DESIGN AND OPERATION

of

PROCESS SUPPLY CHAINS UNDER UNCERTAINTY

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Shailesh Patel, M.Tech. (Chemical Engineering)

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Author:	Shailesh Patel, M.Tech. (Chemical Engineering)
	Indian Institute of Technology - Bombay, Mumbai, India
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Department:	Chemical Engineering
Supervisor	Dr. Christopher L.E. Swartz
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To my Spiritual Guru, H.D.H. Hariprasad Swami, for his selfless love, and guidance

Abstract

This thesis deals with the problems of design and operation of process supply chains. Process supply chains face many challenges due to volatile market conditions, production and transportation delays, and stiff market competition, which ultimately affect their profitability. Supply chain management (SCM) is the process of managing the flow of materials and information within supply chain to optimize the SC performance. SCM is carried out using a hierarchical decision-making framework, where the top most layer looks at network design and the bottom-most layer deals with scheduling day-to-day activities. In this research, the systems engineering principles are applied to devise an improved methodology for supply chain optimization (SCO).

First we consider, the design of supply chain in the presence of demand uncertainty. The representation of network topology plays an important role in deriving the optimal network design. In real practice, the shipping cost for transferring goods from one location to another is determined based on service time and quantity. More importantly, the cost associated for establishing a transportation linkage is relatively small for existing transportation infrastructure, and can be changed if beneficial. The flexibility of changing the transportation routes is included in the network topology representation by the explicit inclusion of time limited transportation contract agreements. Further, the customer demand is volatile and it is very difficult to predict accurately. To handle the demand uncertainty, a two-stage stochastic programming formulation is applied in the SC design approach.

Next, we consider the problem of handling uncertainty in SC planning by applying a system engineering control principle, robust model predictive control (MPC). The uncertainty in model parameters (yield) and demand are captured by stochastic programming. In this approach, the planning activities are represented by a hybrid model with decisions governed by logical conditions/rulesets. An MPC based rolling horizon control framework is used to schedule the planning activities, where the SC performance is expressed using a multi-criterion objective comprising customer service and economics. The uncertainty in demand and yield are propagated by two mechanisms - an open-loop approach, and an approximate closed-loop strategy.

Finally, we consider the problem of integration of SC planning and scheduling. Due to

the use of different time scale models for planning and scheduling, the decision derived at the planning layer may result in infeasibility when those targets are implemented at the scheduling level, which ultimately affects the supply chain efficiency. To address this issue, we model tactical and operational planning activities using an integrated hybrid time modeling approach in which the first few planning periods are formulated using an operational planning model and the remaining time periods are modeled with a tactical planning model. The main rationale for formulating an integrated model is that customer demand forecast becomes less accurate for a future time, therefore making a detailed planning model unnecessary. A key benefit of using a hybrid modeling approach is that it avoids the problem of infeasibility encountered in the hierarchical decision framework, as well as the computational burden associated with the use of a detailed planning model over a long time horizon. We employ an MPC based rolling horizon framework as a tactical decision policy where the integrated model is used to predict the system behaviour.

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Shailesh Patel

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CHAPTER 1

Introduction

In this chapter, we provide a brief overview of supply chain systems and supply chain optimization, which forms the basis of our research work. Next, we give the thesis outline.

1.1 SUPPLY CHAIN SYSTEM

A supply chain (SC) system is a network of suppliers, manufacturing facilities, distribution centers, and retailers and/or customers. The main goal is to achieve high customer satisfaction at low cost. In order to achieve this goal, SC systems perform various functions. The retailer senses customer demand which is transferred to the manufacturing facility via distribution centers. Upon receiving order information, the manufacturer places orders for raw material to suppliers. After receiving raw materials, the manufacturer produces and delivers products to customers through a distribution channel. Thus, the *material* flows from supplier to customer and demand *information* flows in the opposite direction. The tighter integration of the flows of material and information can help to optimize the SC system performance (Beamon, 1998). Figure 1.1 shows the basic activities performed in supply chain management (SCM). These activities can be grouped into three processes: (1) production scheduling and inventory management, (2) production planning, and (3) distribution & logistic management. The *production scheduling and inventory management* comprises the management activities for production scheduling, raw material purchase, and material storage and handling within production network. The *production planning* handles the activities for production and storage facility like production allotment to site, material transfer between the production network and storage facilities, and inventory management. The distribution and logistic management manages the material transportation activities from storage facility (e.g. warehouse) to customer.

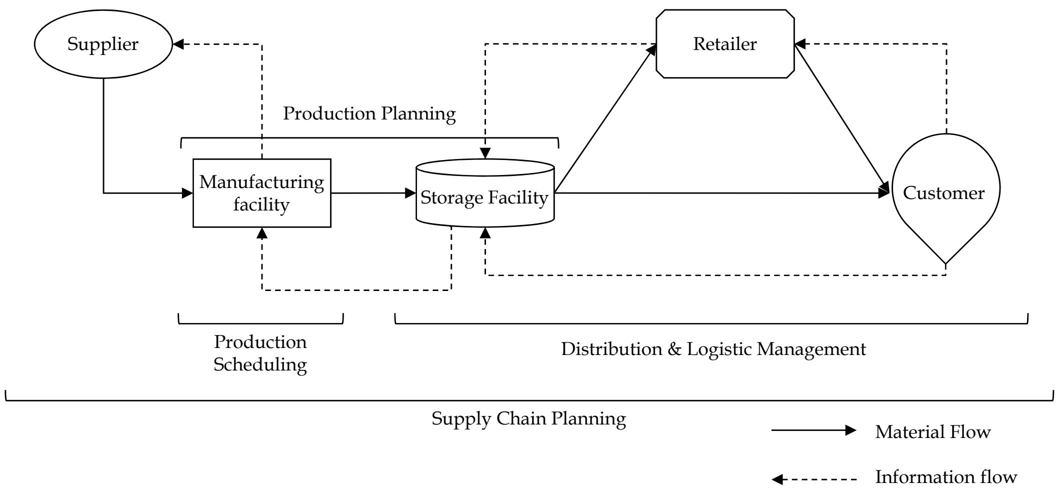

Figure 1.1: A process supply chain. The schematic shows the activities performed in supply chain management.

To achieve the best performance from the system, the material and information flows should be passed efficiently, ideally instantaneously. The material can not flow instantaneously but the information can be passed with negligible delay *theoretically* (Naylor, Naim, and Berry, 1999). Although it appears that the information can flow instantaneously, sometimes it is not possible to achieve due to inherent characteristics of a process system. Another way to achieve higher customer satisfaction is to ensure product availability at all time (Christopher and Towill, 2001). Knowing the customer demand a priori, arrangements can be made to hold sufficient inventory to fulfill customer demand. However the main impeding factor is the demand forecast. Demand prediction is a very involved process because of several reasons, such as market competition, new product introduction, varying product life cycle etc. Therefore in practice, the goal of a SC system is to produce the finished product and deliver it to the customer in minimum time and cost. Thus, the performance of the SC system is generally measured in terms of customer satisfaction, operational cost and lead time, the time duration between when the raw material enters the system and leaves as product from the system.

1.2 SUPPLY CHAIN OPTIMIZATION

The process industry plays an important role in the world industrial economy. In the last decade, the sales of chemicals more than doubled and hit a record 5.4 trillion USD in 2014. In U.S. alone, the chemical process industry had an output of 800 billion USD (America Chemistry Council Inc, 2016). Emerging economies are driving a major share of this growth. In other words, the market has become global and companies must act globally to remain in business. Such global manufacturing and distribution supply chains are constantly seeking to improve efficiency (in terms of lowering operation cost and increasing customer satisfaction). For achieving the *best* performance in such a global market, industries need to change their strategic thinking to, (1) re-define their business model and (2) re-structure manufacturing and transportation activities. The very first step is to identify their supply chain, who the stackholders are and stages of operation (*nodes*); the goal of achieving a greater efficiency can be fulfilled by effective coordination among stakeholders, optimal use of infrastructure and resources allocation. Towards achieving this goal, the concept of supply chain optimization (SCO) has been developed (Grossmann, 2005; Shah, 2005).

The mathematical structure of a supply chain optimization problem considered in this research work can be represented by following general form,

$$\begin{aligned} \min_{x,y} \quad & f(x,y) & \\ s.t. \quad & h(x,y) & = 0 \\ & g(x,y) & \leq 0 \end{aligned} \tag{1.1}$$

where $x \in \mathbb{R}^p$ is vector of continuous variables and $y \in \mathbb{R}^q$ denotes a vector of integer variables. $f(x,y)$ is the objective function written in terms of continuous and integer variables. $g(x,y) = 0$ are equality constraints and $h(x,y) \leq 0$ are inequality constraints. In supply chain optimization, the objective function typically consists of an economic term, reflecting the infrastructure and operating cost and sales. The equality constraints are comprised of a system of governing equations such as material balances, while system feasibility and specifications are written in the form of inequality constraints. Depending on the presence of integer variables and type of equality and inequality constraints, the formulation (1.1) yields a linear programming (LP), non-linear programming (NLP), mixed-integer LP, or mixed-integer NLP problem.

SCO activities are traditionally carried out in a hierarchical decision framework (as shown in Figure 1.2). The top most layer takes care of managing long term activities like supply chain network design and strategic planning. The term network design is very broad and it refers to any strategic activities which involve decisions such as deciding the location of facilities (manufacturing and storage), retrofitting of existing facilities, and allocation decisions (the products to be produced at each location, allocating suppliers for each manufacturing location). A typical time frame involved here is of the scale of months to years. The models are employed to evaluate trade-offs that exist in (1) regional production costs, (2) tax structure and custom duties, (3) complexity of manufacturing processes and transportation, and (4) network structure. The supply chain planning (SCP) comes beneath the design layer. It mostly concerns setting up the medium to long term activities (time frame of a few weeks to months) such as the amount of product produced at each manufacturing plant, the inventory level of each material, level of safety stock, and transportation amount across network nodes. The inputs at this layer comprise of long term demand forecast, long term plant maintenance schedule, production capacity of manufacturing plant(s), the storage and transportation capacity of each network node and node linkages. These decisions are then forwarded to production scheduling layer which refines these decisions considering real time availability of resources and optimally allocates resources to adhere to the production policy decided at the upper layer. The production scheduler works on a time scale of few hours to days.

For supply chain design, many mathematical models have been proposed in the literature with their implementation often relying on the concept of a *rigid* node structure, having certain restrictions on material flow between SC echelons, partly to build tractable optimization problems for a real time application. However, the use of such a *rigid* structure in the design stage results in a lower net present value (NPV) mainly due to limited number of choices given to an optimization problem to explore the profitable space. The problem becomes identifying the optimal location of facilities (manufacturing and storage) and deciding the optimal connectivity between adjacent network nodes. A key contribution of this research is to accommodate time-limited transportation contracts in a SC network design problem to search for a better design and therefore improving the economic performance.

System uncertainty is one of the main important aspects to be considered in SCO. Customer demand and other system parameters (e.g. process yield, machine downtime, transportation time) can not be predicted accurately. Satisfying customer demand is one of the main goals of any supply chain system and thus it should be handled efficiently and appropriately. Many optimization formulations have been discussed in the literature to handle the uncertain parameters in SCO. Among them, two-stage stochastic programming

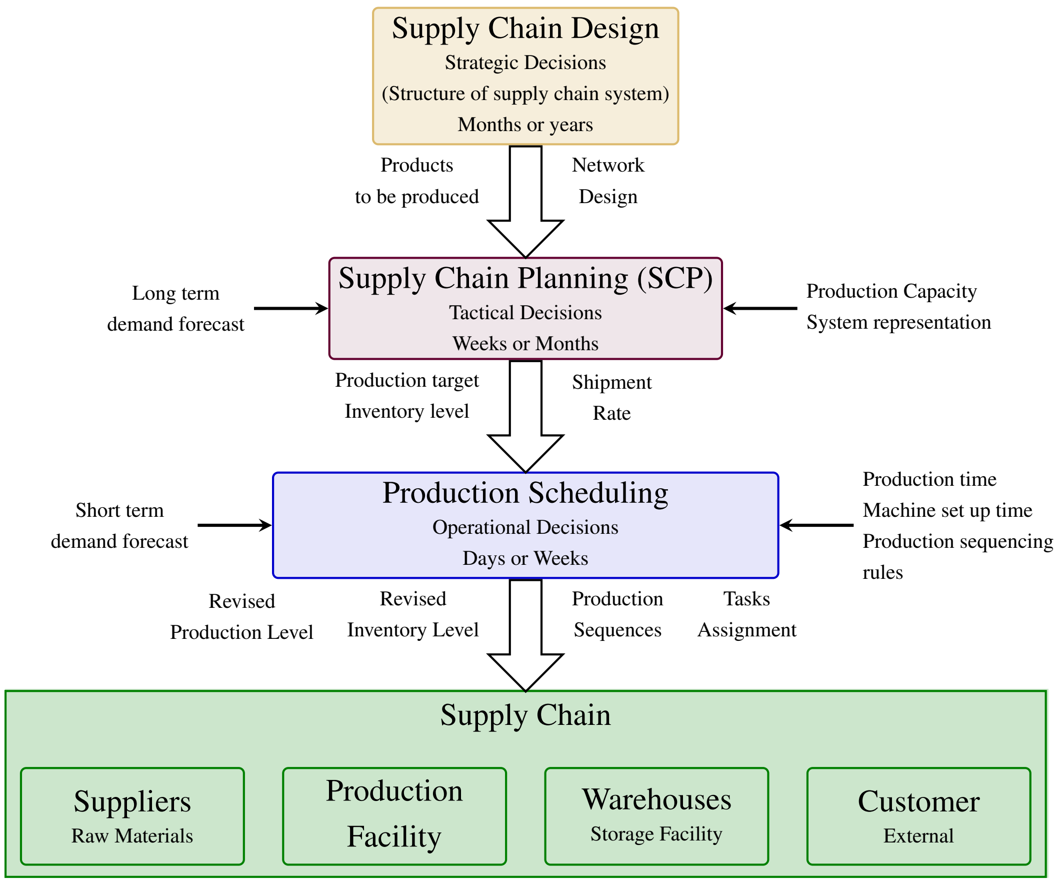

Figure 1.2: Hierarchical decision framework for supply chain optimization

is the most commonly used method to represent demand uncertainty. A scenario based two-stage stochastic programming formulation is used to handle demand uncertainty in the SC design problem. Further, we combine two-stage stochastic programming with a Model Predictive Control (MPC) framework to devise a novel robust-MPC formulation to include the effect of uncertainty in the supply chain planning. A multi-objective optimization problem is formulated for production scheduling of a hybrid supply chain system.

Another problem faced in SC optimization is the coordination among different layers. As discussed previously, a SCO framework considers manufacturing and distribution activities with ranges from hours to years. Each level concentrates on a different time range and therefore it demands use of a different time scale model at each level. However, consideration of different time scale models introduces model inconsistency and therefore decisions derived at upper layer may become sub-optimal or infeasible at the lower layer. While there has been significant work on coordinating these layers, incorporating scheduling information back to the planning level has not gathered much research attention.

Feedback control commonly used in systems engineering, can be utilized to address some of these problems. In this work, we combine two different time scale models, a coarse time-scale tactical planning model and a fine time-scale operational planning model, in an integrated model to address the issue of coordination between planning and scheduling layers, and apply an MPC based rolling horizon decision framework to schedule detailed production and shipment activities.

1.3 THESIS OUTLINE

This thesis is organized in the following chapters.

Chapter 2 – Fundamental concepts: The important concepts and techniques used in supply chain optimization are outlined. We also provide a brief review of each of the aspects, such as supply chain modelling, model predictive control, uncertainty handling.

Chapter 3 – Supply chain design: An approach is presented to design a flexible supply chain network in the presence of demand uncertainty. A network superstructure, i.e. a topology which defines the network nodes and their connectivity, is created where all possible network nodes and their connections are included. A mathematical characterization of a SC design and planning system is developed where time-limited transportation contracts are explicitly included using a novel formulation. Uncertainty in the demand prediction is captured with the use of a scenario representation and two-stage stochastic programming applied to handle the uncertainty. An integrated optimization based approach is formulated for a dynamic discrete time multi-period stochastic MILP model to design a flexible SC network and applied to an industrial case study.

Chapter 4 – Robust control framework for SC Planning: An optimization-based decision support tool is presented for SC planning using a robust MPC strategy. The proposed formulation: (i) captures uncertainty in model parameters and demand by stochastic programming, (ii) accommodates hybrid process systems with decisions governed by logical conditions/rulesets, and (iii) addresses multiple supply chain performance metrics including customer service and economics, within an integrated optimization framework. A nuance in this work is the application of a stochastic forecasting model for generating scenarios to capture demand uncertainty in the optimization formulation. The developed robust framework is applied for the control of a multi-echelon, multi-product supply chain. Additionally, an approach is proposed to reduce the conservativeness of open loop decision making under uncertainty, by approximating the future closed loop prediction of uncertainty propagation with two- and multi-stage stochastic programming.

Chapter 5 – Integrated supply chain planning & scheduling: An integrated hybrid time modeling approach is proposed to characterize tactical and operational planning activities in one mathematical model. The first few planning periods are formulated using an operational planning model and the remaining time periods are modeled with a tactical planning model. A benefit of using a hybrid modeling approach is that it avoids the problem of infeasibility encountered in the hierarchical decision framework, as well the computational burden associated with the use of a detailed planning model over a long time horizon. Further, we employed a model predictive control (MPC) based framework for decision making where the integrated hybrid time model is used to predict the system behaviour and the decisions are implemented in a rolling horizon fashion.

Chapter 6 – Conclusions and Recommendations: The contributions of the research work are summarized and future extensions are presented.

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CHAPTER 2

Fundamental Concepts in Supply Chain Design and Operation

The intent of this chapter is to provide a brief introduction to fundamental concepts used in the research work.

2.1 SUPPLY CHAIN DECISIONS

The problem of supply chain design and operation involves decision variables pertaining to network topology and its operation. The decision variables are those variables which can be adjusted to alter the system behavior in order to achieve desired performance. Thus, the SC performance is constrained by a range of decision variables where they can be changed. Supply chain design and operation decisions can be mainly categorized in two main groups, (1) network decisions, and (2) operational decisions.

1. Network decisions (static): location of facilities (production plants, warehouses, etc.), changes to existing infrastructure (expansion or closure of existing facilities), supplier selection etc.
2. Operational decisions (dynamic) : Production allocation (what products to be produced at each manufacturing location, transportation network selection, production or transportation capacity of each facility, production planning and scheduling,

inventory level of materials across network, transportation amount within supply chain.

The first set of decisions can be changed but not that frequently and thus referred as static decisions. The operational decisions are dynamic and updated at regular time intervals. As process supply chains become global, many trade-offs exist which can be exploited to take advantage in cost reduction. These can be; (1) differences in production and transportation cost, (2) differences in raw materials and product cost, (3) different income tax structure, (4) network flexibility for producing different products etc.

2.2 PERFORMANCE MEASURES

Formation of a performance measure is an essential part in supply chain design and analysis. A performance measure provides a basis to determine the system performance and identifies the best practice. Further it provides a comparison between alternative systems. The performance measured, described here, can be categorized as a qualitative or qualitative measure[1]. The performance of a supply chain can be represented by a single indicator (single-objective SCO) or combination of them (multi-objective).

Cost measure: It is the most commonly used objective in supply chain optimization. It can be presented in various ways; cost minimization, profit maximization, net present value (NPV) maximization, revenue maximization.

Customer satisfaction: It is a qualitative measure by nature and it can not be accurately quantified. However, some of its aspects can be defined and measured (Perea et al., 2000). Typically in supply chains, customer satisfaction is defined as the percentage of orders filled on time.

Flexibility: Flexibility is the ability of the system to withstand demand fluctuation and other parameter variation. Various indices and mathematical expressions are proposed in the literature to represent the SC flexibility (Slack, 1987; Das and Abdel-Malek, 2003; Wang, Mastragostino, and Swartz, 2016).

Responsiveness: SC responsiveness is a measure of how rapidly a process supply chain adapts to a changed condition (typically customer demand). The responsiveness objectives are typically presented as lead time minimization or make-span minimization. The lead

[1] A thorough classification of supply chain performance measures is provided in Beamon (1998)

time is the time difference between when a material enters a supply chain and leaves as a product from a warehouse to satisfy customer demand (Christopher, 2000). A SC with long lead time indicates low responsiveness and vice-versa. The *bullwhip effect* is one of the well-known phenomena seen in supply chains and is generated due to information delay, and is related to how responsive a supply chain is.

Environmental measures: Chemical production systems have a high impact on the environment and, due to tightened regulation it has become important to include environmental concerns in supply chain design (Hugo and Pistikopoulos, 2005). Cano-Ruiz, and McRae (1998) have provided a thorough review on including environmental damage in process design objectives and have shown that, inserting environmental considerations in the design approach yields design alternatives having improved environmental and economical performance. The objective here is to balance the environmental damage against cost saving to design a *green* supply chain which has a low impact on the environment.

2.3 SUPPLY CHAIN MODELING

Supply chain modeling is an activity to represent the structure and operation of a supply chain in a mathematical form. Essentially, it is the set of mathematical equations describing the underlying relationships (e.g., equalities, inequalities, logical conditions) between system variables. These relationships are an abstraction of the real system. The mathematical relationships are mostly algebraic due to a discrete time analysis and can be linear or nonlinear. Based on the type of relationships, the resulting model becomes linear programming (LP), or non-linear programming (NLP) and the presence of integer variables makes them mixed-integer models.

Considering various modeling attributes, supply chain models can be categorized in many different ways (see Figure 2.1). Based on the time attribute, they can be categorized as, (1) *steady state* models, and (2) *dynamic (multi-period)* models. The steady state model assumes steady-state behavior (state of equilibrium) and activities are defined using algebraic equations. For example, the inventory balance equation for a warehouse can be written as the difference between the total mass of material entering a warehouse and leaving it remaining constant and is given by the inventory level. The dynamic model considers process dynamics over time and is referred as multi-period models in supply chain literature. Here, the total time horizon is partitioned into several intervals and each time interval is modeled using steady state models. The time intervals (or time periods) may have demand due dates at future times.

