (x_m^*, T^*) and the values at time t, i.e. $(x_m(t), T(t))$.

Following the descriptions provided for this process [57], the following operational constraints have been applied to impose limits on the temperature of the reactor and the number molecular weight distribution:

$$330 \leq T(t) \leq 420 \quad (4.44)$$

$$500 \leq M_w(t) \leq 3000 \quad (4.45)$$

Process Disturbance

Following the disturbance description presented in (4.2), the disturbance considered for this process, C_m^{in}, is defined as follows:

$$C_m^{in}(t) = 8.63 + 0.8\sin(\omega_{c_{C_{m,i}^{in}}} t) \quad (4.46)$$

For each grade *i*, the critical frequency ($\omega_{c_{C_{m,i}^{in}}}$) that produces the largest variability in x_m and T is obtained from the frequency response analysis of linearized closed-loop process model at the operating conditions specified by the optimization formulation as part of decision variables (**d**) as explained in section 4.2.1.

Table 4.3. Case Study 2: HIPS model parameters

Parameter	Description	Value
T^{in}	Inlet temperature	$294K$
C_m^{in}	Inlet monomer concentration	$8.63 mol/L$
C_i^{in}	Inlet initiator concentration	$0.9814 mol/L$
C_b^{in}	Inlet butadiene concentration	$1.0547 mol/L$
V_C	Jacket volume	$2000L$
ΔH_r	Heat of reaction	$69919.6\ J/mol$
C_{ps}	Monomer heat capacity	$1647.265\ J/kgK$
C_{pcw}	Water heat capacity	$4045.7048\ J/kgK$
U	Heat transfer coefficient	$80\ J/(sKm^2)$
A_{i0}	Pre-exp. factor	$1.1 \text{x} 10^5\ L^2/(mol^2 s)$
A_{i1}	Pre-exp. factor	$1 \text{x} 10^7\ L/(mol\ s)$
A_{i2}	Pre-exp. factor	$2 \text{x} 10^6\ L/(mol\ s)$
A_{i3}	Pre-exp. factor	$1 \text{x} 10^7\ L/(mol\ s)$
A_d	Pre-exp. factor	$9.1 \text{x} 10^{13}\ s^{-1}$
A_{fs}	Pre-exp. factor	$6.6 \text{x} 10^7\ L/(mol\ s)$
A_{fb}	Pre-exp. factor	$2.3 \text{x} 10^9\ L/(mol\ s)$
A_t	Pre-exp. factor	$1.7 \text{x} 10^9\ L/(mol\ s)$
A_p	Pre-exp. factor	$1 \text{x} 10^7\ L/(mol\ s)$
E_{i0}	Activation energy	$27340 cal/mol$
E_{i1}	Activation energy	$7067 cal/mol$
E_{i2}	Activation energy	$7067 cal/mol$
E_{i3}	Activation energy	$7067 cal/mol$
E_d	Activation energy	$29508 cal/mol$
E_{fs}	Activation energy	$14400 cal/mol$
E_{fb}	Activation energy	$18000 cal/mol$
E_t	Activation energy	$843K$
E_p	Activation energy	$7067 cal/mol$
e_f	Efficiency factor	0.57
ρ_s	Monomer density	$0.915 kg/L$
ρ_{cw}	Water density	$1\ kg/L$
A	Heat transfer area	$19.5 m^2$
R	Ideal Gas Constant	$1.9858 cal/(mol\ K)$

The capital cost of the HIPS system consists of the costs associated with the volume of the reactor and the volume of the tanks for product grades produced and can be formulated as follows:

$$CC = 1200(0.1)V + \sum_{i=1}^{I} 1200(0.1)V_i \tag{4.47}$$

where V is the volume for the reactor, while V_i is the volume of product tank for grade *i*. To simplify the analysis, all the costs associated with equipment have been assigned the same value. Following (4.12), $W = 0.1/yr$, Z = \$1,200, $W_P = 0.1/yr$ and Z_P = \$1,200.

Moreover, the variability cost can be calculated by modifying (4.13) as follows:

$$VC = \sum_{i=1}^{I} t_{p_i}((Max(x_{m_i}(t)) - x^*_{m_i}) + (x^*_{m_i} - Min(x_{m_i}(t))))35/t_{total} \tag{4.48}$$

where, $x^*_{m_i}$ is the product grade specification, $x_{m_i}(t)$ is the value at time t for the monomer conversion, while the penalty for variability has been assigned the value of \$35 per unit deviation in conversion set point per unit time. The operating cost for this process can be calculated as follows:

$$OC = \sum_{i=1}^{I} t_{p_i}(20(\overline{q_{cw_i}}) + 30(\overline{q_{m_i}}))/t_{total} \tag{4.49}$$

where $\overline{q_{cw}}$ and $\overline{q_m}$ are the steady-state values for cold water flow and monomer flow at production of each grade *i*, which are weighted by the respective costs per unit, i.e. \$20/(L)-min and \$30/(L)-min.