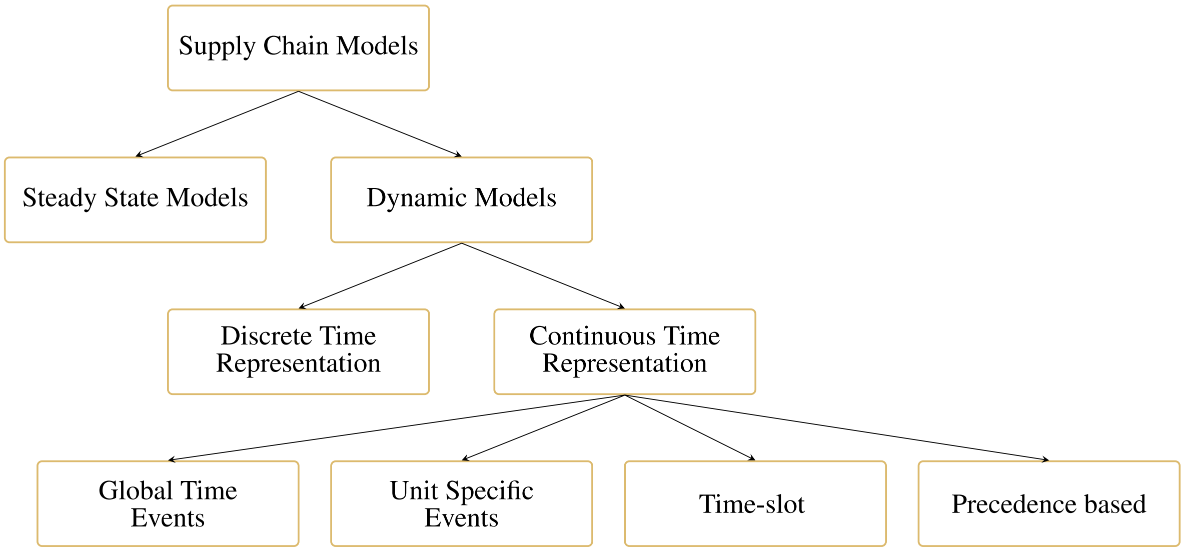

Figure 2.1: Classification of supply chain models

The individual time periods are then connected by formulating dynamic time balance constraints, hence constitutes dynamic models. In multi-period modelling, the most important aspect is time representation. Depending on whether the activity (task) can start at some predefined time or at any moment during the time horizon, modeling approaches can be classified into *discrete* and *continuous time* formulations. In the discrete time formulation, the time horizon is divided into a finite number of intervals of equal or unequal time duration. The task can start or end at beginning or ending of these time periods. Therefore, various activities have to be aligned only at predefined time points.

The fixed time grid formulation makes it simple to represent time dependent activities without changing the structure of the system model. The formulation converts the original problem into pure allocation problem which makes the model structure simpler and easier to handle and thus results in a less complex optimization problem. The number of optimization variables is dependent on the number of time intervals. For a more accurate representation, ideally the length of time intervals should be small so that it can capture required details of the system. However, a small time interval leads to a high number of time periods and eventually generates an optimization problem with a large number of decision variables. The large size makes the problem difficult to solve. Larger time intervals lead to a coarser representation of the system and may lead to sub-optimal or even infeasible solutions. In other words, the size of problem and computational efficiency strongly depend on the number of time intervals. In order to keep the computational complexity low, generally a smaller number of time intervals is used in problem formulations.

In continuous time representations, which are more typical of scheduling than SC formulations, timing decisions are expressed in the form of events. Additional constraints are introduced to define the relationships between these events i.e. when an event can start and end. The variable duration of events can help to generate more flexible models. However, the declaration of activities at these variable time duration events requires more complicated constraints, which makes the model definition relatively hard and leads to complex optimization problems. Moreover, it also requires one to declare the number of time events for given time horizon, which may not be intuitive. The declaration can be avoided by treating it as an additional optimization problem. In this case, the problem has to be solved many times for different values of event points which will again increase the computation load.

Based on the events arrangement, continuous time formulations can be again classified into four classes (Méndez et al., 2006): (1) global time events formulation defines a common time grid across all resources, (2) unit specific time events defines a variable time grid for all resources, (3) time slot formulation sets predefined time events with unknown durations, and (4) precedence rule based formulation employs sequence dependent rules to define the system.

In another classification, the models can be categorized as a deterministic or stochastic. Deterministic models are built on the assumption that all model parameters and inputs are known, whereas stochastic models consider the uncertainty. Depending on the way of incorporating uncertainty in the model, different solution techniques are used. This is discussed further in Section 2.5.

Having presented the general classification of SC modelling approaches, here we discuss the modelling of some of the specific aspects of SC systems.

Network node connections: The node connections define the structure of a supply chain. The mathematical definition of node connections decides the structure of the resulting mathematical problem, which ultimately has a direct impact on solution techniques used to solve an optimization problem. In a supply chain design problem, the facility allocation decisions are defined using binary decision variables, with 1 representing the allocation of a facility (such as a plant, warehouse or retailer) at a given location. Similarly, the connection structure is also formulated using binary variables in most cases. However, the node connectivity can be defined based on facility allocation variables, and in that case the model does not need explicit definition of node connections. Nonetheless, both cases contain binary as well as continuous variables, hence the resulting model structure becomes mixed integer linear program (MILP) or mixed-integer non-linear program (MINLP) depending on the type of system constraints. The presence of binary variables makes the problem non-convex, and therefore far more difficult to solve. The complexity of a mixed-integer programming problem is NP-hard as a large number of possible combinations of integer variables need to be explored to prove optimality. However, careful formulation of the model can result in a tight formulation which significantly decreases solution times. Moreover, recent advancement in computational resources has also contributed solving mixed-integer programming problem in a reasonable time (Lima, and Grossmann, 2011).

Inventory management: Managing inventory plays a crucial role in optimizing the SC performance. Forrester (1961) proposed an inventory control structure based on system dynamics. Inventory is generally kept in two forms, (1) working inventory and (2) safety stock. The safety stock is the buffer amount which is stored in the network to offset the effect of demand uncertainty and increases the SC responsiveness. The working inventory is the amount that is being processed in the system.

In *periodic review based stock policy*, the inventory level is reviewed at the start of each review period and an order is placed for the material to maintain the *base stock*. In a *risk pooling policy*, the safety stock is decided for given service level for all retailers and a single quantity is ordered. A *guaranteed service approach* is used for multi-echelon inventory systems[2] and works on the concept of service time[3]. The inventory level is calculated based on guaranteed service time of the network and orders are placed to manage the inventory[4]. In other approaches, inventory balance constraints are formulated using mass balance equations and optimum inventory levels are calculated from an optimization problem. The mass balance equations can be written as steady state or dynamic time balances. In a dynamic inventory balance, the inventory levels of two time periods are correlated. In the static case, the inventory level is individually optimized at each time period.

Operational (scheduling) activity representation: The supply chain operation activities are formulated using basic governing equations, such as mass balances, capacity constraints, etc. These relationships are written for each node of a network.

[2]A system where the inventory stored at more than one location
[3]The time by which the demand will be fulfilled
[4]A detailed review on inventory management policy is provided in You and Grossmann (2010)

For production nodes, the operation (scheduling) constraints[5] are formulated using two main categories. In the first category, the production scheduling activities are defined using production environments of single-stage, multi-stage, or multi-purpose production. In single-stage production systems, materials go through a single stage production unit and mass balance, production allocation, unit allocations constraints are defined. In multi-stage production, materials are converted to final products through a set of intermediate products, however all material passes through each stage. In multi-purpose production systems, materials pass through only specific stages.

In the second category, the production system is represented either by the state-task network (STN) (Kondili, Pantelides, and Sargent, 1993) or the resource-task network (RTN) (Pantelides, 1994) concept. STN is a directed graph that consists of three key elements: (1) *state nodes* representing feed, intermediates, and final products; (2) *task nodes* representing the process operation which transforms material from one or more input states into one or more output states; and (3) *arcs*, that link states and tasks, indicating the flow of material. It assumes that a processing task produces or consumes states (materials). State and task nodes are represented by circles and rectangles respectively while arcs are represented by arrows. In contrast, the RTN representation gives uniform treatment to all resources (materials and manufacturing resources). The concept is that both processing and storage tasks can consume and produce resources at their beginning and ending times respectively. Thus circles are not only states but they also represent other manufacturing resources (e.g. storage tank).

2.4 MODEL PREDICTIVE CONTROL

Supply chain systems are constantly impacted by disturbances and therefore continuous adjustments should be made to alleviate the effects of disturbances. These effects can be long-term or short-term and require updating strategic, tactical, or operational decisions. Close observation reveals that the problems faced in systems engineering and supply chains are similar in nature. Hence, the theory of optimal control can be applied to harness the benefits of optimal control in supply chain systems. Control theory provides insight to formulating the supply chain problem in mathematical language and helps to design a control structure to circumvent the problems faced by the supply chain system. Due to development of control theory and availability of advanced computational resources, application of many advanced control technologies to supply chain systems becomes more

[5]Harjunkoski et al. (2014) have provided a through review on production planning models

manageable, making it possible to solve the high dimensional supply chain problem in real time. Therefore the interest of the process systems engineering community in supply chain systems is growing rapidly (Perea-López, Ydstie, and Grossmann, 2003; Braun et al., 2003; Bose and Pekny, 2000; Li and Marlin, 2009). The unique hybrid nature (presence of discrete decisions) of supply chain systems makes it a distinct case from general system engineering processes and hence needs special attention, like tailored optimization techniques and solvers for handling mixed-integer programming problem, and model representation to make it suitable for applying advanced control algorithms. In addition, a supply chain system is impacted by unknown disturbances in terms of demand uncertainty. Model predictive control (MPC) is a widely used technology to implement advanced control in process industries and can be used to improve SC planning. The SC decisions can be revised in a rolling horizon fashion using the most recent state of the SC system.

Due to its inherent multivariate nature, ability to handle system constraints, and rolling horizon formulation, MPC has become a preferred advanced control technique in the process industries (Qin and Badgwell, 2003). In MPC, the calculation steps described below, are repeated at each time period once a new measurement (or information) becomes available.

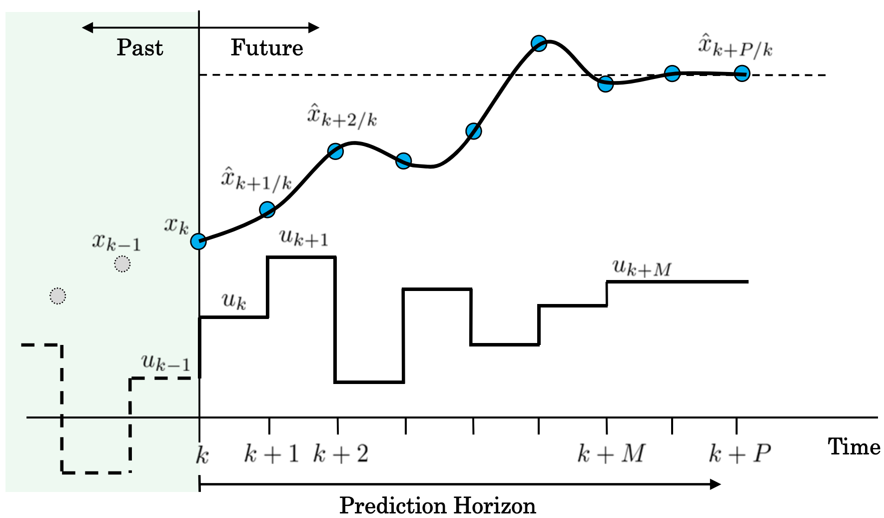

Figure 2.2: Schematic shows the MPC control calculation steps.

1. *Initialization*: The system model is initialized using the system's initial condition (denoted as x_k in Figure 2.2).

2. *Trajectory calculation*: A dynamic optimization problem is solved at each time

period to compute optimal trajectories of control variables by optimizing an objective function while satisfying process constraints. The system model is used to predict the system behavior over a prediction horizon (P). Common examples of process constraints are those that arise from the physical description of system. Any objective function described earlier can be used in the optimization problem.

3. *Implementation*: Only the first control input (denoted by u_k) is implemented and the optimization problem is solved again at the end of the control interval for a new horizon advanced by one time increment.

In supply chain applications, the process model may be linear or nonlinear, and contains both binary and continuous variables or only continuous variables. The presence of mixed-integer variables makes the optimization problem more complex and computationally intensive. The objective function is largely economic and linear in terms of decision variables, hence LP, NLP, MILP, or MINLP solution techniques need to be applied in solving the MPC optimization problem.

2.5 OPTIMIZATION UNDER UNCERTAINTY

Optimality of the decisions derived from an optimization problem is highly dependent on the accuracy of the system characterization used to predict its behavior and its parameters. It is often difficult to accurately estimate or forecast process characteristics and process parameters. In such scenarios, the best possible thing to do is to embrace the impact of uncertainty in the decision making process. The presence of uncertainty affects optimality and sometimes causes infeasibility issues. The aim here is to optimize the expected value of the objective function value for an assumed level of uncertainty (Stochastic Programming Community Home Page, 2016). The source of uncertainties can be classified into four major classes, (1) process inherent uncertainty (such as processing time, yield); (2) model uncertainty (such as mismatch in model parameters); (3) external uncertainty (such as demand, prices); and (4) discrete uncertainty (such as equipment availability).

Uncertainty[6] information can be included in the optimization problem as, (1) bounded form describing uncertain parameters by an interval; (2) probability description using a probabilistic model to represent parameter uncertainties; and (3) fuzzy description that formulates uncertainties by fuzzy set theory. Based on how the uncertainty is described

[6] An overview on theory and methodology for formulating and solving optimization problem under uncertainty is provided in Sahinidis (2004).

in the optimization problem, the solution techniques can be classified into (1) stochastic optimization, (2) robust optimization, (3) fuzzy programming, (4) sensitivity analysis, and (5) parametric programming.

In stochastic optimization, a deterministic model is transformed into a stochastic model by treating uncertain parameters as stochastic variables. In this type of approach, the objective function is set as the expected value of a certain performance criterion with respect to stochastic variables.

The stochastic variables are defined using discrete or continuous probability distribution functions. Based on the type of uncertainty representation, stochastic optimization methods are classified into, (1) scenario based approach (two-stage or multi-stage programming), and (2) probabilistic optimization. The first approach utilizes a discrete probability distribution where the uncertainty space is discretized using sampling techniques, such as Monte-Carlo sampling, to sample random instances of stochastic variables (scenarios). In two-stage optimization, decisions are divided into *first stage* decisions (*here-and-now*) and the *second stage* decisions (*recourse actions*). The first stage decisions are decided before actual realization of uncertain parameters and recourse actions can then be made in the second stage to compensate for the realized uncertainty. Mathematically, a linear two-stage stochastic programming problem is written as follows (Birge and Louveaux, 1997),

$$\begin{aligned} \min_{x} \quad & c^T x + \mathbb{E}_P[Q(x, \xi)] \\ s.t. \quad & Ax = b \\ & x \in \mathbb{X} \end{aligned} \tag{2.1}$$

where, $Q(x, \xi)$ is the optimal value of the second-stage problem,

$$\begin{aligned} Q(x, \xi) := \min_{y} \quad & q^T y \\ s.t. \quad & Wy = h - Tx \\ & y \in \mathbb{Y} \end{aligned} \tag{2.2}$$

where, x and y denotes the *first-stage* and *second-stage* decisions respectively. ξ is the vector formed by the components of q^T, h^T, and T. Both *first* and *second* stage decisions include integer and continuous variables. The set $\mathbb{X}$ and $\mathbb{Y}$ include both real and integer numbers. The problem (2.1) minimizes the *first-stage* cost ($c^T x$) and the *expected* cost of the *second stage* ($\mathbb{E}_P[\cdot]$). In supply chain network design problems, second stage variables are mostly operational decisions and hence continuous variables. Therefore problem (2.2) involves minimizing convex objective function with mixed-integer constraints (Shapiro, Dentcheva, and Ruszczynski, 2014). A two-stage stochastic programming can be extended to a multi-stage programming by considering more stages. At each stage, part of the decisions are made based on the previous stage decisions and uncertain parameter realization occurs at that stage. In a scenario-based approach, the computational load increases substantially with the number of uncertain parameters. If the underlying distribution of uncertain parameters is continuous and can not be approximated by discrete scenarios with sufficient accuracy, the constraints with uncertain parameters can be expressed as probability constraints; the probability of satisfying the constraint is less than or equal to a specified confidence level. These probabilistic constraints are then transformed into deterministic constraints with the use of a probability distribution function (e.g. chance constrained programming). The approach maintains the model size but it is often difficult to solve due to the numerical integration of the probability distribution function which is typically nonlinear.

Robust optimization finds a solution which is robust to the given uncertainty. It describes uncertain parameters through a bounded form formulation. The major distinction between robust optimization and stochastic programming is that in robust optimization no assumption is made regarding the probability distribution of the uncertain parameters. Worst case optimization is a class of methods which handles the parameter uncertainty by considering worst-case values of the uncertain parameters.

Fuzzy programming methods are used when uncertain parameters are described based on a fuzzy description. Constraint violations are allowed and the degree of satisfaction is defined through a membership function. Sensitivity analysis is used to check the sensitivity optimal decisions with respect to uncertain parameters. The main idea is to check the robustness and reliability of optimal solutions derived from deterministic optimization for a given uncertainty. Parametric programming is a technique for obtaining the objective function and optimization decisions as a function of uncertain parameters. The analytical solution can be calculated after actual realization of uncertainty.

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CHAPTER **3**

Flexible Supply Chain Network Design with Time-limited Transportation Contracts

The algorithm and results discuss in this chapter are published and going to appear in:

JOURNAL PAPER

Shailesh Patel and Christopher L.E. Swartz (2016). "Supply chain design under uncertainty with time-limited transportation contracts". In: *Computers & Chemical Engineering* -.-, To be submitted

CONFERENCE PAPERS

Shailesh Patel and Christopher L.E. Swartz (2012). "Flexible supply chain design under demand uncertainty". In: *62nd Canadian Chemical Engineering Conference, Vancouver*

Shailesh Patel and Christopher L.E. Swartz (2013). "Design and operation of supply chain systems under uncertainty". In: *American Institute of Chemical Engineers (AIChE) Annual Meeting, San Francisco*

3.1 INTRODUCTION

A supply chain (SC) is a network of suppliers, manufacturing facilities, warehouses and customers that involves tasks of raw material procurement, product manufacture and delivery to final customers through a channel of distribution centers. A key objective in SC management is to satisfy customer demand at minimal cost. SCs are characterized by forward flow of materials from suppliers to customers, and backward flow of information in the opposite direction. Increased competition in a global marketplace, rising raw material and utility costs, tightening environmental constraints, and increased market volatility all contribute to reduced profit margins in product manufacturing. In order for enterprises to remain competitive, it is imperative that entire SC must be considered, rather than only individual manufacturing processes. These considerations have been at the core of significant research activity in SC design and operation within the process systems engineering community over the past several years. Excellent reviews of the state of the art and challenges in enterprise-wide planning, operation, and design are given in Shah (2005), Grossmann (2005), and Papageorgiou (2009).

Supply chain decision making is typically categorized into three levels - strategic, tactical and operational - based on the time scale under consideration (Papageorgiou, 2009). SC models differ depending on the time scale of interest and the phenomena they are intended to capture, with both steady-state and discrete-time dynamic models in common use. SC studies within the process systems engineering literature are typically posed within an optimization framework, and include objectives based on economics (Tsiakis, Shah, and Pantelides, 2001; Laínez et al., 2009; Georgiadis et al., 2011), environmental impact (Hugo and Pistikopoulos, 2005; Guillén-Gosálbez and Grossmann, 2010), and risk (Gebreslassie, Yao, and You, 2012). The works cited in relation to the last two objectives utilize a multiobjective optimization framework in which the trade-off between economics and the other objective (environmental impact or risk) is evaluated. Recent studies have also included consideration of SC responsiveness (You and Grossmann, 2008a; Mastragostino, Patel, and Swartz, 2014) and flexibility (Mansoornejad, Pistikopoulos, and Stuart, 2011; Wang, Mastragostino, and Swartz, 2016). The decision space may comprise the location and capacities of manufacturing and warehouse facilities, the SC network structure, material flows between the SC nodes, provision for capacity expansion over multiple time periods, or a subset of the above. Inventories may be determined through node material balances written at each time period (Georgiadis et al., 2011; Mastragostino, Patel, and Swartz, 2014), or through empirical relationships, such as a linear relationship between the rate of material leaving a warehouse and its inventory (You and Grossmann, 2008b).

A key issue pertinent to this chapter is how the transportation links between SC nodes are handled. In many SC models, material is restricted to flow from one echelon to the next. However, some works provide for a more flexible arrangement whereby material can move between facilities within an echelon and/or between non-contiguous echelons, such as from a manufacturing site to a customer (You and Grossmann, 2008a; Laínez et al., 2009). A further consideration is the modeling of the linkages themselves and the implication thereof. Several studies include binary variables to indicate the existence of a link between nodes, with constraints that allow for material flow only if a link exists (Tsiakis, Shah, and Pantelides, 2001; Hugo and Pistikopoulos, 2005; You and Grossmann, 2008a; Guillén-Gosálbez and Grossmann, 2010; Georgiadis et al., 2011). As well, a minimum flow may be imposed in order for the link to be established. Other studies do not include binary variables for the transportation links (Guillén et al., 2005; Laínez et al., 2009; Gebreslassie, Yao, and You, 2012); these cases provide more flexibility in the optimization, but may also be unrealistic under circumstances in which there is an appreciable cost associated with the establishment of a transportation link, or when the link is subject to certain types of transportation contract. These considerations are at the core of our study.

Uncertainty in SC operation and design is addressed in many studies. Two key approaches that have been followed are the use of chance constraints and two-stage stochastic programming. In the former, the uncertain parameter is considered to be a random variable, with constraint satisfaction required to a specified probability level. Guillén-Gosálbez and Grossmann (2009) consider uncertainty in the inventories used to compute the LCA-based Eco-indicator 99 environmental metric within their SC design formulation. The environmental impact is expressed as a probabilistic constraint, which is reformulated as a deterministic constraint through use of a probability distribution function. In a subsequent contribution, Guillén-Gosálbez and Grossmann (2010) assume perfect knowledge of the life cycle inventories, but consider instead uncertainty in the damage factors used in the LCA indicator, with environmental impact formulated as a joint chance constraint. In two-stage stochastic programming, decisions are partitioned into first-stage decisions that are made prior to knowledge of uncertainty realizations, and second-stage (recourse) decisions that can be made in response to an uncertainty realization. This approach has been quite widely adopted in SC planning, operation and design. The uncertainty space is typically discretized, with a set of uncertain parameter realizations comprising a scenario. Tsiakis, Shah, and Pantelides (2001) consider demand uncertainty in a SC design formulation in which transportation links are considered as either first-stage (scenario independent) or second-stage (scenario dependent) decisions. Guillén et al. (2005) also consider demand uncertainty in a two-state stochastic programming approach in a multiobjective SC design formulation that considers objectives of NPV, demand satisfaction and financial risk. You, Wassick, and Grossmann (2009) consider uncertainty in customer demand and freight rates in SC planning. They apply a two-stage stochastic programming formulation in which production, distribution and inventory decisions for the current time period comprise the first-stage decisions, with the operating decisions for the remaining time periods constituting second-stage decisions.

In this chapter, we consider SC design under time-limited transportation contracts in which a transportation link, if selected, needs to be active for a specified minimum duration. We consider a flexible network structure in terms of allowable movement of material between nodes, and also account for demand uncertainty through a two-stage stochastic programming framework. The remainder of the chapter is organized as follows. The SC design formulation is presented in Section 3.2, which includes the handling of time-limited transportation contracts. In Section 3.3, the design formulation is applied to a case study, and the impact of different transportation link formulations on the optimal solution is explored. Conclusions are presented in Section 3.4.

3.2 SUPPLY CHAIN DESIGN PROBLEM FORMULATION

3.2.1 Overview of SC Network, Assumptions and Definitions

Figure 3.1 shows the superstructure of a SC system considered in the present work. The network consists of various nodes, such as suppliers (ls), production sites (k), distribution centers (dc), and customers (l). Each production site (k) has multiple production plants (i) to manufacture different products. These nodes are connected by transportation routes which are represented by arcs. The head of an arc shows the direction of material flow. If the material can flow in both directions, the nodes are connected by double headed arc.

The goal here is to determine the configuration of the SC network along with SC operational decisions (long term planning activities) to maximize the net present value (NPV) of the SC system. The decisions to be made are, (1) Network structural decisions : location of each manufacturing and storage facility, material transportation links to be set up and their service periods, production plants to be set up at production facilities, and production and storage capacities, (2) Operational decisions : shipment capacity for each transportation link, production rate of each product at production facilities, storage quantity of materials at each storage facility, and quantity of raw material purchased. Key features of the formulation are the incorporation of time-limited transportation contracts, use of a flexible network superstructure, and consideration of demand uncertainty through a two-stage stochastic programming formulation.

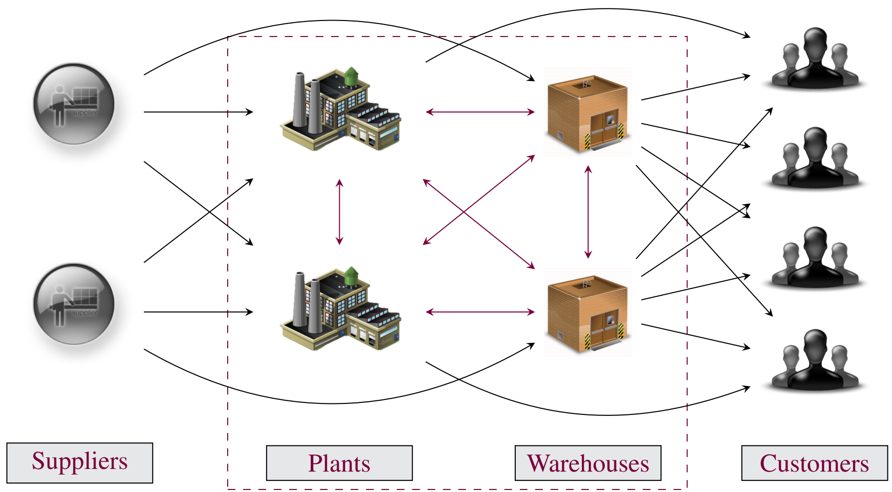

Figure 3.1: Flexible supply chain network superstructure

The production site k encloses several production plants i, which produce intermediate or final product j. If plant i is installed at site k, the binary variable $Y_{k,i}^{P}$ takes the value 1. Similarly, Y_{dc}^{DC} becomes 1, if distribution center dc is set up. The transportation link between supplier ls and plant site k is established that is $y_{j,ls,k,t}^{sp} = 1$, only if supplier ls supplies material j to site k. Shipment lanes between other nodes (plants sites, distribution centers, customers) are similarly defined to set up the material flow linkages within the network. $Q_{j,ls,k,t}^{sp}$ represents the amount of raw material j dispatched to site k from supplier ls in time period t. $W_{k,i,j,m,t}$ units of raw material j is processed at plant i of site k; $I_{j,k,t}^{P}$ is the inventory of material j stored at site k in time period t. $Q_{j,ls,dc,t}^{sd}$ is the amount of material purchase from supplier ls and transferred to distribution center dc. $Q_{j,dc,k,t'}^{dp}$ is the amount of material flow between distribution center dc to site k. If an intermediate product j is used at another plant site k', a quantity $Q_{j,k,k',t}^{pp}$ of material j can be transferred from site k to site k'. A quantity $Q_{j,k,dc,t}^{pd}$ of intermediate or final product j is shipped from plant site k to distribution center dc, and stored with an inventory of $I_{j,dc,t}^{DC}$ units. $D_{j,l,t}$ is the customer demand of product j for customer l at time period t. If sufficient inventory of product j is present at distribution center dc, a quantity $Q_{j,dc,l,t}^{dc}$ is withdrawn and shipped to customer l. If production site k has inventory of product j, a quantity $Q_{j,k,l,t}^{pc}$ of product j can be dispatched to customer l. If there is insufficient inventory at a distribution center or production site to meet the customer demand, the order is partially fulfilled, and remaining unfulfilled portion of the demand treated as a back order $B_{j,l,t}$. The back orders are considered as a business loss and discarded at a specified cost; however there is a requirement of satisfying a certain minimum demand in each time period.

The following assumptions are made:

1. The fixed cost of setting a transportation link is negligible in comparison to the variable transportation cost.
2. The service time of a transportation link is an integer multiple of the sampling time period.
3. The production and transportation delays are negligible in comparison to the sampling time period and hence neglected.

First, we represent the SC design formulation as a discrete-time multiperiod MILP model, and then it is converted to a stochastic MILP model. The formulation is described through two types of constraints, (1) network structure constraints, and (2) operational planning constraints. The network structure dictates the topology of a supply chain and is defined by constraints (3.1) − (3.12). Operational planning activities are modeled by constraints (3.13) − (3.26).

3.2.2 Network Structure Constraints

The SC network is represented by 4 sets of nodes: suppliers, manufacturing facilities, warehouses (distribution centers), and customers. Selection of these nodes and transportation links between these nodes are modeled by binary decision variables. Each material has its own transportation set-up for all node connections. The network structure constraints are adapted from You and Grossmann (2008a) to include time-dependent transportation linkages and potential movement of material between a wider range of nodes (such as between distribution center to plant, plant to customer).

Production sites

These constraints relate the existence of a plant to conditions governing the consumption and production of chemicals.

If a plant i in site k that consumes chemical j is installed $(Y^P_{k,i} = 1)$, then there is another plant i' in same site that produces chemical j, or site k should be connected to one of the suppliers of chemical j ($y^{sp}_{j,ls,k,t}$), or to another site k' that produces chemical j ($y^{pp}_{j,k',k,t}$), or to a distribution center dc ($y^{dp}_{j,dc,k,t}$) that can supply chemical j:

$$Y^P_{k,i} \leq \sum_{i' \in I^P_j} Y^P_{k,i'} + \sum_{ls \in LS_j} \sum_t y^{sp}_{j,ls,k,t} + \sum_{k' \in K_{i':i' \in I^P_j}} \sum_t y^{pp}_{j,k',k,t} + \sum_{dc} \sum_t y^{dp}_{j,dc,k,t}$$
$$\forall\, j \in JR_i, k \in K, i \in I^C_j \tag{3.1}$$

On the other hand, if a plant i in site k that produces chemical j is installed ($Y^P_{k,i} = 1$), then there is another plant i' in same site that consumes chemical j, or there is at least one transportation link to a distribution center dc ($y^{pd}_{j,k,dc,t}$), or to a customer l ($y^{pc}_{j,k,l,t}$), or site k should be connected to another site k' that consumes chemical j ($y^{pp}_{j,k,k',t}$):

$$Y^P_{k,i} \leq \sum_{i' \in I^C_j} Y^P_{k,i'} + \sum_{dc} \sum_t y^{pd}_{j,k,dc,t} + \sum_l \sum_t y^{pc}_{j,k,l,t} + \sum_{k' \in K_{i':i' \in I^C_j}} \sum_t y^{pp}_{j,k,k',t}$$
$$\forall\, j \in JP_i, k \in K, i \in I^P_j \tag{3.2}$$

Plant transportation links

A transportation link for raw material j from supplier ls to production site k exists ($y^{sp}_{j,ls,k,t} = 1$), only if at least one plant that consumes raw material j exists in site k ($Y^P_{k,i}$):

$$y^{sp}_{j,ls,k,t} \leq \sum_{i \in I^C_j} Y^P_{k,i} \qquad \forall\, j \in J^R, ls \in LS_j, k \in K, t \in T \tag{3.3}$$

A transportation link for chemical j from distribution center dc to production site k exists ($y^{dp}_{j,dc,k,t} = 1$), only if plant site k exists:

$$y^{dp}_{j,dc,k,t} \leq \sum_{i \in I_k} Y^P_{k,i} \qquad \forall\, j \in J, dc \in DC, k \in K, t \in T \tag{3.4}$$

An inter-site transportation link from site k to k' is installed for chemical j ($y^{pp}_{j,k,k',t} = 1$), only if both plant sites k and k' exist, and at least one plant i in site k is installed that produces chemical j:

$$y^{pp}_{j,k,k',t} \leq \sum_{i \in I^P_j \cap I_k} Y^P_{k,i} \qquad \forall\, j \in J, k, k' \in K, t \in T \tag{3.5a}$$

$$y^{pp}_{j,k,k',t} \leq \sum_{i' \in I_{k'}} Y^P_{k',i'} \qquad \forall\, j \in J, k, k' \in K, t \in T \tag{3.5b}$$

Any material can be transferred between plant sites, but to keep the computation complexity at reasonable level, inter-site shipment may be restricted to a few chemicals.

A transportation link for chemical j from plant site k to distribution center dc exists ($y^{pd}_{j,k,dc,t} = 1$), only if plant site k exists ($Y^{P}_{k,i}$), and chemical j is a product of plant site k or a final product J^P:

$$y^{pd}_{j,k,dc,t} \leq \sum_{i \in I_k} Y^{P}_{k,i} \qquad \forall\, k, j \in (J^P \cup JP_k), dc \in DC, t \in T \tag{3.6}$$

In principle, any chemical j can be transported from plant site k to distribution center dc. However, to minimize the computation load we allow transfer of only final products and products of a plant site k to distribution center dc.

A transportation link for final product j from plant site k to customer l exists ($y^{pc}_{j,k,l,t} = 1$), only if plant site k exists ($Y^{P}_{k,i}$):

$$y^{pc}_{j,k,l,t} \leq \sum_{i \in I_k} Y^{P}_{k,i} \qquad \forall\, j \in J^P, k \in K, l \in L, t \in T \tag{3.7}$$

Distribution center

These constraints dictate the existence of a distribution center based on the existence of the input and output material flows.

If a distribution center dc is set up ($Y^{DC}_{dc} = 1$), at least one of the transportation links from supplier ls ($y^{sd}_{j,ls,dc,t}$), or from plant site k ($y^{pd}_{j,k,dc,t}$), or from another distribution center dc' to distribution center dc ($y^{dd}_{j,dc',dc,t}$) must exist, and a transportation link from distribution center dc to customer l ($y^{dc}_{j,dc,l,t}$), or to plant site k ($y^{dp}_{j,dc,k,t}$), or to another distribution center dc' ($y^{dd}_{j,dc,dc',t}$) must exist:

$$Y^{DC}_{dc} \leq \sum_{j \in J^R} \sum_{ls} \sum_{t} y^{sd}_{j,ls,dc,t} + \sum_{j} \sum_{k} \sum_{t} y^{pd}_{j,k,dc,t} + \sum_{j} \sum_{dc'} \sum_{t} y^{dd}_{j,dc',dc,t} \qquad \forall\, dc \in DC \tag{3.8a}$$

$$Y^{DC}_{dc} \leq \sum_{j \in J^P} \sum_{l} \sum_{t} y^{dc}_{j,dc,l,t} + \sum_{j} \sum_{k} \sum_{t} y^{dp}_{j,dc,k,t} + \sum_{j} \sum_{dc'} \sum_{t} y^{dd}_{j,dc,dc',t} \qquad \forall\, dc \in DC \tag{3.8b}$$

It is worth mentioning that the transportation links $y^{pd}_{j,k,dc,t}$ and $y^{dp}_{j,dc,k,t}$ are not same and considered to have separate transportation contracts. The first link represents the material flow from a plant to a distribution center, while the second corresponds to the opposite direction of flow.

Distribution center transportation links

A transportation link to distribution center dc for chemical j from supplier ls ($y^{sd}_{j,ls,dc,t}$), or from plant site k ($y^{pd}_{j,k,dc,t}$), or from distribution center dc' ($y^{dd}_{j,dc',dc,t}$) can exist only if distribution center dc exists ($Y^{DC}_{dc} = 1$). Similarly, a transportation link for chemical j from distribution center dc to plant site k ($y^{dp}_{j,dc,k,t}$), or to customer l ($y^{dc}_{j,dc,l,t}$) can exist, only if distribution center dc exists:

$$y^{sd}_{j,ls,dc,t} \leq Y^{DC}_{dc} \qquad \forall\, j \in J^R, ls \in LS, dc \in DC, t \in T \tag{3.9a}$$
$$y^{pd}_{j,k,dc,t} \leq Y^{DC}_{dc} \qquad \forall\, j \in J, k \in K, dc \in DC, t \in T \tag{3.9b}$$
$$y^{dd}_{j,dc',dc,t} \leq Y^{DC}_{dc} \qquad \forall\, j \in J^P, dc, dc' \in DC, t \in T \tag{3.9c}$$
$$y^{dp}_{j,dc,k,t} \leq Y^{DC}_{dc} \qquad \forall\, j \in J, dc \in DC, k \in K, t \in T \tag{3.9d}$$
$$y^{dc}_{j,dc,l,t} \leq Y^{DC}_{dc} \qquad \forall\, j \in J^P, dc \in DC, l \in L, t \in T \tag{3.9e}$$

A transportation link between distribution centers dc and dc' exists for final product j ($y^{dd}_{j,dc,dc',t} = 1$), only if distribution center dc receives chemical j from a plant site k ($y^{pd}_{j,k,dc,t}$) and distribution center dc' supplies chemical j to a plant site k' ($y^{dp}_{j,dc',k',t}$), or to a customer l ($y^{dc}_{j,dc',l,t}$). These requirements can be mathematically represented by the inequalities,

$$y^{dd}_{j,dc,dc',t} \leq \sum_k y^{pd}_{j,k,dc,t} \qquad \forall\, j \in J^P, dc, dc' \in DC, t \in T \tag{3.10a}$$
$$y^{dd}_{j,dc,dc',t} \leq \sum_k y^{dp}_{j,dc',k,t} + \sum_l y^{dc}_{j,dc',l,t} \qquad \forall\, j \in J^P, dc, dc' \in DC, t \in T \tag{3.10b}$$

To minimize computational complexity, we permit the establishment of inter-distribution center transportation links only for the final product.

A transportation link from distribution center dc to plant site k exists for chemical j ($y^{dp}_{j,dc,k,t} = 1$) only if distribution center dc receives chemical j from another plant site k' ($y^{pd}_{j,k',dc,t}$), or from supplier ls ($y^{sd}_{j,ls,dc,t}$), or from another distribution center dc' ($y^{dd}_{j,dc',dc,t}$). In addition, site k should supply chemical j to distribution center dc' ($y^{pd}_{j,k,dc',t}$), or to customer l ($y^{pc}_{j,k,l,t}$), or to another site k' ($y^{pp}_{j,k,k',t}$), or consume chemical j:

$$y^{dp}_{j,dc,k,t} \leq \sum_{k'} y^{pd}_{j,k',dc,t} + \sum_{ls \in LS_j} y^{sd}_{j,ls,dc,t} + \sum_{dc':dc' \neq dc, j \notin J^R_k} y^{dd}_{j,dc',dc,t}$$
$$\forall\, k \in K, j \in (J^P \cup JR_k), dc \in DC, t \in T \tag{3.11a}$$
$$y^{dp}_{j,dc,k,t} \leq \sum_{dc':dc' \neq dc} y^{pd}_{j,k,dc',t} + \sum_{k':k' \neq k} y^{pp}_{j,k,k',t} + \sum_l y^{pc}_{j,k,l,t} + \sum_{i \in I^C_j} Y^P_{k,i}$$
$$\forall\, k \in K, j \in (J^P \cup JR_k), dc \in DC, t \in T \tag{3.11b}$$

We allow the shipment of only final product (J^P) or raw material for plant site k (J_k^R) from distribution center dc to plant site k.

A transportation link from distribution center dc to customer l exists for chemical j $(y_{j,dc,l,t}^{dc} = 1)$, only if distribution center dc receives chemical j from plant site k $(y_{j,k,dc,t}^{pd})$ or from another distribution center dc' $(y_{j,dc',dc,t}^{dd})$:

$$y_{j,dc,l,t}^{dc} \leq \sum_{k} y_{j,k,dc,t}^{pd} + \sum_{dc':dc' \neq dc} y_{j,dc',dc,t}^{dd} \qquad \forall\, j \in J^P, dc \in DC, l \in L, t \in T \tag{3.12}$$

3.2.3 Operational Planning

The operation planning model includes constraints related to production, transportation, and mass balance relationships. It also defines the production capacity of plants and storage capacity of plants and distribution centers.

Production constraints

Flow $W_{k,i,j,m,t}$ of chemical j associated with production scheme m in plant i at site k is calculated from the production amount of main product j^* of scheme m, and is given by the mass balance coefficient $\mu_{i,j,m}$ times the production flow of main product j^*:

$$W_{k,i,j,m,t} = \mu_{i,j,m} W_{k,i,j*,m,t} \qquad \forall\, k \in K, i \in I_k, j \in J_m, j^* \in J_m^{MP}, m \in M_i, t \in T \tag{3.13}$$

The total production amount of main product j from all production schemes m installed at plant i of site k should be within the production capacity of plant i $(Q_{k,i}^{prod})$:

$$\sum_{m \in M_i} \sum_{j \in J_m^{MP}} \eta_{k,i,m} W_{k,i,j,m,t} \leq Q_{k,i}^{prod} \qquad \forall\, k \in K, i \in I_k, t \in T \tag{3.14}$$

where $\eta_{k,i,m}$ represents the relative production amount of main product j of production scheme m in plant i in terms of plant capacity.

The design production capacity of plant i at site k $(Q_{k,i}^{prod})$ is constrained by a specified maximum allowable installation capacity $Q_{k,i}^{prod,max}$:

$$Q_{k,i}^{prod} \leq Q_{k,i}^{prod,max} \qquad \forall\, k \in K, i \in I \tag{3.15}$$

Mass balance constraints

The mass balance for chemical j at plant site k during time period t is given by,

$$
\begin{aligned}
I^{P}_{j,k,t} = I^{P}_{j,k,t-1} + \sum_{ls \in LS_j} Q^{sp}_{j,ls,k,t} + \sum_{k'} Q^{pp}_{j,k',k,t} + \sum_{dc} Q^{dp}_{j,dc,k,t} + \underbrace{\sum_{i \in I^P_j} \sum_{m \in M_i} W_{k,i,j,m,t}}_{\text{production}} \\
- \sum_{dc} Q^{pd}_{j,k,dc,t} - \sum_{l} Q^{pc}_{j,k,l,t} - \sum_{k'} Q^{pp}_{j,k,k',t} - \underbrace{\sum_{i \in I^C_j} \sum_{m \in M_i} W_{k,i,j,m,t}}_{\text{consumption}} \\
\forall\ k \in K_i, j \in J, t \in T \qquad (3.16)
\end{aligned}
$$

where $I^{P}_{j,k,t}$ is the inventory level of chemical j at plant site k, $Q^{sp}_{j,ls,k,t}$ is the purchase amount, $Q^{pp}_{j,k',k,t}$ and $Q^{pp}_{j,k,k',t}$ are inter-site shipment quantities to plant site k from site k' and from plant site k to site k' respectively, $Q^{dp}_{j,dc,k,t}$ is the shipment amount from a distribution center to plant site, $Q^{pd}_{j,k,dc,t}$ is the shipment amount from a plant site to distribution center, and $Q^{pc}_{j,k,l,t}$ is the shipment amount to customer l.

The mass balance for chemical j at distribution center dc at time period t is given by,

$$
\begin{aligned}
I^{DC}_{j,dc,t} = I^{DC}_{j,dc,t-1} + \left(\sum_{ls \in LS_j} Q^{sd}_{j,ls,dc,t} + \sum_{k} Q^{pd}_{j,k,dc,t} + \sum_{dc'} Q^{dd}_{j,dc',dc,t} \right) \\
- \left(\sum_{k} Q^{dp}_{j,dc,k,t} + \sum_{l} Q^{dc}_{j,dc,l,t} + \sum_{dc'} Q^{dd}_{j,dc,dc',t} \right) \qquad \forall\ dc \in DC, j \in J, t \in T \qquad (3.17)
\end{aligned}
$$

where $I^{DC}_{j,dc,t}$ is the inventory level of chemical j at distribution center dc, $Q^{sd}_{j,ls,dc,t}$ is the purchase amount from supplier ls, $Q^{dc}_{j,dc,l,t}$ is shipment amount to customer l, and $Q^{dd}_{j,dc',dc,t}$ is the inter-distribution center shipment.

Inventory constraints

The average inventory at distribution center dc $(IL^{DC}_{dc,t})$ during time period t is equal to the outlet flow from distribution center dc divided by the residence time (TOR - turn over ratio), with an analogous expression for the average inventory at plant site k (Guillén-Gosálbez and Grossmann, 2010):

$$
IL^{DC}_{dc,t} = \frac{\sum_{j} \sum_{l} Q^{dc}_{j,dc,l,t} + \sum_{j} \sum_{k} Q^{dp}_{j,dc,k,t} + \sum_{j} \sum_{dc'} Q^{dd}_{j,dc,dc',t}}{TOR^{DC}_{dc}} \qquad \forall\ dc \in DC, t \in T \qquad (3.18a)
$$

$$IL^P_{k,t} = \frac{\sum_j \sum_{dc} Q^{pd}_{j,k,dc,t} + \sum_j \sum_l Q^{pc}_{j,k,l,t} + \sum_{k'} Q^{pp}_{j,k,k',t}}{TOR^P_k} \qquad \forall\, k \in K, t \in T \qquad (3.18b)$$

where TOR^{DC}_{dc} and TOR^P_k are the turn over ratio of distribution center dc and plant k respectively. The turn over ratio is defined as the number of times the total inventory is replenished in one time period.

Equation (3.19) enforces the distribution center and plant site inventories at the end of each time period, and the average inventories, to be maintained within capacity limits:

$$\sum_j I^{DC}_{j,dc,t} \leq Q^{DC}_{dc} \qquad \forall\, dc \in DC, t \in T \qquad (3.19a)$$

$$\psi\, IL^{DC}_{dc,t} \leq Q^{DC}_{dc} \qquad \forall\, dc \in DC, t \in T \qquad (3.19b)$$

$$\sum_j I^P_{j,k,t} \leq Q^P_k \qquad \forall\, k \in K, t \in T \qquad (3.19c)$$

$$\psi\, IL^P_{k,t} \leq Q^P_k \qquad \forall\, k \in K, t \in T \qquad (3.19d)$$

where ψ (> 1) represents a storage capacity safety factor. Q^{DC}_{dc} and Q^P_k are the storage capacities of distribution center dc and plant site k respectively.

Equation (3.20) imposes upper limits on the design storage capacities at the distribution centers (Q^{DC}_{dc}) and plant sites (Q^P_k):

$$Q^P_k \leq Q^{P,max}_k \qquad \forall\, k \in K \qquad (3.20a)$$

$$Q^{DC}_{dc} \leq Q^{DC,max}_{dc} \qquad \forall\, dc \in DC \qquad (3.20b)$$

where $Q^{DC,max}_{dc}$ and $Q^{P,max}_k$ are the design capacity of distribution center and plant site respectively.