Furthermore, the transition cost can be calculated from (4.15) as follows, i.e.

$$TC = \sum_{i=1}^{I} 35 t_i SSE_i / t_{total} \tag{4.50}$$

where SSE_i is the sum of squared errors during transition period of the grade i. The penalty for waste production has been assigned the value of \$35 per unit squared error in conversion per unit time. The decision variables related to the design, control and scheduling aspects are evaluated for the optimal solution. The volume of the reactor and inlet temperature T^{in} $(\boldsymbol{\kappa} = [V, T^{in}])$ are the design decision variable, while tuning parameters for the two PI controllers $(\boldsymbol{\Lambda} = [K_{C_1}, K_{C_2}, \tau_1, \tau_2])$ are the control decision variables to be evaluated. The scheduling decision variables include slopes for transition of each grade i.e. $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ and optimal sequence of production i.e. **s**.

Following the developments described above, the optimization formulation shown in (4.16) is solved with the specifications of HIPS system described above. The specifications of four different grades are shown in Table 4.4 along with the information related to the critical scenarios created for uncertainty in the product demands. The results obtained for the integration of scheduling, design and control of the HIPS case study are shown in Table 4.5.

Figure 4.7(a) depicts the transition and production of various grades under the critical realizations in the disturbance (C_m^{in}) for the production demand uncertainty scenario that presented the maximum variability in the monomer conversion. In order to validate the linear approximation used to generate worst-case variability, a test has been performed where process constraints have been evaluated for the range of frequencies.

Table 4.4. Case Study 2: Product Specifications and demand scenarios, HIPS

Grade	**Monomer conversion**	
1	0.25	
2	0.30	
3	0.35	
4	0.40	
Scenario	**Demands of Product Grades: 1,2,3,4 (L)**	**Probability**
1	10,000, 10,000, 10,000, 10,000	0.4
2	15,000, 12,000, 7,000, 5,000	0.3
3	7,000, 15,000, 5,000, 12,000	0.2
4	5,000, 12,000, 15,000, 7,000	0.1

The range includes minimum, maximum and the critical frequency obtained from the linear approximation proposed in this work.

For this range of frequencies the profiles of number-average molecular weight for the uncertain demand scenario that correspond to the maximum variability in the controlled variable are shown in Figure 4.7(b). It is clear from the figure that the largest variability in this variable corresponds to the critical frequency and constraints are not violated over a range of frequencies and thus the linear approximation is valid.

Table 4.5. Case Study 2: HIPS results

Decision Variables and Costs	Optimal Values
Design: V (L) T^{in} (K)	 7174 387.74
Control: $K_{C_1}, K_{C_2}, \tau_1, \tau_2$	 -1.732, -0.0183, 1132, 23
Scheduling: **s** (sequence of grades) $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ (transition slopes)	 2-3-4-1 0.0124, 0.0386, 0.0213,-0.0311
Capital Cost($/yr)	5,256,360.641
Operating Cost($/yr)	1,766,102.077
Variability Cost($/yr)	19,317.941
Transition Cost($/yr)	87,042.738
Total Cost($/yr)	7,128,822.82

The CPU time required for the second case study was very high as compared to case study 1 because of the presence of non-linearity and the size of the problem. Each single function evaluation takes around 205 seconds, while it took approximately 8 hours to generate the solution for this case study. The approach presented here assumes a fixed flow-sheet of the process as well as a fixed control scheme, while the scheduling decisions (sequence of product grades) were made for 3-4 grades in the case studies. The application of multi-scenario approach to handle uncertainty increases the computational time as more uncertain parameters are added into the analysis, while adding more integer decision variables in the analysis for the structural decisions related to flow-sheet and control structure can further increase the methodology's computational time.