The total shipment amount of chemical j to each customer ls at time period t is equal to the amount shipped from plant site k $(Q^{pc}_{j,k,l,t})$ plus the shipment dispatched from distribution center dc $(Q^{dc}_{j,dc,l,t})$:

$$SA_{j,l,t} = \sum_{k \in K} Q^{pc}_{j,k,l,t} + \sum_{dc \in DC} Q^{dc}_{j,dc,l,t} \qquad \forall\, j \in J, l \in L, t \in T \qquad (3.21)$$

The sale amount SA must be less than or equal to the demand D for any time period. However, there is a requirement of satisfying a minimum customer satisfaction level φ for each product j at each time period:

$$\varphi D_{j,l,t} \leq SA_{j,l,t} \leq D_{j,l,t} \qquad \forall\, j \in J, l \in L, t \in T \tag{3.22}$$

Any unsatisfied customer demand (back-order) will not be carried further and discarded with some penalty cost. The back order quantity of product j at time period t is given by,

$$BO_{j,l,t} = D_{j,l,t} - SA_{j,l,t} \qquad \forall\, j \in J^P, l \in L, t \in T \tag{3.23}$$

Transportation flow constraints

Transportation of chemical j between two locations takes place only if the transportation link between them is set up. Moreover, there is usually a minimum flow rate of material that is needed to justify the establishment of a transportation link between two locations. These considerations can be modeled by,

$$y^{sp}_{j,ls,k,t}\, Q^{sp,L}_{ls,k} \leq Q^{sp}_{j,ls,k,t} \leq y^{sp}_{j,ls,k,t} Q^{sp,U}_{j,ls,k} \qquad \forall\, j \in J^R, ls \in LS, k \in K, t \in T \tag{3.24a}$$

$$y^{sd}_{j,ls,dc,t}\, Q^{sd,L}_{ls,dc} \leq Q^{sd}_{j,ls,dc,t} \leq y^{sd}_{j,ls,dc,t} Q^{sd,U}_{j,ls,dc} \qquad \forall\, j \in J^R, ls \in LS, dc \in DC, t \in T \tag{3.24b}$$

$$y^{p}_{j,k,k',t}\, Q^{pp,L}_{k,k'} \leq Q^{pp}_{j,k,k',t} \leq y^{pp}_{j,k,k',t} Q^{pp,U}_{j,k,k'} \qquad \forall\, j \in J, k, k' \in K, t \in T \tag{3.24c}$$

$$y^{dp}_{j,dc,k,t}\, Q^{dp,L}_{dc,k} \leq Q^{dp}_{j,dc,k,t} \leq y^{dp}_{j,dc,k,t} Q^{dp,U}_{j,dc,k} \qquad \forall\, j \in J, dc \in DC, k \in K, t \in T \tag{3.24d}$$

$$y^{pd}_{j,k,dc,t}\, Q^{pd,L}_{k,dc} \leq Q^{pd}_{j,k,dc,t} \leq y^{pd}_{j,k,dc,t} Q^{pd,U}_{j,k,dc} \qquad \forall\, j \in J, k \in K, dc \in DC, t \in T \tag{3.24e}$$

$$y^{dd}_{j,dc,dc',t}\, Q^{dd,L}_{dc,dc'} \leq Q^{dd}_{j,dc,dc',t} \leq y^{dd}_{j,dc,dc',t} Q^{dd^U}_{j,dc,dc'} \qquad \forall\, j \in J, dc, dc' \in DC, t \in T \tag{3.24f}$$

$$y^{pc}_{j,k,l,t}\, Q^{pc,L}_{k,l} \leq Q^{pc}_{j,k,l,t} \leq y^{pc}_{j,k,l,t} Q^{pc,U}_{j,k,l} \qquad \forall\, j \in J^P, k \in K, l \in L, t \in T \tag{3.24g}$$

$$y^{dc}_{j,dc,l,t}\, Q^{dc,L}_{dc,l} \leq Q^{dc}_{j,dc,l,t} \leq y^{dc}_{j,dc,l,t} Q^{dc,U}_{j,dc,l} \qquad \forall\, j \in J^P, dc \in DC, l \in L, t \in T \tag{3.24h}$$

3.2.4 Contractual Agreement Constraints - Transportation Routes

The contractual agreement constraints track the transportation linkages' service time and restrict their minimum duration to a specified contract time. In order to check the contract duration, the contract start and end time have to be recorded. The contract starts $(Cs^{pd}_{j,k,dc,t} = 1)$ when the binary variable $y^{pd}_{j,k,dc,t}$ changes value from 0 to 1 and ends $(Ce^{pd}_{j,k,dc,t} = 1)$ when its value changes back to zero. In order to relate the contract start and end times to the binary transportation linkage variables, we utilize a formulation presented in Kelly and Zyngier (2007) for sequence-dependent switchovers in scheduling problems that was also applied in Chong and Swartz (2016) to track plant unit shutdown durations. For illustration purposes, the formulation is expressed for the link from a plant to a distribution center:

$$y^{pd}_{j,k,dc,t} - y^{pd}_{j,k,dc,t-1} = Cs^{pd}_{j,k,dc,t} - Ce^{pd}_{j,k,dc,t} \quad \forall\, j \in J, k \in K, dc \in DC, t \in T \quad (3.25a)$$

$$y^{pd}_{j,k,dc,t} + y^{pd}_{j,k,dc,t-1} = Cs^{pd}_{j,k,dc,t} + Ce^{pd}_{j,k,dc,t} + 2\,Cd^{pd}_{j,k,dc,t} \quad \forall\, j \in J, k \in K, dc \in DC, t \in T \quad (3.25b)$$

$$Cs^{pd}_{j,k,dc,t} + Ce^{pd}_{j,k,dc,t} + Cd^{pd}_{j,k,dc,t} \leq 1 \quad \forall\, j \in J, k \in K, dc \in DC, t \in T \quad (3.25c)$$

Here, $Cs^{pd}_{j,k,dc,t} \in [0,1]$ is a contract start marker (1 when true, 0 otherwise); $Ce^{pd}_{j,k,dc,t} \in [0,1]$ is an end marker; and $Cd^{pd}_{j,k,dc,t} \in [0,1]$ is an auxiliary variable. Equation (3.25) results in

- $Cs^{pd}_{j,k,dc,t} = 1$ and $Ce^{pd}_{j,k,dc,t} = 0$ when the transportation link changes status from inactive ($y^{pd}_{j,k,dc,t-1} = 0$) to active ($y^{pd}_{j,k,dc,t} = 1$),
- $Cs^{pd}_{j,k,dc,t} = 0$ and $Ce^{pd}_{j,k,dc,t} = 1$ when the transportation link changes status from active ($y^{pd}_{j,k,dc,t-1} = 1$) to inactive ($y^{pd}_{j,k,dc,t} = 0$), and
- $Cs^{pd}_{j,k,dc,t} = 0$ and $Ce^{pd}_{j,k,dc,t} = 0$ when there is no change in transportation link status.

Equation (3.25) also preserves the integrality of the marker variables, which are treated as continuous variables within the interval $[0,1]$. Figure 3.2 provides a pictorial representation of the formulation (3.25).

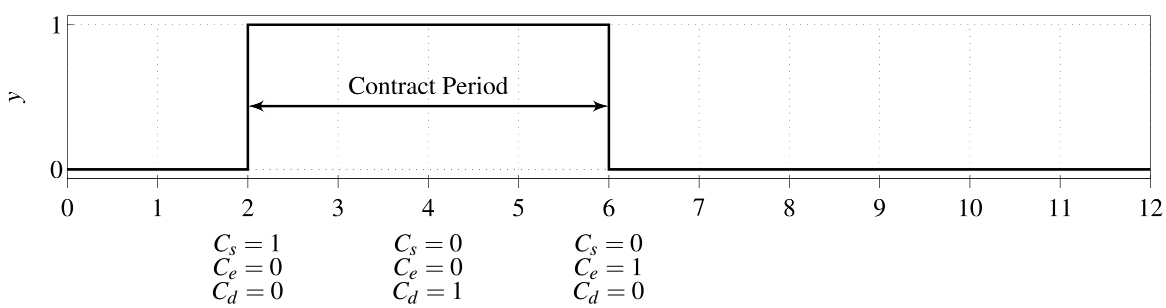

Figure 3.2: Transportation link contract period with marker variables.

Minimum contract service time

When a transportation contract starts, it has to be in service for a specified minimum contract period. Following the formulation presented in Chong and Swartz (2016) in the context of plant shutdown durations, we model the contract service time requirement that the shipment lane from plant site k to distribution center dc has a minimum service time of τ^{pd} time periods as

$$Cc^{pd}_{j,k,dc,t} = \sum_{t}^{t+\tau^{pd}_{k,dc}-1} y^{pd}_{j,k,dc,t} \qquad \forall\, j \in J, k \in K, dc \in DC, t = 1, \ldots, N - \tau^{pd}_{k,dc} + 1 \tag{3.26a}$$

$$Cc^{pd}_{j,k,dc,t} \geq \tau^{pd}_{k,dc}\, Cs^{pd}_{j,k,dc,t} \qquad \forall\, j, k, dc, t = 1, \ldots, N - \tau^{pd}_{k,dc} + 1 \tag{3.26b}$$

Here, N is the total number of time periods and $Cc^{pd}_{j,k,dc,t}$ represents a τ^{pd}-step ahead summation of $y^{pd}_{j,k,dc,t}$. It is worth noting that the formulation does not require the introduction of any new binary variables, hence does not appreciably increase the computation burden of the MILP problem.

Constraint sets (3.25) and (3.26) are written for a plant site to distribution center transportation link. Similar sets of constraints are written for other transportation links (supplier to plant site, plant site to customer, etc.).

3.2.5 Economic Performance Metrics

In the SC design literature, net present value (NPV) is a widely used economic objective for strategic decisions. In the present formulation, we also use NPV as an economic performance measure, calculated from the total revenue generated from sales and the SC cost. The cost can be classified into operating cost and investment cost.

Operating revenue

The operating revenue is calculated from the total sale of products.

$$\text{Revenue} = \sum_{j} \sum_{l} \sum_{t} SA_{j,l,t}\, \gamma^{P}_{j,l,t} \tag{3.27}$$

where γ^P is the selling price of the product.

Operating cost

The cost for operating the SC is computed by summing (1) raw material purchasing cost ($\mathcal{C}^{purchase}$), (2) production cost ($\mathcal{C}^{prod}$), (3) transportation cost ($\mathcal{C}^{trans}$), (4) inventory cost ($\mathcal{C}^{inv}$), and (5) back order cost ($\mathcal{C}^{boc}$). The purchasing cost is calculated from the total quantity of raw material purchased from suppliers. The production cost is calculated from the amount of product produced at each production facility. The inventory cost is reckoned based on the amount of material stored at plants and warehouses. The unmet demand in each time period is discarded with a back order penalty cost and included in the SC operating cost. The transportation cost is the cost incurred for moving materials across SC nodes. The formulation assumes that the unit cost of transportation is independent of amount of material transported and distance between locations. In practice, the cost usually decreases with distance and transportation quantity, but for simplicity we assumed constant unit transportation cost. Similarly, we considered constant unit cost for inventory handling, and production process.

$$\mathcal{C}^{purchase} = \sum_{j\in J^R}\sum_{ls}\sum_{t}\left(\sum_{k} Q^{sp}_{j,ls,k,t} + \sum_{dc} Q^{sd}_{j,ls,dc,t}\right)\gamma^{R}_{j,ls,t} \tag{3.28a}$$

$$\mathcal{C}^{prod} = \sum_{k}\sum_{i\in I_k}\sum_{m\in M_i}\sum_{j\in J^{MP}_m}\sum_{t} W_{k,i,j,m,t}\ \pi_{k,i,m,t} \tag{3.28b}$$

$$\mathcal{C}^{trans} = \sum_{t}\Bigg(\sum_{j\in J^R}\sum_{ls}\sum_{k} Q^{sp}_{j,ls,k,t}\lambda^{sp}_{j,ls,k,t} + \sum_{j\in J^R}\sum_{ls}\sum_{dc} Q^{sd}_{j,ls,dc,t}\lambda^{sd}_{j,ls,dc,t} \tag{3.28c}$$

$$+ \sum_{j}\sum_{k}\sum_{k'} Q^{pp}_{j,k,k',t}\lambda^{pp}_{j,k,k',t} + \sum_{j}\sum_{dc}\sum_{k} Q^{dp}_{j,dc,k,t}\lambda^{dp}_{j,dc,k,t} \tag{3.28d}$$

$$+ \sum_{j}\sum_{k}\sum_{dc} Q^{pd}_{j,k,dc,t}\lambda^{pd}_{j,k,dc,t} + \sum_{j}\sum_{dc}\sum_{dc'} Q^{dd}_{j,dc,dc',t}\lambda^{dd}_{j,dc,dc',t} \tag{3.28e}$$

$$+ \sum_{j}\sum_{k}\sum_{l} Q^{pc}_{j,k,l,t}\lambda^{pc}_{j,k,l,t} + \sum_{j}\sum_{dc}\sum_{l} Q^{dc}_{j,dc,l,t}\lambda^{dc}_{j,dc,l,t}\Bigg) \tag{3.28f}$$

$$\mathcal{C}^{inv} = \sum_{k}\sum_{t} IL^{P}_{k,t}\ \rho^{P}_{k,t} + \sum_{dc}\sum_{t} IL^{DC}_{dc,t}\ \rho^{DC}_{dc,t} \tag{3.28g}$$

$$\mathcal{C}^{boc} = \sum_{j\in J^P}\sum_{l}\sum_{t}(D_{j,l,t} - SA_{j,l,t})\ \nu_{j,l,t} \tag{3.28h}$$

Investment cost

The investment cost is determined from the installment cost of production and storage facilities at candidate locations, and given by the sum of fixed ($\mathcal{C}^{finvst}$) and variable ($\mathcal{C}^{vinvst}$) costs as shown in Equation (3.29).

$$\mathcal{C}^{invst} = \mathcal{C}^{finvst} + \mathcal{C}^{vinvst} \tag{3.29}$$

The investment cost includes the infrastructure cost associated with the facility design and construction, which is assumed to be equally distributed over total service time of the facility. The depreciation of the investment capital (infrastructure cost) is determined through Equation (3.30). We ignore any infrastructure cost associated with developing customer zones.

$$\mathcal{C}^{finvst} = (1-\psi) \times N \left\{ \sum_{k}\sum_{i} \frac{Y^{P}_{k,i}\ \alpha^{P}_{k,i}}{ST_k} + \sum_{dc} \frac{Y^{DC}_{dc}\ \alpha^{DC}_{dc}}{ST_{dc}} \right\} \tag{3.30}$$

where ψ is the salvage value, ST is service life time of facility (plant and distribution center), and N is the length of design horizon.

The variable investment cost is calculated based on the installed capacity of production and storage facilities, and given by,

$$\mathcal{C}^{finvst} = \sum_{k}\sum_{i \in I_k} Q^{prod}_{k,i}\beta^{PS}_{k,i} + \sum_{k} Q^{P}_{k}\beta^{P}_{k} + \sum_{dc} Q^{DC}_{dc}\beta^{DC}_{dc} \tag{3.31}$$

The NPV of a supply chain is computed as,

$$\text{NPV} = \text{Revenue} - \left(\mathcal{C}^{invst} + \mathcal{C}^{purchase} + \mathcal{C}^{prod} + \mathcal{C}^{trans} + \mathcal{C}^{inv} + \mathcal{C}^{boc}\right) \tag{3.32}$$

The cost parameters pertaining to product sales, investment, and network operation (such as raw material purchase, production, material storage, back-order) are discounted at a specified interest rate (You and Grossmann, 2008a).

The deterministic flexible SC design problem is posed with an objective of maximizing NPV subject to Equations (3.1) − (3.26).

3.2.6 Two-stage Stochastic Formulation

In this work, uncertainty in the customer demand is handled by a scenario based approach using two-stage stochastic programming. The network structure decisions, such as locations of facilities, and transportation routes between these facilities, are treated as first stage decisions which retain the same values across all demand scenarios, while the operational planning decisions, such as production and transportation amounts are considered as second stage decisions.

Uncertainty information in the demand is captured by generating a number of discrete realizations of uncertain demand, where each complete realization gives rise to a scenario. In this work, we assume equal probability of occurrence of all scenarios. Ideally, a large number of scenarios should be included in the optimization formulation to effectively capture the uncertainty; however it results in a large-size problem which is not only complex to handle but difficult to solve. Monte Carlo sampling can be used to reduce the number of scenarios required to achieve desired performance. The objective function is set as the expected value of the NPV over all scenarios. The mathematical formulation [1] of a two-stage stochastic network design model is given by,

$$\begin{aligned}
\max \quad & \mathbb{E}[\text{NPV}] = \sum_{s} \xi_s \ \text{NPV}_s \\
\text{subject to:} \quad & f(x_{t,s}, z_t, u_t, d_{t,s}, c_1) \le 0 && \forall\ s, t \\
& g(x_{t,s}, z_t, u_t, d_{t,s}, c_2) = 0 && \forall\ s, t \\
& x_{t,s} \in \mathbb{R}^{+n_x} && \forall\ s, t \\
& u_t \in \mathbb{R}^{+n_u} && \forall\ t \\
& z_t \in \{0,1\}^{n_z} && \forall\ t
\end{aligned} \tag{3.33}$$

where, objective function $\mathbb{E}[\text{NPV}]$ represents the expected value of NPV over all scenarios, the index $s \in S := \{1, \ldots, NS\}$ represents the scenarios, NS is the total number of scenarios, ξ_s is the probability of scenario s occurring. $f(\cdot)$ and $g(\cdot)$ represent the linear inequality and equality constraints respectively of a dynamic supply chain model. z_t are the *first* stage discrete decisions, u_t are the *first* stage continuous decisions, and $x_{t,s}$ are the *second* stage decisions. $d_{t,s}$ is the demand profile realization for scenarios s, and c_1 and c_2 are the set of parameters. n_x, n_u, and n_z indicate the dimension of corresponding vector x, u, and z. The definition of *second stage* stochastic variables are given by extending their equivalent deterministic variables over a scenario index s. The variable sets x, z, u and d are defined as,

$$\begin{aligned}
x =[\ & W_{K,I,J,M,T,S},\ I^{P}_{J,K,T,S},\ I^{DC}_{J,DC,T,S},\ IL^{DC}_{DC,T,S},\ IL^{P}_{K,T,S},\ SA_{J,L,T,S},\ BO_{J,L,T,S}, \\
& Q^{sp}_{J,LS,K,T,S},\ Q^{sd}_{J,LS,DC,T,S},\ Q^{pp}_{J,K,K,T,S},\ Q^{dp}_{J,DC,K,T,S},\ Q^{pd}_{J,K,DC,T,S},\ Q^{pc}_{J,K,L,T,S},\ Q^{dc}_{J,DC,L,T,S}, \\
& Q^{dd}_{J,DC,DC,T,S}\ ] \\
z =[\ & Y^{P}_{K,I},\ Y^{DC}_{DC},\ y^{sp}_{J,LS,K,T},\ y^{sd}_{J,LS,DC,T},\ y^{pp}_{J,K,K,T},\ y^{dp}_{J,DC,K,T},\ y^{pd}_{J,K,DC,T},\ y^{pc}_{J,K,L,T},\ y^{dc}_{J,DC,L,T}, \\
& y^{dd}_{J,DC,DC,T}\ ] \\
u =[\ & Q^{prod}_{K,I},\ Q^{P}_{K},\ Q^{DC}_{DC}, \\
& Cs^{sp}_{J,LS,K,T},\ Cs^{sd}_{J,LS,DC,T},\ Cs^{pp}_{J,K,K,T},\ Cs^{dp}_{J,DC,K,T},\ Cs^{pd}_{J,K,DC,T},\ Cs^{pc}_{J,K,L,T},\ Cs^{dc}_{J,DC,L,T}, \\
& Ce^{sp}_{J,LS,K,T},\ Ce^{sd}_{J,LS,DC,T},\ Ce^{pp}_{J,K,K,T},\ Ce^{dp}_{J,DC,K,T},\ Ce^{pd}_{J,K,DC,T},\ Ce^{pc}_{J,K,L,T},\ Ce^{dc}_{J,DC,L,T}, \\
& Cd^{sp}_{J,LS,K,T},\ Cd^{sd}_{J,LS,DC,T},\ Cd^{pp}_{J,K,K,T},\ Cd^{dp}_{J,DC,K,T},\ Cd^{pd}_{J,K,DC,T},\ Cd^{pc}_{J,K,L,T},\ Cd^{dc}_{J,DC,L,T}, \\
& Cc^{sp}_{J,LS,K,T},\ Cc^{sd}_{J,LS,DC,T},\ Cc^{pp}_{J,K,K,T},\ Cc^{dp}_{J,DC,K,T},\ Cc^{pd}_{J,K,DC,T},\ Cc^{pc}_{J,K,L,T},\ Cc^{dc}_{J,DC,L,T},
\end{aligned}$$

[1] Refer Birge and Louveaux (1997) for detailed explanation of stochastic programming methods.

$Cs^{dd}_{J,DC,DC,T},\ Ce^{dd}_{J,DC,DC,T},\ Cd^{dd}_{J,DC,DC,T},\ Cc^{dd}_{J,DC,DC,T}\ ]$
$d = [\ D_{J,L,T,S}\ ]$

The variable indices shown above indicate their maximum dimensions and would be defined over the sets described in the model formulation section using the notation,

$$W_{K,I,J,M,T,S} := \Big\{ W_{k,i,j,m,t,s}, \quad \forall\, k \in K, i \in I, j \in J, m \in M, t \in T, s \in S \Big\}$$

Similarly other variables are defined on their corresponding sets.

In the above formulation, the time-dependent transportation linkages are treated as first stage decisions. However, other alternatives are possible, such as choosing linkages for a prescribed horizon as first-stage decisions and treating them as second-stage decisions for the remainder of the horizon.