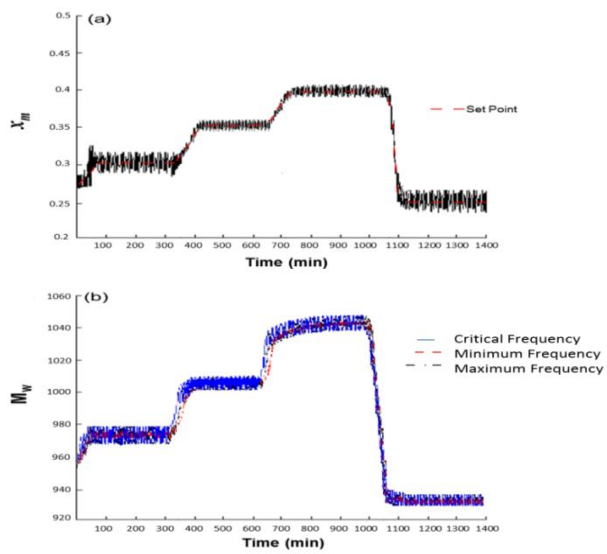

Figure 4.7. (a) transition and production of grade for the scenario with maximum variability (b) process constraints evaluated for the range of frequencies

Similarly, increasing the number of scheduling decisions can also make the task computationally more challenging. Thus, in the future work, the trade-off needs to be taken into account in order to control the computational time while adding more integer decision variables in the analysis.

The results from the case study demonstrate the capability of the methodology to be applied to a large scale non-linear problem in the presence of process disturbances with oscillatory behavior at critical frequency determined for production each grade, while uncertainty has been addressed in product demands.

4.4 Chapter Summary

A new methodology for the simultaneous scheduling, design and control of multi-product processes has been presented in this chapter. The characteristics of the multi-product processes along with the optimization formulation proposed in this study to address the simultaneous design of these plants have been presented in detail. The methodology has been presented with mathematical details describing the key features. The specification of process disturbances has been presented which is based on the sinusoidal function operating at a critical frequency obtained from the frequency response analysis of the linearized closed loop process model. The limitation of this approach is use of fixed disturbance function, while generic distributions can be used to increase the applicability of the methodology. The disturbances specified at this critical frequency generate the maximum variability in the controlled variable which has been justified in case study 2. Another key feature of the methodology presented in this chapter is use of ramp functions for the smooth transitions between grades of product. The slopes of these ramp functions form part of the decision variables. Moreover, uncertainty in the parameters has also been considered in this methodology. A multi-scenario approach has been used, where critical uncertain scenarios have been created and probabilities have been assigned to each of them. Descriptions of all these features have been provided in this chapter with mathematical details. A simple CSTR case study has been developed in order demonstrate an application of the simultaneous methodology and compare the results obtained against the semi-sequential approach. A larger scale process has also been used for another application of the methodology in order to show the capability of the methodology in handling larger problems. Thus, the methodology that integrates scheduling, design and control for multi-product processes has been successfully developed and tested.

Chapter 5

Conclusions and Recommendations

Optimal scheduling is paramount in many chemical process industries where several operations are involved which depend upon each other while their schedule affects the economics of the industry. Applications of scheduling in actual industries need to be designed in order to develop practical and efficient methods that can improve the process economics. Along with this, research that is focused on the integration of scheduling with other aspects of the process economics also needs development of methodologies. The work presented in this thesis focuses on these two areas. A summary of the findings concluded from this work is presented in Section 5.1; while the scope of future work in this field is discussed through recommendations in Section 5.2.

5.1 Conclusions

Part of the research work developed in this thesis focuses on an application of optimal scheduling in an analytical services industry. In this work, an optimization-based scheduling algorithm was developed for better scheduling of operations in the facility owned by the industrial partner. The optimization framework is an application of integer programming (IP) and multi commodity flow, where each process at each time unit is tracked as a flow node. The proposed mathematical formulation has an objective function to minimize the turnaround time of the operations subject to resource, capacity and flow constraints. Flow constraints ensure the balance of samples across the processes, while the resource and capacity constraints make sure that design capacities of the processes are not violated. One of the key contributions of the work is addressing the scheduling issues of commercial scale plants in the analytical services sector with operational characteristics that are less studied, which include large number of simultaneous scheduling decisions on the location of samples, the specific sequences of processes followed by large number of samples and varying processing times. This makes the problem size extensive in terms of number of decision variables with their specific nature. Two case studies were considered to demonstrate the performance of the scheduling algorithm developed in this study. The first case study is an illustrative process where the working principles of the scheduling algorithm are discussed through small examples. Effects of various parameters used in the model on the results have been demonstrated via different scenarios. The second case study is the comparison between results obtained via the present optimization algorithm against historical plant data and the results obtained by simulating the current policy implemented in the real plant, i.e. first-come first-served basis. The analysis of the latter study shows potential improvement in the turnaround time of the operations. The results also show significantly less variance in the operations in terms of work performed each day, which is an additional positive outcome besides the objective of the study. The CPU time required to generate schedules each day (an eight hour shift) is 130 seconds on an average depending on the number of samples under consideration for scheduling.