3.3 CASE STUDY

In order to demonstrate the applicability and benefits of the proposed SC design approach, we consider a case study presented in Guillén-Gosálbez and Grossmann (2010), adapted to incorporate characteristics of our flexible SC design problem. The original case study represents the optimal retrofit design of an existing European supply chain. As the problem in the present work addresses the new design of SC, we treat the location and capacity of existing production and storage facility as decision variables in the design problem, along with other potential new plant and storage facilities locations. Further, in the present study, capacity expansion is not considered, upper and lower bounds on material flows between suppliers and plant sites are included, and transportation contract information is incorporated. The network superstructure of the case study is shown in Figure 3.3

The case study involves the design of a European supply chain consisting of 2 raw material suppliers, 2 production sites, 6 production plants, 2 distribution centers, and 4 customers over a time horizon of 12 months with a discretization period of 1 month. There are 6 different production schemes ($M_1, \ldots, M_6$) available to produce 6 products: acetaldehyde, acetone, acrylonitrile, cumene, isopropanol, and phenol from 9 raw materials: ammonia, benzene, ethylene, hydrochloric acid, hydrogen cyanide, oxygen, propylene, sodium hydroxide, and sulfuric acid. The production network structure is shown in Figure 3.4. The number indicated on each arrow shows the mass balance coefficient of the material

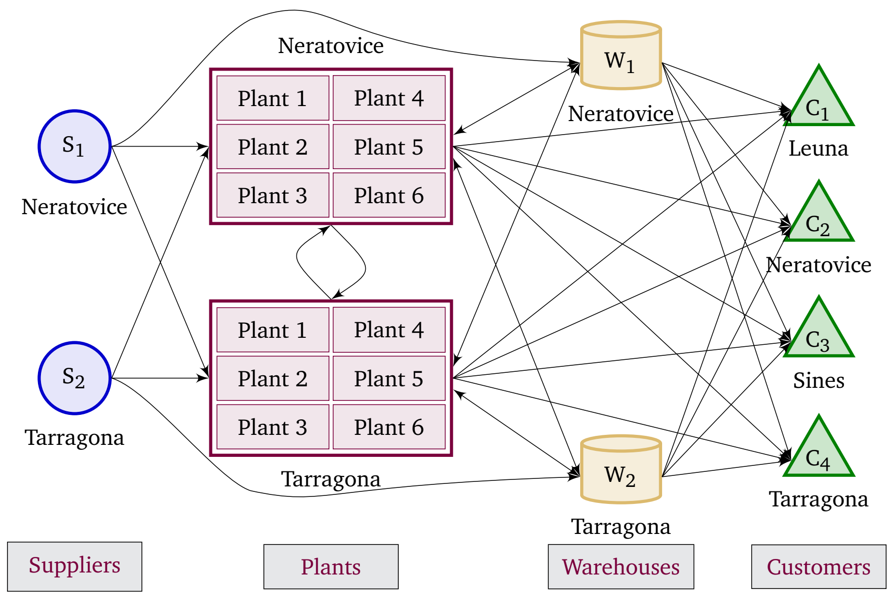

Figure 3.3: Network superstructure of the European supply chain case study

for the corresponding production scheme.

The potential location for raw material suppliers, production sites, and distribution centers are Tarragona (Spain) and Neratovice (Czech Republic). The 4 final markets are located at Leuna (Germany), Neratovice (Czech Republic), Sines (Portugal), and Tarragona (Spain). The customer demand is treated as an uncertain parameter in the optimization formulation. A minimum demand satisfaction target level is considered as 40%. The production capacities of the plants are considered as design variables with an

Table 3.1: Variable and fixed investment cost of production facilities for the European supply chain

Plant/Site	$\beta^{PS}_{k,i}$ (\$/ton/month)		$\alpha^{P}_{k,i}$ (thousand \$)	
	Neratovice	Tarragona	Neratovice	Terragona
I_1	48.68	91.28	4430.11	8306.45
I_2	49.83	93.43	4534.83	8502.82
I_3	125.76	235.81	11445.06	21459.49
I_4	55.86	104.73	5083.10	9530.80
I_5	24.71	46.34	2248.92	4216.72
I_6	88.31	165.59	8036.80	15069.01

upper limit of 10 kton/month and no minimum production capacity specified. The fixed and variable investment costs of opening a new plant and distribution center are given in

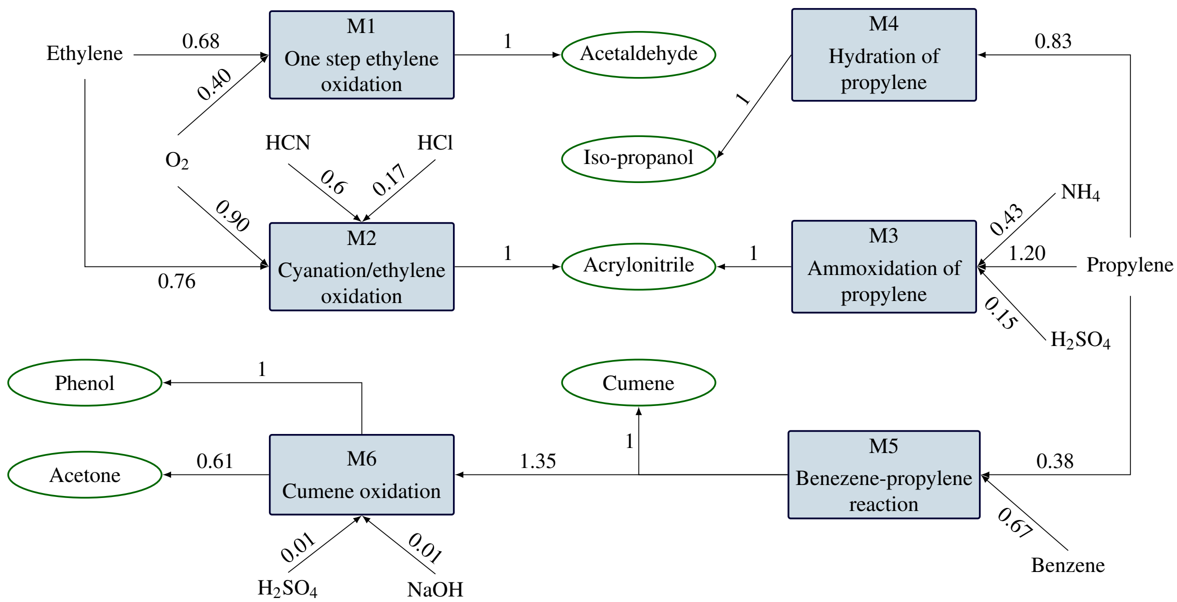

Figure 3.4: Production network within production site of the European supply chain case study

Tables 3.1 and 3.2. The safety factor for plant and distribution center storage capacity is taken as 2.

The cost of on-site storage is set higher than the most costly warehouse storage; thus the traditional network structure will be favored, and the more flexible options used only if economically advantageous. Considering limited space availability at a plant site, the storage capacity at plant sites is restricted to 4 kton, whereas a warehouse has a capacity of 12 kton. The variable investment cost of building a storage facility at a plant site is taken as 3 \$/ton which is higher than the most costly option (2.38 \$/ton) of building a warehouse. Similarly, the inventory cost at the plant sites is taken as 0.3 and 0.5 \$/ton at Neratovice and Tarragona respectively, higher than cost at corresponding warehouses. The total service time of each facility is taken as 4 years and salvage value is taken as 20% of fixed cost. The production cost data are given in Table 3.3.

The minimum and maximum transportation quantities for each transportation link are restricted to 0.15 and 11 kton/month respectively, except for the customer shipping lane for which no minimum transportation quantity is enforced. The transportation cost of all linkages are taken as 0.021 \$/(ton-km). The turnover ratio (TOR) for the storage facilities located at each plant site and distribution center is taken as 10. Table 3.4 provides the distance between plants, warehouses, and markets. The purchase cost of raw materials and the selling price of products are given in Tables 3.5 and 3.6 respectively.

Table 3.2: Investment and operating costs of storage facilities for the European supply chain

Warehouse or plant site	β_k^P ($/ton)	β_{dc}^{DC} ($/ton)	α_{dc}^{DC} (thousands $)	$\rho_{k,t}^P$ ($/ton)	$\rho_{dc,t}^{DC}$ ($/ton)
Neratovice	3	1.06	96.31	0.3	0.1
Tarragona	3	2.38	216.69	0.5	0.22

Note: The inventory costs are the same for each time period.

Table 3.3: Production costs for the European supply chain

Scheme/Plant	$\pi_{k,i,m,t}$ ($/ton)	
	Neratovice	Tarragona
M_1	7.12	16.03
M_2	19.43	43.71
M_3	4.86	10.93
M_4	12.30	27.68
M_5	1.94	4.37
M_6	12.30	27.68

Note: The production costs are same for each time period.

Table 3.4: Inter-node distances for the European supply chain

Facilty / Facility or Market	Distances (km)			
	Leuna	Neratovice	Sines	Tarragona
Neratovice	295.45	0	2970.72	1855.47
Tarragona	1781.36	1855.47	1212.82	0

3.3.1 Results and Discussion

In order to demonstrate the proposed SC design approach and its impact, we present three design cases initially: (1) Single transportation contract formulation (SCF): single transportation contract over the entire time horizon (base case), (2) Fixed contract formulation (FCF): transportation links with contractual agreement having a minimum lock-in period of 4 months, and (3) No contract formulation (NCF): transportation links with no contract agreement. A fourth case is introduced later. The design case FCF represents the proposed SC design formulation. We treat design case SCF as the base case against which we compare and analyze the performance of the proposed design approach.

Table 3.5: Price of raw materials for the European supply chain case study

Chemical/Plant	$\gamma^R_{j,ls,t}$ ($/ton)	
	Neratovice	Tarragona
Ammonia	140.54	148.81
Benzene	200.51	212.30
Ethylene	233.68	247.42
Hydrochloric acid	116.18	123.02
Hydrogen cyanide	468.47	496.03
Oxygen	29.98	31.75
propylene	159.28	168.65
Sodium hydroxide	140.54	148.81
Sulfuric acid	42.16	44.64

Note: The raw materials cost are same for each time period.

Table 3.6: Price of final products for the European supply chain case study

Chemical/Market	$\gamma^P_{j,l,t}$ ($/ton)			
	Leuna	Neratovice	Sines	Tarragona
Acetaldehyde	509.26	487.43	491.07	500.17
Acetone	432.87	414.32	417.41	425.14
Acrylonitrile	36.40	34.84	35.10	35.75
Cumene	401.23	384.04	386.90	394.07
Isopropanol	401.23	384.04	386.90	394.07
Phenol	709.88	679.45	684.52	697.20

Note: The products selling cost are same for each time period.

Considering smaller storage facilities available at plant sites, it will deliver the part of customer orders to the extent that it is cost-effective, while warehouses will deliver the remaining orders. We expect that, in the absence of transportation link contractual agreements (as in NCF case), the optimization should take advantage of switching the transportation links whenever profitable. It provides an additional degree of freedom within optimization formulation and thus represents the most flexible SC design. By contrast, in the presence of link contracts (cases SCF and FCF), it is not possible to change transportation links without satisfying minimum contract times and hence it will result in a lower NPV value. For case SCF, the transportation links can not be changed across time periods and hence represents the least flexible formulation. As explained earlier, the uncertainty in demand is handled by a scenario-based, two-stage stochastic optimization approach. We consider seasonal demand pattern for each product and

Table 3.7: Nominal demand of products for the European supply chain case study

Chemical/Market	$D_{j,l,t}$ (kton/month)			
	Leuna	Neratovice	Sines	Tarragona
Acetaldehyde	1.125	3.125	1.0	0.625
Acetone	0.9	2.5	0.8	0.5
Acrylonitrile	1.5	4.167	1.333	0.833
Cumene	1.125	3.125	1.0	0.625
Isopropanol	0.75	2.083	0.667	0.417
Phenol	1.050	2.917	0.933	0.583

assume that the seasonal characteristic remains same across customer zones. However, the nominal demand of each product is different for different customer zones. Figure 3.5 shows representative demand profiles of all products, where zero shows the nominal demand values. The demand of acetaldehyde shows peak during time periods 6 and 7, whereas acetone shows peak demand in early time periods and acrylonitrile attains the peak in the later time periods. Likewise, acetone demand increases in the first few time periods and then it forms a peak. It creates another peak with lesser value in the later time periods before it tapers off. Isopropanol and phenol show linear increase in demand. We assume that the seasonal demand pattern for all product will repeat in each year, and limit the design horizon to one year. However, to capture the demand uncertainty over the entire design period, we generate demand scenarios by introducing variation around mean demand profiles. 15 demand scenarios are selected using a Monte-Carlo sampling technique assuming a uniform distribution with a variation of $\pm$10% around mean demand profile as a balance between capturing the uncertainty and generating a computationally tractable optimization problem. The nominal demand values of each product are tabulated in Table 3.7. The model is implemented in `AMPL` and solved with the MILP solver `CPLEX 12.5` to a 0.5% optimality gap. The optimization problems are solved on a 3.00 GHz Intel®Core^{TM} i7 machine with 8 GB of RAM.

Table 3.8 summarizes the network design results. The 3rd and 4th column show the problem size for each design case. The number of binary variables remains same for all cases, however the number of continuous variables are different depending on transportation contract period, and NCF has the highest number of continuous variables. The NPV comparison graph is shown in Figure 3.6. The design case NCF shows an NPV value that is 10.37% greater than design case SCF, while case NCF has a 13.08% higher NPV than case SCF. The NPV results falls in line of expectation as design cases, FCF and NCF, both utilize the freedom of altering transportation links between facilities if it reduces the

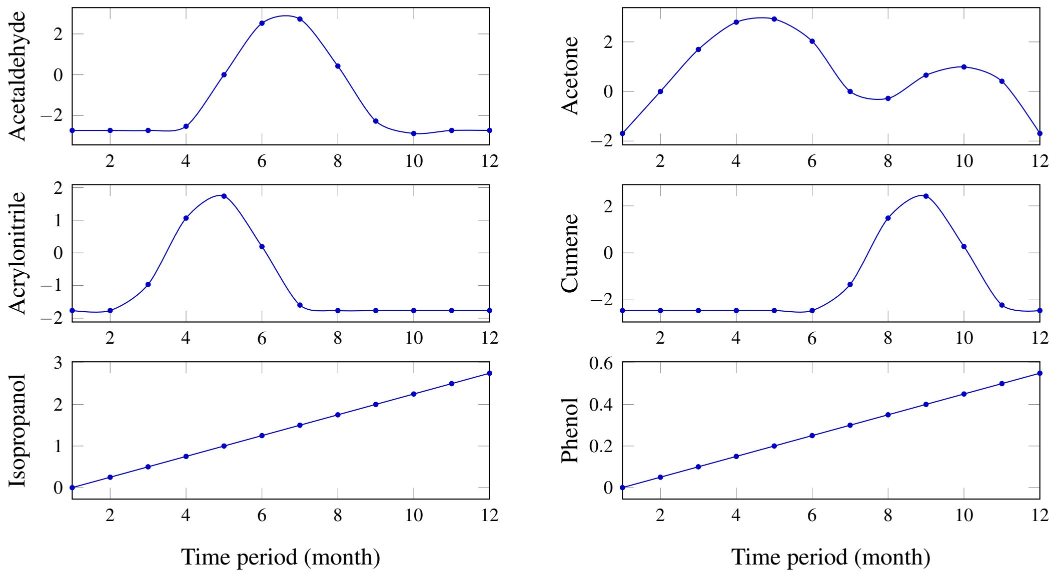

Figure 3.5: Nominal demand profile of each product with zero mean

Table 3.8: Comparison between three design formulations: SCF, FCF, and NCF

Design Case	Contract period	Continuous Variables	Discrete Variables	NPV (million $)	% NPV improvement	Revenue (million $)
SCF	12	89007	3326	59.8857	–	144.0463
FCF	4	93423	3326	66.0939	10.37	144.2719
NCF	–	95079	3326	67.7240	13.09	144.4278
FNF	4	80393	2928	57.2070	-4.47	135.9745

- The NPV improvement percentage is indicated in reference to base case SCF. A design horizon of 12 months is considered for all design cases.
- In SCF, only single transportation contract is allowed, so contract period is equal to design horizon.

operating cost, and thus result in a higher NPV value than the base case SCF.

The network structures obtained from design cases SCF, FCF and NCF are presented in Figures 3.7 to 3.9 respectively. The number shown in a rectangular box (plant) indicates the installed capacity of the corresponding production plant. A blank box indicates that plant is not installed at the corresponding location. The design formulations, presented here, consider a separate transportation link for each material between each pair of echelons, however for brevity of representation, the design structures (Figures 3.7 to 3.9) show one combined link between facilities if at least one link is set up between these locations to transport material.

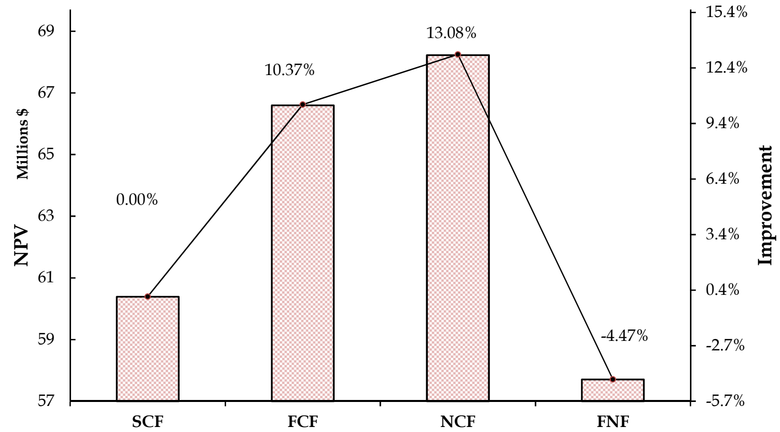

Figure 3.6: NPV comparison between design cases SCF, FCF, NCF, and FNF

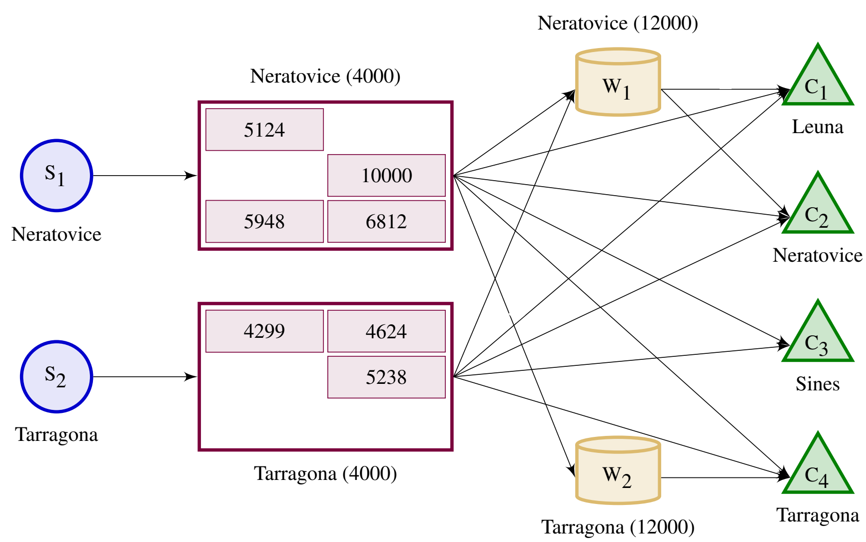

Figure 3.7: Network structure of the SCF (single transportation contract) case - Base case

The number written beside each transportation link specifies the time period(s) for which the link is active for some chemical. If no number is specified, that means the transportation link is active for the entire time horizon.

Formulations FCF and NCF provide similar network structures with few exceptions but differ largely in terms of selecting transportation links between network nodes. They both chose to set up the production plants I_4, I_5 and I_6 at the Neratovice production site and I_1 and I_5 at the Tarragona site. The case NCF also sets up a plant I_1 at Neratovice location. It is worth to mention that, for the same set of plants, both design cases choose to allocate different production capacities. On the other hand, design case SCF chose to install I_1,

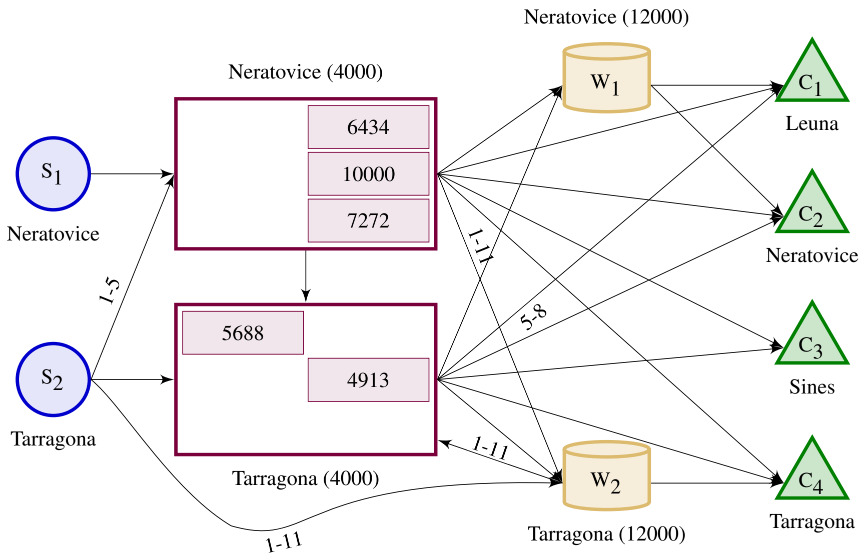

Figure 3.8: Network structure of the FCF (transportation contract agreements) case - proposed approach : 4 months of transportation contract period

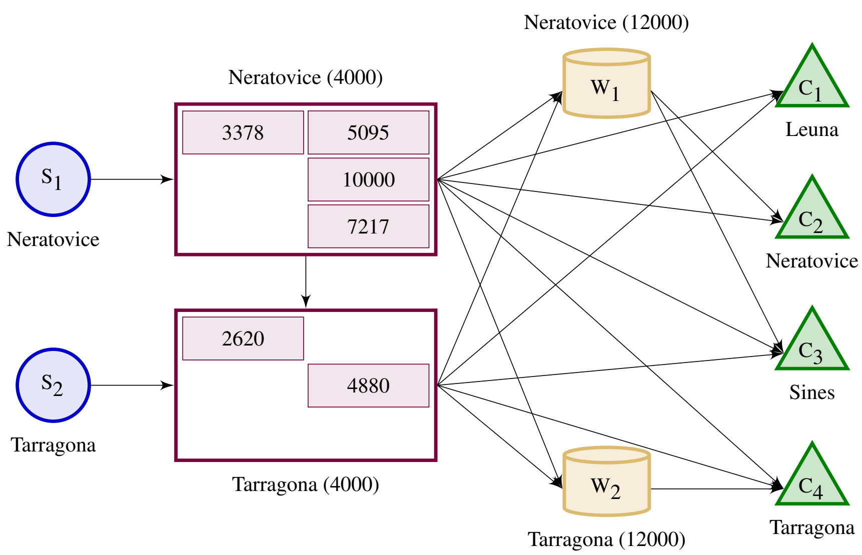

Figure 3.9: Network structure of the NCF (No transportation contract) case - Totally flexible case

I_3, I_5 and I_6 at Neratovice and I_1, I_4 and I_5 at the Tarragona plant site. All design cases propose to install warehouse at both locations with highest allowable capacity. Further, all design cases take advantage of storing materials at plant site and directing them to customers and therefore use the highest storage capacity that can be installed at both plant sites. The design case FCF takes the advantage of flexible node connectivity and transports the raw materials to Tarragona plant through distribution center located at Tarragona during design periods 1-11 to reduce the operating cost. It also uses a direct shipment path to send raw materials to the Tarragona plant site during time periods 1-5. Design cases SCF and NCF propose to use suppliers located at the plant vicinity to supply raw materials, however case FCF uses supplier located at Tarragona to provide raw materials to both plant sites. Thus, the main distinction between these three design networks lies in terms of material distribution channels.

The cost contribution of each component towards total network cost for design case FCF is shown in pie chart 3.10. The purchase cost accounts for the most (68%) of the total cost while the inventory holding cost accounts for the least (0.05%). The share of transportation cost is 8.4% of the total cost, while the fixed and variable investment cost contributions are 7.22% and 2.64% respectively. The back order cost accounts for 9.76% which is even higher than the production cost 4.02%.