Apart from an industrial application of optimal scheduling, the research work performed in this thesis also consists of the development of a methodology for integration of scheduling, design and control for the multi-product processes. The key novelty introduced by this methodology is that it explicitly addresses the scheduling, design and control simultaneously while taking into account the influence of process disturbances and uncertainty in the parameters, which aims to represent the actual operation of these processes. The process disturbances are specified as sinusoidal signals at critical frequency, which are determined via frequency response analysis. The uncertainty in the parameters has been addressed via multi-scenario approach, where critical scenarios were created and probability of occurrence was assigned for each of them. Another feature of study is in terms of smooth transitions between different product grades. Ramp functions have been used for the transition and the slopes of these ramps which determine the rate of transitions were part of decision variables. Two case studies were developed with first case study focusing in the comparison of a semi-sequential approach to the simultaneous methodology developed in this work for the integration of scheduling, design and control. The improved results obtained from the simultaneous methodology in this case study demonstrate the need of integration of scheduling, design and control. The second case study tests the capability of the methodology in the application of larger non-linear process. This case study is larger in size and requires larger computational time, where solutions are generated in approximately 8 hours. The results from the case studies show that the methodology developed in this work is a practical approach that can integrate the scheduling, design and control aspects of the large multi-product processes.

5.2 Recommendations

The research work presented in this thesis has contributed in the field of optimal scheduling as well as integration of scheduling with design and control. The work can be further extended in several ways which involves working on the assumptions considered during the development of this work as well as taking into account some new factors. The following text discusses the possible way forward in the presented work.

- **Optimal Scheduling in an Analytical Services Industry**

  The case studies presented in the Chapter 3 have demonstrated the potential of the scheduling algorithm developed in this work; however, there is scope to extend the work to address several factors that are present as operational characteristics of the analytical services industry. These characteristics include uncertainties in processing times, resource availability and account for re-analyses. The uncertainties can be addressed using stochastic programming techniques. The investigation of the uncertainties present in historical data can be the first step towards developing a formulation that can handle uncertainty in the process. The identification of the distribution that may possibly describe the uncertainty present in processing times or availability of resources can be very useful in this regard. As described in Chapter 3, one of the assumptions made is same characteristics for all the resources, i.e., all resources for a process have the same formulation which requires further investigation in the available literature with similar capacities. In an actual analytical service facility, resources having different characteristics may be used and therefore, there is a need to investigate further in order to make the algorithm robust. The size of the problem considered in this study is fairly large involving 8,256 decision variables for location of samples per day and 304 decision variables for the resources, therefore, techniques can be employed/ developed in order to control the problem size. One of the methods to do this may be the development of a continuous time applications. Furthermore, another potential extension to the current work may be personnel reallocation. As the analytical services industry involves several processes which require different skills to operate the available machinery/programs, there is dedicated group of operators to work on each process, while there may be human resources possessing multiple skills to work on different processes. The scheduling problem can be augmented with the decisions on human resources (labor) available to operate various machines as per the availability of the work staff. This feature can potentially be developed considering multiple skill sets of the staff in order to address the optimal assignment of tasks. However, development of these features may add extra complexity to the existing problem and increase the computational costs associated with it.

- **Integration of Scheduling, Design and Control for Multi-product Processes**

  The methodology developed in this work and that was successfully tested with a CSTR case study has demonstrated the advantages of the simultaneous methodology over the semi-sequential approach, while a larger case study with HIPS process proved the applicability of the proposed methodology to a larger problem. Although, the features developed as parts of the methodology depict its importance, several factors can be considered in the future path of this work. In term of process disturbances, the methodology can be tested with specification of disturbances with functions other than sinusoid so as to increase the applicability of the methodologies to the processes with disturbances following different distributions/functions. Uncertainty considered for the case studies was limited to product demands, while in actual processes the uncertainty is also present in different parameters, which may include reaction parameters, heat transfer parameters, etc. Another area that can be considered for potential extension is the control scheme. The case studies developed within this work only considered traditional Proportional-Integral (PI) controllers, while the methodology can be further tested using advanced control schemes like Model Predictive Control (MPC). Another potential extension to this study is accounting for structural decisions in the process/control schemes.

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Appendix (A)

The content of Chapter 3 has been accepted for publication in the Industrial Engineering & Chemistry Research Journal [109]. The author of this thesis is the first and main author of this publication and contributed all the technical aspects of the work as well as writing the manuscript.