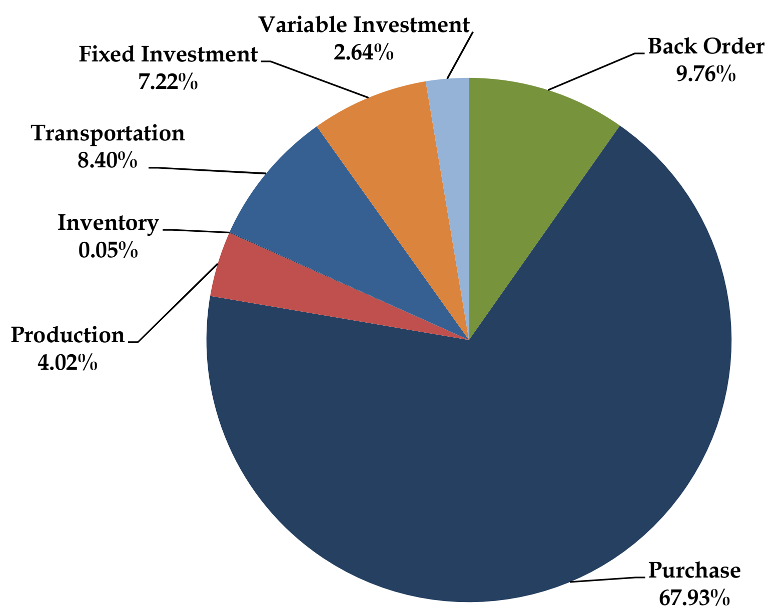

Figure 3.10: Cost contribution chart for the design case FCF

Figure 3.11 shows a cost comparison chart between design cases. Notably, the fixed-investment cost for SCF case is much higher than the rest of the cases. The fixed investment cost is 41.88% lower in FCF case than SCF. The FCF case also managed to slash its variable investment cost by 12.59% than the SCF. The Neratovice production site offers a lower production cost for all production schemes and therefore the optimizer chose to produce most of the products at the Neratovice production site in all design

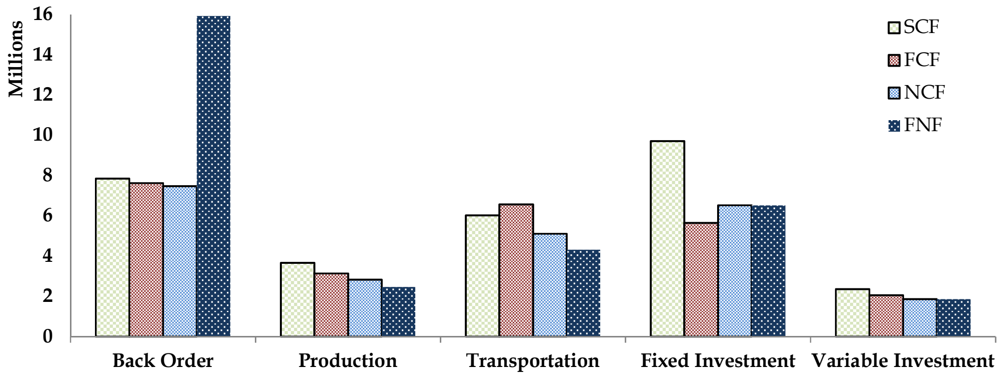

Figure 3.11: Comparison of cost components between design cases SCF, FCF, SCF, and FNF

case. Because of having the freedom of selecting different transportation routes after satisfying a specified minimum contractual service time, design case FCF and NCF make better use of investment cost to generate extra revenue from higher sales and reduce operating cost. However, the enforcement of a single contract agreement in design case SCF does not favour this situation and yields lower NPV value. The extra freedom allowed in case FCF results in savings of 14.23% in production cost. The design case NCF exploits this flexibility even further and offers savings of 22.8% in production cost. Similarly, the purchase cost is decreased by 2.61% and 4.86% for FCF and NCF respectively. On the other hand, inventory and transportation cost is increased in FCF case by 3.42% and 9.06% respectively, however NCF has managed to save 2.01% and 15.04% in the corresponding cost components. The revenue generated from case NCF is $144.42 million, $0.1558 million higher than case FCF and $0.3815 million higher than SCF.

While the design case NCF provides a more economically beneficial design in terms of higher NPV, the SC performance of case NCF may worsen when executing the time-limited contractual agreement on the resulting network configuration. To analyze the supply chain performance in this scenario, we fixed the network design obtained in case NCF, imposed a contractual agreement of 4 months, and re-optimizes SC performance. We refer it as fixed network with contractual agreement enforcement formulation (FNF). As the NCF network structure is fixed, the variables that define the structure; location of storage facilities (Y_{dc}^{DC}), plants that are installed at plant site ($Y_{k,i}^{P}$), production capacity of installed plants ($Q_{k,i}^{prod}$), storage capacities at plant site (Q_{k}^{P}), and storage capacity at distribution center dc (Q_{dc}^{DC}) are considered as parameters in the FNF optimization problem, and their values are fixed from the NCF case. The result for FNF case is shown in Figure 3.6. Surprisingly, the FNF case generates an NPV value less than the base case SCF. The drop in NPV value is 4.47% from SCF and 14.84% from FCF case. The network's demand satisfaction level drops which results in an increase in backorder cost by a factor of two in comparison with SCF case. The backorder cost accounts for 21% total cost of running a supply chain. This clearly shows that the network structure designed for no transportation contract is not able to handle them effectively if they have to be implemented due to a business requirement. For the present case study, this translates to losing an opportunity to improve the profit by $2.6787 million per year with respect to the base case. This result emphasizes the importance of considering transportation contractual agreements, if any, during SC network design phase.

3.4 CONCLUSIONS

In this work, we presented a novel SC design approach which provides flexibility by allowing contiguous and non-contiguous node connections, and incorporates time-limited transportation contracts. Uncertainty in the customer demand prediction was considered in the optimization formulation using a scenario based two-stage stochastic programming approach. The proposed approach is illustrated through application to an industrially-based case study. The network structures and economics under different transportation contracts were compared. The main inferences drawn from the case study are, (i) including different transportation contracts yielded different network structures, (ii) transportation link flexibility that satisfies contract periods gives a higher NPV than single-contract case but lower than no contract restrictions, and (iii) no restriction on transportation service time generated a higher NPV, however it may be unrealistic from a management perspective, and if time-limited contracts are subsequently imposed on the resulting network, lower economics are achieved than with a SC structure that considered time-limited contracts in the design formulation.

NOMENCLATURE

Indices

dc	distribution centers
i	plants
j	chemicals
k	production sites

l	customers
ls	suppliers
m	production schemes
s	demand scenarios
t	time periods

Sets

I	set of plant i
J	set of chemical j
K	set of production site k
L	set of customer l
LS	set of supplier ls
M	set of production scheme m
S	set of scenario s
T	set of time period t
I_j^C	set of plants that consume chemical j
I_j^P	set of plants that produce chemical j
I_k	set of plants that can install at site k
J_m	set of materials for scheme m
J^P	set of final products
JP_i	set of products for plant i
JP_k	set of products that could potentially produced at site k
J_m^{MP}	set of main product for scheme m
J^R	set of main raw materials
JR_i	set of raw materials for plant i
JR_k	set of raw materials that can potentially use at site k
LS_j	set of suppliers that supply chemical j
K_i	set of production sites that can set up plant i
M_i	set of production schemes for plant i

Binary Variables

Y^{DC}_{dc}	1 if warehouse dc is to be established
$Y^{P}_{k,i}$	1 if plant i is to be established at site k
$y^{dc}_{j,dc,l,t}$	1 if a transportation link from warehouse dc to customer l for chemical j is set up
$y^{dd}_{j,dc,dc',t}$	1 if an inter-warehouse transportation link from warehouse dc to warehouse dc' for chemical j is set up
$y^{dp}_{j,dc,k,t}$	1 if a transportation link from warehouse dc to site k for chemical j is set up
$y^{pc}_{j,k,l,t}$	1 if a transportation link from site k to customer l for chemical j is set up
$y^{pd}_{j,k,dc,t}$	1 if a transportation link from site k to warehouse dc for chemical j is set up
$y^{pp}_{j,k,k',t}$	1 if an inter-site transportation link from site k to another site k' for chemical j is set up
$y^{sd}_{j,ls,dc,t}$	1 if a transportation link from supplier ls to warehouse dc for chemical j is set up
$y^{sp}_{j,ls,k,t}$	1 if a transportation link from supplier ls to site k for chemical j is set up

Continuous Variables

$BO_{j,l,t}$	amount of back order (unsatisfied demand) of chemical j for customer l accumulated at time period t
$Cc^{pd}_{j,k,dc,t}$	1 if site k sends chemical j to distribution center dc during time period t
$Ce^{pd}_{j,k,dc,t}$	1 if site k stops supplying chemical j to warehouse dc at time period t
$Cs^{pd}_{j,k,dc,t}$	1 if site k starts supplying chemical j to warehouse dc at time period t
$I^{DC}_{j,dc,t}$	inventory level of chemical j at warehouse dc during time period t
$I^{P}_{j,k,t}$	inventory level of chemical j at site k during time period t
$IL^{DC}_{dc,t}$	average inventory of chemical j at warehouse dc during time period t
$IL^{P}_{k,t}$	average inventory of chemical j at site site k during time period t
$Q^{dc}_{j,dc,l,t}$	shipping amount of chemical j from distribution center dc to customer l during time period t

$Q^{dd}_{j,dc,dc',t}$	shipping amount of chemical j from distribution center dc to distribution center dc' during time period t
$Q^{dp}_{j,dc,k,t}$	shipping amount of chemical j from distribution center dc to site k during time period t
Q^{DC}_{dc}	storage capacity of distribution center dc
$Q^{pc}_{j,k,l,t}$	shipping amount of chemical j from site k to customer l during time period t
$Q^{pd}_{j,k,dc,t}$	shipping amount of chemical j from site k to distribution center dc during time period t
$Q^{pp}_{j,k,k',t}$	shipping amount of chemical j from site k to site k' during time period t
$Q^{prod}_{k,i}$	production capacity of plant i at site k
Q^{P}_{k}	storage capacity of plant site k
$Q^{sd}_{j,ls,dc,t}$	shipping amount of chemical j from supplier ls to distribution center dc during time period t
$Q^{sp}_{j,ls,k,t}$	shipping amount of chemical j from supplier ls to site dc during time period t
$SA_{j,l,t}$	sale of chemical j to customer l during time period t
$W_{k,i,j,m,t}$	amount of chemical j produced in plant i at site k for scheme m in time period t

Parameters

$D_{j,l,t}$	nominal demand of chemical j for customer l during time period t
N	total number of time periods
NS	total number of demand scenarios
$Q^{DC,max}_{dc}$	maximum allowable storage capacity of distribution center dc
$Q^{dc,L}_{dc,l}$	lower bound on total transportation quantity for warehouse dc to customer l link
$Q^{dd,L}_{dc,dc'}$	lower bound on total transportation quantity for warehouse dc to warehouse dc' link
$Q^{dp,L}_{dc,k}$	lower bound on total transportation quantity for warehouse dc to site k link
$Q^{pc,L}_{k,l}$	lower bound on total transportation quantity for site k to customer l link

$Q^{pd,L}_{k,dc}$	lower bound on total transportation quantity for site k to warehouse dc link
$Q^{pp,L}_{k,k'}$	lower bound on total transportation quantity for site k to site k' link
$Q^{sd,L}_{ls,dc}$	lower bound on total transportation quantity for supplier ls to warehouse dc link
$Q^{sp,L}_{ls,k}$	lower bound on total transportation quantity for supplier ls to site k link
$Q^{dc,U}_{j,dc,l}$	upper bound on transportation quantity of chemical j for warehouse dc to customer l link
$Q^{dd,U}_{j,dc,dc'}$	upper bound on transportation quantity of chemical j for warehouse dc to warehouse dc' link
$Q^{dp,U}_{j,dc,k}$	upper bound on transportation quantity of chemical j for warehouse dc to site k link
$Q^{pc,U}_{j,k,l}$	upper bound on transportation quantity of chemical j for site k to customer l link
$Q^{pd,U}_{j,k,dc}$	upper bound on transportation quantity of chemical j for site k to warehouse dc link
$Q^{pp,U}_{j,k,k'}$	upper bound on transportation quantity of chemical j for site k to site k' link
$Q^{sd,U}_{j,ls,dc}$	upper bound on transportation quantity of chemical j for supplier ls to warehouse dc link
$Q^{sp,U}_{j,ls,k}$	upper bound on transportation quantity of chemical j for supplier ls to site k link
$Q^{prod,max}_{k,i}$	maximum allowable production capacity of site i at site k
$Q^{P,max}_{k}$	maximum allowable storage capacity of site k
ST_k	service time of production facility k in years
ST_{dc}	service time of storage facility dc in years
TOR^{DC}_{dc}	turn over ratio of warehouse dc
TOR^{P}_{k}	turn over ratio of site k

α^{DC}_{dc}	fixed cost of installation of distribution center dc
$\alpha^{P}_{k,i}$	fixed cost of installation of plant i in site k
β^{DC}_{dc}	variable cost of installation of distribution center dc
β^{PS}_{k}	variable cost of installation of building storage capacity at plant site k

$\beta^{P}_{k,i}$	operating cost of storage capacity of plant i at site k
$\gamma^{P}_{j,l,t}$	selling price of product j for customer l at time period t
$\gamma^{R}_{j,ls,t}$	purchase price of raw material j from supplier ls at time period t
$\eta_{k,i,m}$	relative production amount of main product j of production scheme m in site i in terms of plant capacity
$\lambda^{dc}_{j,dc,l,t}$	unit shipping cost of chemical j from warehouse dc to customer l during time period t
$\lambda^{dd}_{j,dc,dc',t}$	unit shipping cost of chemical j from warehouse dc to dc' during time period t
$\lambda^{dp}_{j,dc,k,t}$	unit shipping cost of chemical j from warehouse dc to site k during time period t
$\lambda^{pc}_{j,k,l,t}$	unit shipping cost of chemical j from site k to customer l during time period t
$\lambda^{pd}_{j,k,dc,t}$	unit shipping cost of chemical j from site k to warehouse dc during time period t
$\lambda^{pp}_{j,k,k',t}$	unit shipping cost of chemical j for inter-site shipping from site k to site k' during time period t
$\lambda^{sd}_{j,ls,dc,t}$	unit shipping cost of raw material j from supplier ls to warehouse dc during time period t
$\lambda^{sp}_{j,ls,k,t}$	unit shipping cost of raw material j from supplier ls to site k during time period t
$\mu_{i,j,m}$	mass balance coefficient of chemical j in production scheme m of plant i
$\nu_{j,l,t}$	back order penalty cost of product j for customer l at time period t
ξ_{s}	probability of demand scenario s
$\pi_{k,i,m,t}$	production cost of scheme m at plant i in site k at time period t
$\rho^{P}_{k,t}$	inventory cost of site k at time period t
$\rho^{DC}_{dc,t}$	inventory cost of warehouse dc at time period t
ψ	salvage value
$\tau^{pd}_{k,dc}$	contract period for transportation link from plant site k to warehouse dc
φ	minimum customer satisfaction level
ψ	safety factor for storage capacity located at plant site and distribution center

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CHAPTER 4

Robust Multi-stage Model Predictive Control of Process Supply Chains

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4.1 INTRODUCTION

A supply chain (SC) is a network of system nodes connected to each other to perform different undertakings with a target of fulfilling customer needs. The network nodes include mainly raw material suppliers, production facilities, storage facilities, and product distribution channels. The system works to attain its main goal by minimizing the operational and production cost of running a supply chain. Industries forecast their customer demand based on market surveys, and plan production activities to produce the right amount of product such that the overall cost of production, inventory stock, and transportation is minimized. For chemical supply chain systems, it is pertinent to remain competitive to survive in today's global marketplace and therefore chemical process industries strive to reduce their operational cost by a lean management fashion by reduced working inventory and lower production cost (Grossmann, 2012).

Supply chain management (SCM) can be seen as a set of activities that looks at the various business activities carried out by a supply chain and attempts to achieve a coordination across various business and operation functions, such as raw materials purchase, production, material storage, and transportation across the network. The primary objective is to minimize the total cost of running a supply chain while improving customer service. Research shows that having a coordinated view on a supply chain rather than looking each node as a separate entity yields greater benefits (Sousa, Shah, and Papageorgiou, 2008) and therefore integration efforts between SC members should be invested in optimizing process supply chain operations.

The efficiency of any SC system relies upon the level of integration within the system; poor integration leads to sub-optimal performance and many times results in infeasible operation. The "*Bullwhip effect*", which refers to an increased swing in inventory in response to variation in customer demand when we move further right in the supply chain (from distribution center to suppliers), is such a phenomenon that occurs due to poor management. A tighter integration can smooth the *Bullwhip effect* and results in substantial saving in cost (Lee, Padmanabhan, and Whang, 1997). From a systems engineering point of view, a supply chain system can be viewed as a process having a set of inputs, such as production and transportation amounts, and a set of outputs such as inventory levels, customer service, and acted upon by set of disturbances in the form customer demand. This transformational view makes it possible to apply optimal control theory to supply chain systems to gain tighter control on SC operation. In a pioneering work, Forrester (1961) applied an inventory control structure on a supply chain, and demonstrated the *bullwhip phenomenon* on a case study. Literature acknowledges that a major cause of the occurrence of the phenomenon is the artificial shortage that is created due to demand forecast handling, delays in transportation and production, and a decentralized decision making process (Lee, Padmanabhan, and Whang, 1997; Geary, Disney, and Towill, 2006). Applications of classical control theory for supply chain management are cited in Towill (1982); Perea et al. (2000); Perea-López et al. (2001); Lalwani, Disney, and Towill (2006) to reduce inefficiencies, where a feedback control law is applied for inventory and production control for improving the demand satisfaction level. In a review paper, Sarimveis et al. (2008) provide a comprehensive coverage on modelling and control of supply chain systems, and discuss the limitation of classical control theory, such as the inability to consider system constraints, that results in poor performance of supply chain systems and can be improved by applying advanced control techniques such as model predictive control (MPC). Because of inherent ability to handle system constraints explictly and consideration of system dynamics, model predidctive control is widely accepted within process industries applications (García, Prett, and Morari, 1989; Qin and Badgwell, 2003).

An early application of an advanced process control technique to a SC system utilizing MPC was carried out by Tzafestas, Kapsiotis, and Kyriannakis (1997). They use a production planning model which comprises sales level and inventory level as states variables, and advertising effort and production as decision variables. Bose and Pekny (2000) study three different control configurations for production planning and scheduling, (1) centralized, (2) de-centralized, and (3) distributed MPC framework, and use an integrated model to derive a detailed production schedule for the first time period and capacity planning for the rest of the time periods. Seferlis and Giannelos (2004) study a two layer MPC - PID control framework for supply chain control, where a PID inventory controller is embedded within an MPC framework and optimizes system economics. They investigate the effects of transportation delays, move suppresion, and control horizon on controller performance. Braun et al. (2003) develop a decentralized MPC framework where a dedicated MPC is assigned for each node (production, warehouse, retailer), and study the effect of model mismatch and demand forecast error for a semiconductor supply chain. They further demonstrate that move suppression can be used as a means to hedge against system uncertainty. The semiconductor manufacturing industry exhibits a high stochasticity in demand and nonlinear process dynamics. Wang, Rivera, and Kempf (2007) study the application of MPC to manage a semiconductor supply chain and show that proper selection of move suppression parameters, MPC controller parameters (e.g. control horizon, prediction horizon), and model parameters leads to desired system performance and achieves robustness. Wang and Rivera (2008) further extend the formulation by including a *multiple-degree-of-freedom observer* to gain robustness and performance in the presence of uncertain demand and model nonlinearity. Dunbar and Desa (2005) implement a distributed nonlinear MPC to manage a supply chain involving only continuous variables, and proved stability and feasibility of control actions if the system remains within a neighbourhood. Further, they observe the *bullwhip effect* in their simulations. Subramanian et al. (2012) propose a cooperative distributed MPC framework for supply chain management and proved guaranteed closed-loop stability. Through a two-node SC network simulation study, they compare the cooperative distributed MPC against decentralized and noncooperative configurations, and show that the proposed framework provides superior performance.

MPC uses a process model to predict the system response to determine optimal decisions. Therefore accuracy of a process model plays an important role in MPC performance. In SCM literature, various modelling approaches have been proposed, starting from a simple model to capture inventory and production dynamics based on the transfer of material between echelons to a rigorous model that addresses the hybrid nature of a supply chain. An SC system exhibits hybrid dynamics due to existence of disjunctive logical conditions/rulesets which governs decision making process (e.g. production allocation, assignment of production task to a production unit). Hybrid dynamics are generally formulated using integer variables and yield a mixed-integer programming (MIP) formulation. Bemporad and Morari (1999a) present a mixed-integer predictive control (MIPC) framework for hybrid systems, that describes both dynamics and logic conditions denoted as mixed logical dynamical (MLD) systems. These MLD systems are depicted by linear dynamic equations subject to linear inequalities including real and integer variables. Perea-López, Ydstie, and Grossmann (2003) model supply chain members and their interactions with a discrete time dynamic mixed-integer linear programming (MILP) model, and develop a general dynamic optimization framework to update SC decision variables in a rolling horizon fashion using an MPC strategy. The proposed framework is shown to effectively control a gas supply system represented in MLD form. Mestan et al. (2006) utilized a Mixed Logical Dynamical (MLD) model to describe an SC system and optimize the SC operation using an MPC framework. They study centralized and de-centralized MPC configurations, and conclude that lack of coordination causes the bullwhip effect in a decentralized scheme. Bemporad and Giorgetti (2006) present a logic-based solution methodology for optimal control of hybrid systems by combining numerical optimization techniques with symbolic techniques for centralized supply chain management. Liu, Shah, and Papageorgiou (2012) adopt an MPC approach for planning of a multiechelon SC with sequence-dependent changeovers and price elasticity to tackle the uncertainty present in demand and price. They consider an objective function consisting of profit, inventory deviations, and price changes, and study the effect of control horizon, price elasticity, and objective function weights on system performance.

Process disturbances, acting on the process, degrade MPC controller performance. Process disturbances (uncertainty) form another important aspect to be considered within an MPC optimization problem. For a SC system, the most common source of uncertainty is product demand forecast. Maintaining a safety stock (excess inventory) is one of the methods generally employed to hedge against demand uncertainty (Gupta and Maranas, 2003). To address the demand uncertainty for SC planning and scheduling, multi-stage stochastic programming approaches have been utilized. In the multi-stage stochastic approach, uncertainty evolution is depicted by a scenario tree. A scenario tree is one of many plausible ways the uncertainty may evolve with time. In the approaches, the decision variables are classified into two sets, (1) “*here-and-now*" decisions prior to the uncertain event taking place, and (2) “*wait-and-see*" recourse actions postponed until uncertainty information is resolved and more information becomes available. The objective is to optimize the cost of decisions and expected cost of recourse actions over all scenarios. In the review paper, Grossmann (2012) mentions that stochastic programming is best qualified when recourse actions can be adapted to the uncertainty evolution. As SC planning problems are multi-period in nature, multistage stochastic programming can be easily framed for SCM problems. However, problem complexity increases rapidly with the number of stages and hence two-stage stochastic problems are usually used for reasonable computation times.

You, Wassick, and Grossmann (2009) use a two-stage stochastic programming approach for risk management within mid-term planning of a multi-product chemical SC under demand and freight rate uncertainty. They further quantify the percentage savings achieved by using a stochastic approach compared to deterministic optimization. If real time uncertainty evolution can be perfectly modeled by a scenario tree, a multi-stage programming model provides a more accurate solution than a two-stage model; however the computational expense is much higher than the latter (Lucia, Finkler, and Engell, 2013). Thus, a tradeoff exists between model complexity and solution accuracy. Nonetheless, an efficient approximation strategy based on a two-stage programming or decomposition strategy (Gupta and Grossmann, 2011) can be employed to solve large-scale multi-stage programming models. Balasubramanian and Grossmann (2004) apply multistage stochastic optimization for multiperiod multiproduct batch plant scheduling under demand uncertainty. In order to reduce the computational cost in solving a complex multistage stochastic problem, they use an approximate strategy based on solving a number of two-stage programming problem within a shrinking horizon framework and obtain expected profit within a few percent of the multistage stochastic result. For sawmill production planning, Masoumeh, Mustapha, and Daoud (2010) develop a multi-period, multi-product production planning model with uncertain raw material quality, yield and demand using multistage stochastic programming. They indicate that the multistage solution significantly outperforms deterministic and two-stage solutions. Körpeoğlu, Yaman, and Aktürk (2011) use a multi-stage stochastic programming approach for master production scheduling and indicate that it generates higher profit than a deterministic model.

In nominal MPC, the decisions are calculated using a process model under the assumption that no disturbances are acting on the process and the controller model exhibits the true dynamics of underlying process. Robust MPC is a class of methods that accounts for model uncertainties and disturbances in designing the control law. MPC inherently incorporates a feedback mechanism and therefore future control actions are different depending on the uncertainty evolution i.e. they are non-deterministic. However, an open-loop robust MPC neglects the feedback mechanism in generating the predicted response and computes a single control trajectory rather than a set of different control trajectories. Because of inadequate compensation of future controller actions against uncertainty, the open-loop approach generates conservative decisions.

Bemporad and Morari (1999b) provide a thorough review of robust MPC literature and discuss the closed-loop prediction within MPC in detail. Lee and Yu (1997) present min-max based robust MPC approaches for time-varying state-space systems with uncertain parameters using open-loop and closed-loop prediction. The closed-loop prediction is achieved using dynamic programming, however it becomes numerically demanding as number of states and time period increases. They further demonstrate that open-loop control prediction yields poor performance in compare to closed-loop prediction. Kothare, Balakrishnan, and Morari (1996) utilize a linear matrix inequalities (LMI) framework and propose a robust MPC method that characterizes the uncertainty description in a state-feedback control law calculation by minimizing an upper bound on a *worst-case* objective function. To reduce the online computation for a closed-loop LMI based robust MPC, Kouvaritakis, Rossiter, and Schuurmans (2000) use a fixed state-feedback control law but an additional degree of freedom is introduced in the control law through a perturbation term. The method shifts the major part of computations offline and therefore online computation can be performed very quickly.

Robust explicit MPC is an another class of methods to manage system uncertainty where optimal control actions are calculated as a set of system state functions. It offloads online computation with the use of multiparametric programming. Sakizlis et al. (2004) handle input uncertainties as additive state disturbances with an explicit MPC framework. Bemporad, Borrelli, and Morari (2003) use a dynamic programming based explicit robust MPC to handle input disturbances and parametric uncertainties. Later, Pistikopoulos et al. (2009) design a multiparametric robust feedback control law by combining robust optimization and a dynamic programming, and avoid the need of global optimization in the dynamic programming step. Nonetheless, while the multiparametric MPC lowers the online computation, its offline computational effort is significant.

In order to include the effect of new measurements that become available at future times on future control actions, Pena, Bempora, and Alamo (2005) investigate a multistage stochastic programming based robust MPC formulation for a linear state space system and compare its performance to nominal MPC and min-max MPC. On a similar thread, Lucia, Finkler, and Engell (2013) use multistage stochastic programming within a robust nonlinear MPC framework for a semi-batch polymerization reactor. The stage-wise evolution of uncertainty is captured through a scenario tree, which helps to adapt future control inputs and reduces the conservativeness of the computed control action. Through a simulation case study, they shown that multi-stage nonlinear MPC (NMPC) performs better than standard and min-max MPC. However, they noted that the resulting problem size grows exponentially with number of stages and number of uncertain parameters, and hence efficient computation techniques need to be devised to handle problem complexity and to reduce computation time. To reduce the conservativeness of open-loop robust MPC, Warren and Marlin (2003) devise a robust MPC approach where the future closed-loop response is modeled with unconstrained nominal MPC and output constraints are replaced by probabilistic constraints to model closed-loop propagation of uncertainty. Simulation studies demonstrate that robust closed-loop MPC shows improved dynamic constraint-handling performance against nominal MPC and robust open-loop MPC. Li and Ierapetritou (2009) extend the prior work and include a constrained nominal MPC within robust closed-loop MPC. They formulate the problem as a bi-level stochastic optimization problem which translates into a single level problem by assuming that bounds on manipulated variables are either active or inactive for all uncertainty realizations. They use the “DMC" heuristic to decide active bounds on manipulated variables. The approach is implemented for supply chain optimization and shown to achieve significant improvement in performance in reducing back-orders against nominal MPC. However, the formulation does not involve any integer variables which is typical in an SC system that is governed by logical conditions.

The main contribution of the present work is the application of MPC-based tools to address system uncertainty explicitly for control of hybrid SC systems. The proposed approach handles process disturbances and model uncertainty explicitly for supply chain systems governed by hybrid process dynamics, and uses multiple SC performance measures within the optimization framework. In this work, a scenario based approach is applied to describe uncertainty and a stochastic forecasting model is used to generate demand scenarios. Further, a multistage stochastic program is applied to predict the closed-loop response and used within a robust MPC framework to compute control actions, which reduce the conservativeness of the approach.

The part of the research discussed in this chapter has been published in Mastragostino, Patel, and Swartz (2014). First author of the above paper developed a mixed-logical dynamic process supply chain model. My contributions are as follows. The model was entirely reformulated and recoded in order to accommodate a more complex case study, and all case study results were generated using the new model formulation. In addition, the multi-stage stochastic programming formulation is added within the robust MPC framework.

The remainder of the chapter is organized as follows. Section 4.2 describes the supply chain system and the general problem statement. Section 5.2 describes the mathematical formulation of the dynamic model of the system. Section 5.2.5 presents the details of the open-loop and closed-loop approach to robust MPC applied to SCM. Section 4.6 presents a case study, where the developed robust MPC approaches are applied for controlling a multi-product, multi-echelon supply chain. Finally, Section 4.7 concludes with some remarks.

4.2 PROBLEM STATEMENT

We consider the supply chain system illustrated in Figure 5.1, which was adapted from a case study originally presented in Li and Ierapetritou (2009) and extended to address purchasing and manufacturing delays, production scheduling in the plant, and multiple raw material suppliers, production schemes, and plant sites. An overview of the system follows.

The box encompassing several echelons represents a plant site m. Each plant site includes

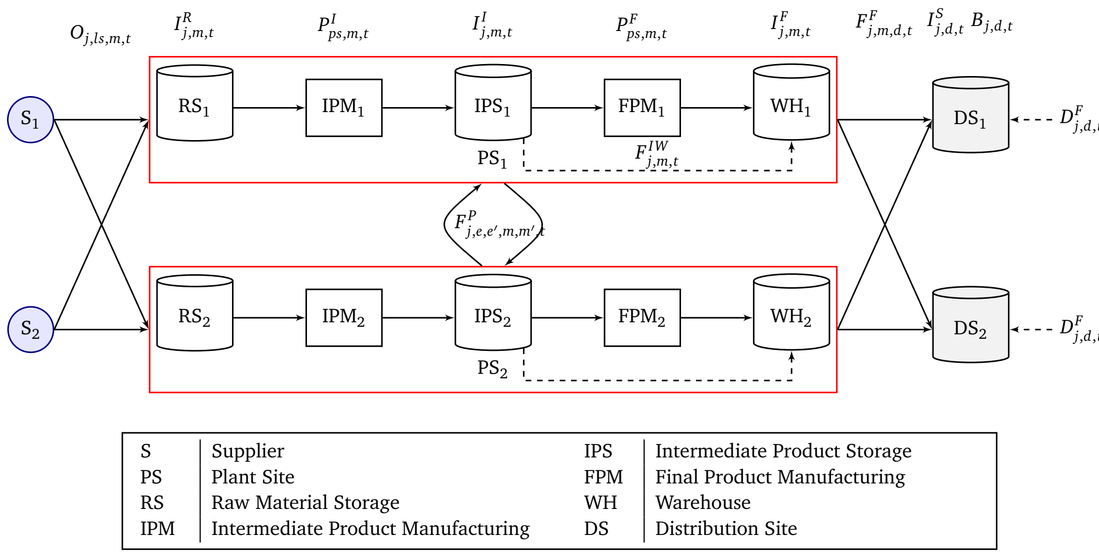

Figure 4.1: Schematic of a process supply chain system for robust MPC study.

the following echelons: raw material storage (RS), intermediate product manufacturing (IPM) and storage (IPS), final product manufacturing (FPM), and a warehouse (WH) for final product storage. A purchase of $O_{j,ls,m,t}$ units of raw material j is made to supplier ls from plant site m at time period t. The order arrives at the plant site after a delivery delay of $\delta^R_{ls,m}$ days. Raw material is stored with inventory of $I^R_{j,m,t}$ units. A quantity of $P^I_{ps,m,t}$ units of main raw material is withdrawn from inventory and processed into intermediate product by the IPM echelon in plant site m via production scheme ps. The conversion of raw material into intermediate product is a single stage batch process, with a manufacturing delay of δ^M_{ps} days. Intermediate product j is stored with inventory of $I^I_{j,m,t}$ units. If material j acts as one of the raw materials at another plant site m', a quantity $F^P_{j,e,e',m,m',t}$ units is transferred from inventory echelon e of plant site m to echelon e' of plant site m'. If material j is one of the final products, a quantity $F^{IW}_{j,m,t}$ units is transferred from the IPS to the warehouse in plant site m. A quantity of $P^F_{ps,m,t}$ units of main raw material is withdrawn from the remaining inventory and processed further into final product j by the FPM echelon in plant site m via production scheme ps. The production of final product j from intermediate product is a single stage batch process, with a manufacturing delay of δ^M_{ps} days. During the manufacturing duration of final product j, the production of an alternate product cannot begin at the FPM echelon. A similar restriction applies in the manufacture of intermediate products. Final product j is stored with inventory of $I^F_{j,m,t}$ units at the warehouse in plant site m. A quantity of $F^F_{j,m,d,t}$ units is withdrawn from inventory and shipped from plant site m to distribution site d. The final product arrives at the distribution site after a delay of $\delta^S_{m,d}$ days, which reflects the transportation and material handling delay. Product within the distribution site which does not fulfill demand or accumulated back orders at time period t, is stored as "safety stock" with inventory of $I^S_{j,d,t}$ units. Safety stock is excess inventory held for hedging against uncertainty. The customer demand of final product j at distribution site d at time period t is $D^F_{j,d,t}$. If sufficient inventory does not exist at the distribution site, product shortfall occurs, and the unfulfilled portion of demand is accumulated as a back order of $B_{j,d,t}$ units. Back orders must be fulfilled before new demand requests can be satisfied. The objective of the SCO problem to be solved at each execution of the model predictive controller is to minimize system wide operating costs, while preventing back orders in the presence of uncertain demand and process yield. The following system assumptions are introduced:

(i) Raw materials are procured from the set of LS different suppliers.

(ii) The IPM and FPM echelons in plant site m represent batch process units, which convert raw materials into intermediate products, and intermediate products into final products j within the set J^P.

(iii) Changeover times at manufacturing units are negligible in comparison to manufacturing times.

(iv) Procurement, production, and transportation decision making occur at equivalent time intervals.

(v) Intermediate product can be transferred directly and stored at a warehouse if it is one of the final products.

It is worth mentioning that the formulation is flexible with regard to the supply chain system considered. Additionally, the supply chain model presented in the paper can be readily revised to relax assumptions, or add additional details (if needed).

4.3 PROCESS SUPPLY CHAIN MODEL

A discrete-time supply chain model is presented to describe the dynamic behavior of material and information flow within the supply chain. The discrete-time formulation divides the horizon into equal length intervals, ΔT, where each time period is indexed by t. A discrete-time representation facilitates the inclusion of time delays (lags), and restricts decision-making to occur at the beginning of each time period. The model is based on a material balance around each storage echelon in the supply chain.

4.3.1 Raw Material Storage

The mass balance of raw material around the RS echelon in plant site m is given by Equation (4.1). The delay of $\delta^R_{ls,m}$ reflects the time between when an order for raw material j ($O_{j,ls,m,t}$) is made to a supplier and the corresponding delivery. The term $F^P_{j,e',e,m',m,t}$ represents the inter-plant shipment amount of chemical j from storage echelon e' in plant m' to storage echelon e in plant m with time delay of $\delta^P_{m',m}$. Product storage echelons rs, ips, and fps designate the raw material, intermediate product and final product storage echelons in inventory echelon set E. Constraint (4.2) represents the maximum order which can be made to supplier ls for material j ($\lambda^R_{ls,m}$) during a time period. The total inventory of all raw materials at plant site m is restricted to a maximum storage capacity of Ω^R_m, as given by constraint (4.3). The quantity of raw material j that begins to be consumed in a production task ps in plant site m at time period t is expressed in terms of the consumption amount of its main raw material and is given by $\mu_{j,ps}\, P^I_{ps,m,t}$, where $\mu_{j,ps}$ is the mass balance coefficient of chemical j. Similarly, the production amount of intermediate product j in a production task ps in plant site m at time period t is given by $\mu_{j,ps}\,\beta^P_{ps}\,P^I_{ps,m,t}$, where β^P_{ps} is the process yield of production scheme ps. The binary variable $u^I_{m,ps,t}$ is introduced to model a disjunction in the continuous variable $P^I_{ps,m,t}$. Equations (4.4) and (4.5) restrict the consumption amount of main raw material $P^I_{ps,m,t}$ to lie between a lower ($\gamma^{M^l}_{m,ps}$) and upper ($\gamma^{M^u}_{m,ps}$) bound, if $u^I_{m,ps,t}$ is 1. $u^I_{m,ps,t}$ is 1 if the IPM process unit in plant site m begins a production task ps at time period t; and 0 otherwise. The basic assignment constraints included in the model capture the logical conditions/rulesets that regulate production scheduling in the plant site. Similar constraints are proposed in Shah, Pantelides, and Sargent (1993), where the authors reformulated the assignment constraint originally derived in Kondili, Pantelides, and Sargent (1993) to improve computational performance. Equation (4.6) is the *full backward* constraint that restricts the start of another production task ps at the IPM process unit at time period t, if a task has already begun within the backward interval $[t-(\delta^M_{ps}/\Delta T)+1, t]$.

$$\begin{aligned} I^R_{j,m,t+1} = {} & I^R_{j,m,t} + \sum_{ls} O_{j,ls,m,t-(\delta^R_{ls,m}/\Delta T)} - \sum_{ps} \mu_{j,ps}\, P^I_{ps,m,t} \\ & + \sum_{m':m'\neq m} \sum_{e'} F^P_{j,e',rs,m',m,t-(\delta^P_{m',m}/\Delta T)} - \sum_{m':m'\neq m} \sum_{e'} F^P_{j,rs,e',m,m',t} \\ & \qquad \forall\, j \in J^{RI}_m, m, t \end{aligned} \tag{4.1}$$

$$O_{j,ls,m,t} \le \lambda^R_{ls,m} \qquad \forall\, j \in J^R, ls, m, t \tag{4.2}$$

$$\sum_{j:j\in J^{RI}_m} I^R_{j,m,t} \le \Omega^R_m \qquad \forall\, m, t \tag{4.3}$$

$$P^{I}_{ps,m,t} \leq \gamma^{M^u}_{m,ps}\ u^{I}_{m,ps,t} \qquad \forall\ m, ps \in PS^{I}_{m}, t \qquad (4.4)$$

$$P^{I}_{ps,m,t} \geq \gamma^{M^l}_{m,ps}\ u^{I}_{m,ps,t} \qquad \forall\ m, ps \in PS^{I}_{m}, t \qquad (4.5)$$

$$\sum_{ps} \sum_{t'=t}^{t-(\delta^{M}_{ps}/\Delta T)+1} u^{I}_{m,ps,t'} \leq 1 \qquad \forall\, m, t \qquad (4.6)$$

4.3.2 Intermediate Product Storage

The mass balance of material j around the IPS echelon in plant site m is given by Equation (4.7). The total inventory of materials at IPS unit is restricted to a maximum storage capacity of Ω^{I}_{m} as given by Equation (4.8). $F^{IW}_{j,m,t}$ represents the amount of material transferred from IPS to the warehouse in plant site m. The amount of chemical j generated or consumed in the production task ps at FPM process unit in plant site m at time period t is expressed in terms of the consumption amount $P^{F}_{ps,m,t}$ of its main raw material. Equations (4.9) and (4.10) are required to model the disjunction in the variable $P^{F}_{ps,m,t}$. The binary variable $u^{F}_{m,ps,t}$ is 1 if the FPM process unit in plant site m begins a production task at time period t to produce final product through production scheme ps; and 0 otherwise. Equation (4.11) is a full backward constraint for representing production scheduling at the FPM process unit, that restricts the start of another production task at the FPM unit at time period t, if another task has already begun within the backward interval $[t - (\delta^{M}_{ps}/\Delta T) + 1, t]$.

$$\begin{aligned} I^{I}_{j,m,t+1} = I^{I}_{j,m,t} + \sum_{ps} \mu_{j,ps}\ \beta^{P}_{ps}\ P^{I}_{ps,m,t-(\delta^{M}_{ps}/\Delta T)} + \sum_{m':m\neq m'} \sum_{e'} F^{P}_{j,e',ips,m',m,t-(\delta^{P}_{m',m}/\Delta T)} \\ - \sum_{m':m\neq m'} \sum_{e'} F^{P}_{j,ips,e',m,m',t} - \sum_{ps} \mu_{j,ps}\ P^{F}_{ps,m,t} - F^{IW}_{j,m,t} \end{aligned}$$

$$\forall\, j \in J^{PI}_{m} \cup J^{RF}_{m}, m, t \qquad (4.7)$$

$$\sum_{j} I^{I}_{j,m,t} \leq \Omega^{I}_{m} \qquad \forall\, j \in J^{PI}_{m} \cup J^{RF}_{m}, m, t \qquad (4.8)$$

$$P^{F}_{ps,m,t} \leq \gamma^{M^u}_{m,ps}\ u^{F}_{m,ps,t} \qquad \forall\, m, ps \in PS^{F}_{m}, t \qquad (4.9)$$

$$P^{F}_{ps,m,t} \geq \gamma^{M^l}_{m,ps}\ u^{F}_{m,ps,t} \qquad \forall\, m, ps \in PS^{F}_{m}, t \qquad (4.10)$$

$$\sum_{ps} \sum_{t'=t}^{t-(\delta^{M}_{ps}/\Delta T)+1} u^{F}_{m,ps,t'} \leq 1 \qquad \forall\, m, t \qquad (4.11)$$

4.3.3 Warehouse

The mass balance of final product j around the WH echelon within plant site m is given by Equation (4.12). The shipment of products from plant site m to distribution site d is restricted by a maximum transportation capacity of $\lambda^F_{m,d}$ during a time period as given by Equation (4.13). The inter-plant shipment quantity is restricted to a maximum quantity of λ^P during a time period [Equation (4.14)]. Equation (4.15) restricts the inventory of final product j to a maximum storage capacity of $\Omega^F_{j,m}$.

$$I^F_{j,m,t+1} = I^F_{j,m,t} + \sum_{ps} \beta^P_{ps}\, \mu_{j,ps}\, P^F_{j,ps,m,t-(\delta^M_{ps}/\Delta T)} + \sum_{m':m'\neq m} \sum_{e} F^P_{j,e,fps,m',m,t-(\delta^P_{m',m}/\Delta T)} + F^{IW}_{j,m,t} - \sum_{m':m\neq m'} \sum_{e} F^P_{j,fps,e,m,m',t} - \sum_{d} F^F_{j,m,d,t} \quad \forall\, j \in J^{PF}_m, m, t \tag{4.12}$$

$$\sum_{j\in J^{PF}_m} F^F_{j,m,d,t} \leq \lambda^F_{m,d} \quad \forall\, m, d, t \tag{4.13}$$

$$\sum_{j} F^P_{j,e,e',m,m',t} \leq \lambda^P_{m,m'} \quad \forall\, e, e', m, m', t \tag{4.14}$$

$$I^F_{j,m,t} \leq \Omega^F_{j,m} \quad \forall\, j \in J^{PF}_m, d, t \tag{4.15}$$

4.3.4 Distribution Site

The mass balance of final product j in distribution site d is given by Equation (4.16), where $\delta^S_{m,d}$ is the transportation delay between plant site m and distribution site d, and $F^S_{j,d,t}$ is the quantity of final product j delivered from d at time period t to satisfy customer demand and accumulated back orders. Equation (4.17) represents the back order balance for final product j at distribution site d.

$$I^S_{j,d,t+1} = I^S_{j,d,t} + \sum_{m} F^F_{j,m,d,t-(\delta^S_{m,d}/\Delta T)} - F^S_{j,d,t} \quad \forall\, j \in J^P, d, t \tag{4.16}$$

$$B_{j,d,t+1} = B_{j,d,t} - F^S_{j,d,t} + D^F_{j,d,t} \quad \forall\, j \in J^P, d, t \tag{4.17}$$

The distribution sites operate with a "best I can do" policy (Perea-López, Ydstie, and Grossmann, 2003) indicated by Equation (4.18),

$$F^S_{j,d,t} = \begin{cases} D^F_{j,d,t} + B_{j,d,t}, & \text{if } I^S_{j,d,t} \geq D^F_{j,d,t} + B_{j,d,t} \\ I^S_{j,d,t}, & \text{if } I^S_{j,d,t} < D^F_{j,d,t} + B_{j,d,t} \end{cases} \quad \forall\, j \in J^P,\ d, t \tag{4.18}$$

where all the demand and accumulated back orders at time period t are satisfied if sufficient stock is available; otherwise the available stock will be shipped. To capture this logical condition a binary variable is required; however, a construct was posed in Li and Ierapetritou (2009) to avoid additional integer variables by eliminating $F^S_{j,d,t}$ in the model through the substitution, $I^{S*}_{j,d,t} = I^S_{j,d,t} - B_{j,d,t}$. Equations (4.16) and (4.17) are then transformed into Equation (4.19), where back orders exist for final product j at d if $I^{S*}_{j,d,t}$ is negative, and inventory of final product j exists at d, if $I^{S*}_{j,d,t}$ is positive. We can now impose an upper bound on $I^{S*}_{j,d,t}$, which reflects the maximum storage capacity of final product j at distribution site d, as given by Equation (4.20).

$$I^{S*}_{j,d,t+1} = I^{S*}_{j,d,t} + \sum_m F^F_{j,m,d,t-(\delta^S_{m,d}/\Delta T)} - D^F_{j,d,t} \qquad \forall\, j \in J^P, d, t \tag{4.19}$$

$$I^{S*}_{j,d,t} \leq \Omega^S_{j,d} \qquad \forall\, j \in J^P, d, t \tag{4.20}$$

4.3.5 Variable Bounds

Inventory variables and back order variables are non-negative as given by Equation (4.21). Equations (4.22) and (4.23) force the back order variable $(B_{j,d,t})$ to be non-zero when $I^{S*}_{j,d,t}$ is negative and the variable representing inventory in the distribution site $(I^S_{j,d,t})$ to be non-zero when $I^{S*}_{j,d,t}$ is positive.

$$I^R_{j,m,t},\ I^I_{j,m,t},\ I^F_{j,m,t},\ I^S_{j,d,t},\ B_{j,d,t} \geq 0 \qquad \forall\, j, m, d, t \tag{4.21}$$

$$B_{j,d,t} \geq -I^{S*}_{j,d,t} \qquad \forall\, j \in J^P, d, t \tag{4.22}$$

$$I^S_{j,d,t} \geq I^{S*}_{j,d,t} + B_{j,d,t} \qquad \forall\, j \in J^P, d, t \tag{4.23}$$

Equations (4.22) and (4.23) are valid if $I^S_{j,d,t}$ and $B_{j,d,t}$ are minimized in the objective function of the SCO problem, and have the effect of setting $B_{j,d,t} = -I^{S*}_{j,d,t}$ and $I^S_{j,d,t} = 0$ if $I^{S*}_{j,d,t}$ is negative, and $B_{j,d,t} = 0$ and $I^S_{j,d,t} = I^{S*}_{j,d,t}$ if $I^{S*}_{j,d,t}$ is positive. The continuous decision variables associated with ordering, production and shipment are non-negative as given by Equation (4.24),

$$O_{j,ls,m,t},\ P^I_{ps,m,t},\ P^F_{ps,m,t},\ F^P_{j,e,e',m,m't},\ F^F_{j,m,d,t},\ F^{IW}_{j,m,t} \geq 0 \quad \forall\, j, ls, ps, m, m', e, e', d, t \tag{4.24}$$

and binary decision variables can take a value of 1 or 0 as given by Equation (4.25),

$$u^I_{m,ps,t},\ u^F_{m,ps,t} \in \{0,1\} \qquad \forall\, m, ps \in PS^I_m \cup PS^F_m, t \tag{4.25}$$

4.3.6 System Representation

For brevity of representation and ease of explanation, the supply chain model presented in above section can be equivalently represented in the following form.

$$f(x_t, u_t, h_t, \ldots, h_{t-q}, d_t, c_1) \leq 0 \qquad \forall\, t \tag{4.26a}$$

$$g(x_{t+1}, x_t, u_t, \ldots, u_{t-q}, d_t, c_2) = 0 \qquad \forall\, t \tag{4.26b}$$

$$x_t \in \mathbb{R}^{n_x} \qquad \forall\, s, t \tag{4.26c}$$

$$u_t \in \mathbb{R}^{n_u} \qquad \forall\, t \tag{4.26d}$$

$$h_t \in \{0, 1\} \qquad \forall\, t \tag{4.26e}$$

where inequality constraint set $f(\cdot)$ and equality constraint set $g(\cdot)$ constitute discretized dynamic linear supply chain model and associated constraints. x_t is the vector of state variables, u_t is the vector of continuous decision variables, h_t is the vector of binary decision variable, d_t is the vector of uncertain disturbance parameter realizations, and c_1 and c_2 are the vectors of parameters. The state vector (x), decision vectors (u and h), and disturbance parameter vector (d) are defined as,

$$\begin{aligned}
x =& [\ I^R_{1,1}, \ldots, I^R_{|J|,|M|},\ I^I_{1,1}, \ldots, I^I_{|J|,|M|},\ I^F_{1,1}, \ldots, I^F_{|J|,|M|},\ I^{S*}_{1,1}, \ldots, I^{S*}_{|J|,|D|}, \\
& I^S_{1,1}, \ldots, I^S_{|J|,|D|},\ B_{1,1}, \ldots, B_{|J|,|D|}\ ]^\mathsf{T} \\
u =& [\ O_{1,1,1}, \ldots, O_{|J|,|LS|,|M|},\ P^I_{1,1}, \ldots, P^I_{|PS|,|M|},\ P^F_{1,1}, \ldots, P^F_{|PS|,|M|}, \\
& F^P_{1,1,1,1,1}, \ldots, F^P_{|J|,|E|,|E|,|M|,|M|},\ F^F_{1,1,1}, \ldots, F^F_{|J|,|M|,|D|}, F^{IW}_{1,1}, \ldots,\ F^{IW}_{|J|,|M|}\ ]^\mathsf{T} \\
h =& [\ u^I_{1,1}, \ldots, u^I_{|M|,|PS|},\ u^F_{1,1}, \ldots, u^F_{|M|,|PS|}\ ]^\mathsf{T} \\
d =& [\ D^F_{1,1}, \ldots, D^F_{|J|,|D|}\ ]^\mathsf{T}
\end{aligned}$$

The maximum dimension of the variables is indicated in the above. In practice, the variables would be defined over the sets indicated in the SC problem formulation, which in some cases are subsets of the full sets J, etc. In Equations (4.26a) and (4.26b), q represents the longest delay associated with transportation and production, i.e.

$$q = \left\lceil \max \{\delta^M_1, \ldots, \delta^M_{|PS|}, \delta^R_{1,1}, \ldots, \delta^R_{|LS|,|M|}, \delta^P_{1,2}, \ldots, \delta^P_{|M|,|M|}, \delta^S_{1,1}, \ldots, \delta^S_{|M|,|D|}\} - 1 \right\rceil$$

Of particular importance is that some of the decisions variables (u_t and h_t) in Equation (4.26a) are not defined when the time period t is less than or equal to q, since they reflect time periods *in the past*. When solving the SCO problem at the execution of the model predictive controller, decisions made in previous time periods (i.e. procurement amount dispatched from supplier, to begin a production task or not) influence decisions made at the current time period or in the future, so they are introduced as parameters in the optimization, and are included in c_1 and c_2.

4.4 REPRESENTATION OF SCENARIOS

In this section, we discuss the demand forecast model and provide an overview of the scenario tree representation within multi-stage stochastic programming.

4.4.1 Demand Forecast Model

Demand is considered as an input disturbance in the supply chain control model, and therefore an accurate prediction of demand greatly increases the controller performance. In the process supply chain literature, time series modeling is employed to predict the demand (e.g., Seferlis and Giannelos, 2004; Wang, Rivera, and Kempf, 2007). In this work, we use a nonstationary integrated moving average model, indicated by Equation (4.27), to forecast the stochastic disturbance (demand) over the prediction horizon n. ∇ is a backward difference operator, $\theta_{j,d}$ is a model parameter and $a_{j,d,t}$ is a white noise process described by a normal distribution with zero mean and variance of $\sigma_{j,d}^2$. It is worth mentioning that the proposed multi-stage MPC is flexible enough to handle any kind of time series model for demand prediction. Additionally, the accuracy of the demand prediction depends on the identification of a correct model. Generally, historical data are employed for finding correct order and parameters for the time-series model. However that is beyond the scope of this work.

$$\nabla D^F_{j,d,t} := D^F_{j,d,t} - D^F_{j,d,t-1} = a_{j,d,t} - \theta_{j,d}\ a_{j,d,t-1} \qquad \forall\ j \in J^P, d, t \tag{4.27}$$

4.4.2 Scenario Generation

In this work, uncertainty is characterized by discrete probability measures, which represents the uncertain parameter by scenario trees. The scenario-based approach has been regularly applied in optimization for capturing uncertainty. Furthermore, scenario-based approaches allow for flexible uncertainty representations, since the underlying structure of the model is unchanged and independent of how scenarios are generated (Gupta and

Maranas, 2003). Moreover, a discrete probability distribution permits the problem representation as a large scale deterministic mathematical optimization program having special structure which can be exploited to reduce the computation time (Lucia, Finkler, and Engell, 2013). A Monte Carlo sampling method is applied for generating scenarios (Hammersley and Handscomb, 1964). The Monte Carlo method entails generating a discrete set of scenarios by sampling from the continuous probability distribution, where the complete realization of all uncertain parameters in the model gives rise to a scenario.

Figure 4.2 shows a standard representation of scenario tree having one uncertain parameter with three discrete values for two time periods. At each time period, the uncertain parameter can take one of three possible discrete values, which generates a total of 9 scenarios. The root node of a tree represents the initial time period $t = 1$. The value of uncertain parameters ξ_1 and ξ_2 is revealed at the end of first ($t = 1$) and second ($t = 2$) time period respectively. In the scenario tree, each node branches off into several nodes

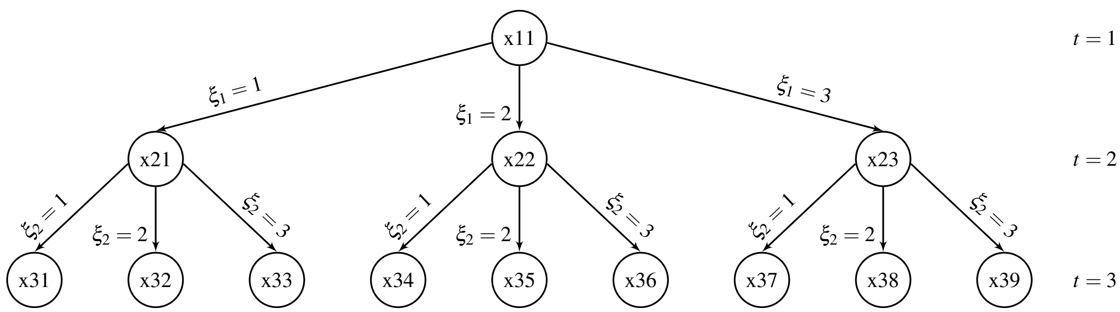

Figure 4.2: Scenario tree with three possible events for two time periods

depending on the number of discrete probability realizations. The nodes (e.g. x21, x22, and x23) that branch from the same node (e.g. x11) are called *child* nodes of the corresponding *parent* node. The *arc* depicts the probability transition from one time period to the next time period of that state. A path that connects the root node to *leaf* node constitute a scenario (e.g. {x11, x21, x31}). Figure 4.3 is an alternate representation of scenario tree given in Figure 4.2. In this representation, each scenario has unique nodes. The horizontal line connecting nodes at each time period indicate identical nodes and have same amount of information. These horizontal lines represent *non-anticipativity constraints*, which state that decisions that emerge from a same parent nodes are the same (Lucia, Finkler, and Engell, 2013). The stage is defined as the set of time periods which has same amount of information. A tree having more than two stages are termed as multi-stage representation and consequently results in a multi-stage stochastic problem.

The forecasting model given by Equations (4.28) and (4.29) is used to generate demand

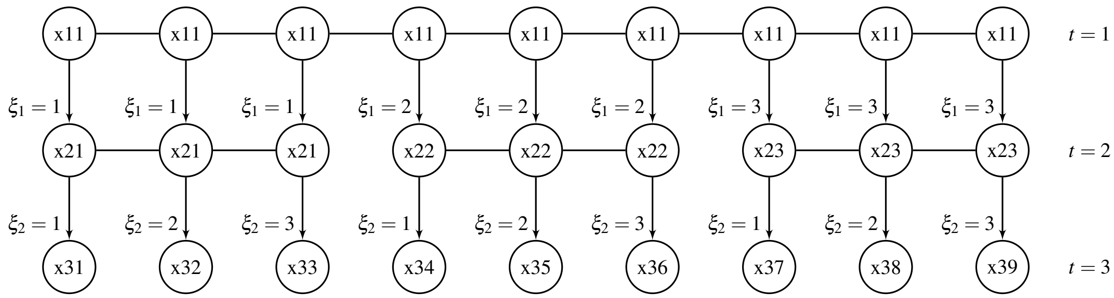

Figure 4.3: An alternate representation of scenario tree with three possible events for two time periods

scenarios,

$$D^F_{j,d,t^*+l,s} = D^F_{j,d,t^*+l-1} + a_{j,d,t^*+l,s} \qquad \forall\ j \in J^P, d, s, l = 0 \quad (4.28)$$

$$D^F_{j,d,t^*+l,s} = D^F_{j,d,t^*+l-1,s} + a_{j,d,t^*+l,s} - \theta_{j,d}\ a_{j,d,t^*+l-1,s}, \forall\ j \in J^P, d, s, l = 1, \ldots, n-1 \quad (4.29)$$

where l is the forecast lead time, and the input $a_{j,d,t^*+l,s}$ is sampled from a normal distribution, $a \sim \mathcal{N}(\mu, \sigma^2)$. The demand forecast depends on the demand resolved at the previous time period ($t^* - 1$) as illustrated by Equation (4.28). This strategy addresses the autocorrelation and moving average nature typically apparent with demand. This is expected to lead to less conservative control action than assuming independent demand uncertainty at each future time period. The process yield of intermediate and final product j at each plant site m is approximated by a normal distribution. Independent process yield scenarios are generated by sampling from the continuous distribution. Each scenario s represents an outcome of both the demand trajectory and process yield parameters of the model. Each scenario is then assigned an equivalent probability of occurrence, with the summation of probabilities for all scenarios equal to 1, i.e. $\rho_s = 1/ns$, where ns is the number of scenarios generated for capturing uncertainty.

4.5 CONTROL PROBLEM FORMULATION

4.5.1 Performance Function

A number of quantitative metrics exist for evaluating the performance of a supply chain, a comprehensive review of which is given in Beamon (1999). Two key criteria considered here are an evaluation of economics and customer service. Equation (4.30) represents the total summation of back orders, denoting a measure of customer service. Equation (4.31) represents the total operating cost in terms of the variables defined in the state-space model, where C_x is a vector of cost coefficients for the held inventory in the plant and distribution site, and C_u is a vector of costs associated with the decision variables (i.e. raw material procurement, production and transportation). Operating cost denotes a measure of economic performance.

$$\mathfrak{J}_1 := \sum_{t=1}^{n-1} \left[\sum_{j,d} B_{j,d,t+1} \right] \tag{4.30}$$

$$\mathfrak{J}_2 := \sum_{t=1}^{n-1} \left[C_x^{\mathsf{T}} x_{t+1} + C_u^{\mathsf{T}} u_t \right] \tag{4.31}$$

The multi-objective optimization problem is solved by applying the weighted-sum method indicated by Equation (5.66),

$$\mathfrak{J}^* := \omega_1 \mathfrak{J}_1 + \omega_2 \mathfrak{J}_2 \tag{4.32}$$

where ω_1 and ω_2 are the weighting parameters for performance metrics. The ratio of ω_1 to ω_2 is a tunning parameter in the optimization, defined here as $\kappa := \omega_1/\omega_2$. Finally, it is important to mention that the performance function ($\mathfrak{J}^*$) is linear, thus giving rise to a linear MPC framework.

4.5.2 Nominal MPC

The primary objective of MPC is to determine the trajectory of future inputs that optimizes a performance criterion over a specific prediction horizon. Once the optimal input trajectory is computed, only the first control action is implemented on the process at the current time period. This reflects a key benefit over open-loop optimization, because at the next sampling instance, new state information is available from the process, and the optimal input trajectory is re-computed. In the presence of plant-model mismatch and unmeasured disturbances, the current solution trajectory is likely no longer an optimal or even feasible solution for subsequent time periods.

4.5.3 Open-loop Approach to Robust MPC

The open-loop approach denoted here as ROF (robust open-loop formulation), utilizes a stochastic supply chain model and disturbance parameter to predict future system behavior. A scenario-based approach is applied to capture the uncertainty in product demand and process yield. A control trajectory is computed that is robust for all scenarios, and the entire control trajectory is computed before uncertainty is resolved (i.e. no recourse action). The ROF is given by,

$$
\begin{aligned}
\min_{u_t,\, h_t} \quad & \mathbb{E}[\mathfrak{J}^*] := \textstyle\sum_s \rho_s \mathfrak{J}^*_s && && (4.33a)\\
\text{s.t.} \quad & f(x_{t,s}, u_t, h_t, \ldots, h_{t-q}, d_{t,s}, c_1) \leq 0 && \forall\ s,\ t && (4.33b)\\
& g(x_{t+1,s}, x_{t,s}, u_t, , \ldots, u_{t-q}, d_{t,s}, c_2) = 0 && \forall\ s,\ t && (4.33c)\\
& x_{1,s} = \tilde{x} && \forall\ s && (4.33d)\\
& x_{t,s} \in \mathbb{R}^{n_x} && \forall\ s, t && (4.33e)\\
& u_t \in \mathbb{R}^{n_u} && \forall\ t && (4.33f)\\
& h_t \in \{0, 1\} && t && (4.33g)
\end{aligned}
$$

where, objective function, $\mathbb{E}[\mathfrak{J}^*]$ represents the expectation of the dynamic performance of the supply chain system, which is a Monte Carlo estimator of the true expected value of $\mathfrak{J}^*$ (Liu and Sahinidis, 1996). Unlike *min-max* robust MPC where the worst-case performance is optimized, the open-loop approach optimizes the expectation over all scenarios which is less conservative. s refers to the scenario resolved, ρ_s is the probability of scenario s occurring, n is the length of the prediction horizon, and $\tilde{x}$ represents the initial value of the state variables. Optimizing the expectation of the dynamic performance is typically less conservative than optimizing the worst-case performance (i.e. min-max) used in some robust MPC formulations.

The uncertainty in customer demand is characterized by the uncertain elements within the disturbance vector $d_{t,s}$. Demand uncertainty is resolved after decisions in the current time period are computed, i.e., after the execution of the model predictive controller. Uncertainty in the intermediate and final product yield within the manufacturing sites (i.e β^P_{ps}) is captured by the model function $g(\cdot)$. The yield can be thought of as an end-point quality of the batch (resolved after the batch operation is complete). The uncertainty in yield is resolved after the batch is complete.

We consider the current time period for which control actions need to be computed correspond to $t = 1$, with the prediction horizon extending to $t = n$. As discussed earlier, the production constraints use a backward time formulation that involves binary variables corresponding to a number of previous time periods. These discrete inputs, h_t for $t < 1$, are known and treated as parameters which are embedded within c_1 and c_2 in Equation (4.33c). At the end of the control period, ΔT, the control horizon shifts relative to the actual time period, denoted by t^*, with the controller time periods again running from 1 to n.

4.5.4 Two-stage Stochastic Programming Robust MPC

The ROF proposed in Section 4.5.3 may result in overly conservative control action causing excess safety stock, because in actual operation the effect of uncertainty is partly mitigated by feedback. To rigorously model the future closed-loop behavior, a multi-stage stochastic approach can be applied. The basic idea of a multi-stage approach is to make a decision before an uncertain event occurs, and then to take some corrective actions after uncertainty is resolved and more information is available by keeping previous stage decisions unchanged. In SCM, where decisions are made over multiple time periods as uncertainty is revealed over time, the decision-making procedure naturally lends to a multi-stage stochastic formulation. In a multi-stage approach, future control actions are taken in response to how the states have been evolved over time to resolve uncertainty and hence tends to take more optimal realistic actions. As the name suggests, the decision-maker takes corrective measures over a sequence of stages. If the process happens only in two stages, then the problem corresponds to a two-stage stochastic program. Naturally, multi-stage decision-making step demands a high computation burden, thus the resulting problem becomes computationally expensive and intractable when the number of stages and scenarios become large. In such cases, a two-stage framework can be employed to approximate the multi-stage decision-making procedure. First, we present a two-stage stochastic programming framework for clarity of model representation and then introduce a multi-stage stochastic programming framework.

In two-stage stochastic programming, decision making for the first time period occurs before uncertainty realization, and the decisions for the remaining time periods are postponed until uncertainty resolved (i.e. second stage). As with MPC, only the first time period decisions are implemented, it approximates a closed-loop approach though decisions computed after the first time period no longer hedge against the possibility that another scenario can resolve. The closed-loop approach to robust MPC, denoted here as RCF (robust closed-loop formulation) is given by,

$$\min_{\Gamma} \quad \mathbb{E}[\mathfrak{J}^*] := \mathfrak{J}^{(1)^*} + \textstyle\sum_s \rho_s \mathfrak{J}_s^{(2)^*} \tag{4.34a}$$

$$\text{s.t.} \quad f(x_{1,s}^{(1)}, x_{t,s}^{(2)}, u_1^{(1)}, u_{t,s}^{(2)}, h_1^{(1)}, h_{t,s}^{(2)}, \ldots, h_{t-q,s}^{(2)}, d_{t'}^s, c_1) \leq 0 \quad \forall\, s,\ t', t = 2, \ldots, n \tag{4.34b}$$

$$g(x_{1,s}^{(1)}, x_{t+1,s}^{(2)}, x_{t,s}^{(2)}, u_1^{(1)}, u_{t,s}^{(2)}, \ldots, u_{t-q,s}^{(2)}, d_{t'}^s, c_2) = 0 \quad \forall\, s,\ t', t = 2, \ldots, n \tag{4.34c}$$

$$x_{1,s}^{(1)} = \tilde{x} \quad \forall\, s \tag{4.34d}$$

$$x_{1,s}^{(1)} \in \mathbb{R}^{n_x} \qquad \forall\ s \tag{4.34e}$$
$$u_1^{(1)} \in \mathbb{R}^{n_u} \qquad \forall\ s \tag{4.34f}$$
$$x_{t,s}^{(2)} \in \mathbb{R}^{n_x} \qquad \forall\ s,\ t = 2,\ldots,n \tag{4.34g}$$
$$u_{t,s}^{(2)} \in \mathbb{R}^{n_u} \qquad \forall\ s,\ t = 2,\ldots,n \tag{4.34h}$$
$$h_1^{(1)} \in \{0,1\}^{n_h} \tag{4.34i}$$
$$h_{t,s}^{(2)} \in \{0,1\}^{n_h} \qquad \forall\ s, t = 2,\ldots,n \tag{4.34j}$$

where superscript (1) denotes a first stage variable, and (2) denotes a second stage variable. Γ represents the decision variables: $u_1^{(1)}$, $h_1^{(1)}$, $u_{t,s}^{(2)}$, and $h_{t,s}^{(2)}$ for $t = 2,\ldots,n$. $\mathfrak{J}^{(1)^*}$ represents the first stage performance objective defined as,

$$\mathfrak{J}^{(1)^*} := \omega_2 \left[C_u^\mathsf{T} u_1^{(1)}\right] \tag{4.35}$$

and $\mathfrak{J}_s^{(2)^*}$ represents the second stage performance objective for scenario s, defined as,

$$\mathfrak{J}_s^{(2)^*} := \omega_1 \mathfrak{J}_{1,s} + \omega_2 \left[\sum_{t=1}^{n-1}\ C_x^\mathsf{T} x_{t+1,s}^{(2)} + \sum_{t=2}^{n-1}\ C_u^\mathsf{T} u_{t,s}^{(2)}\right] \tag{4.36}$$

with $\mathfrak{J}_1$ as defined in Equation (4.30).

4.5.5 Multi-stage Stochastic Programming Robust MPC

The accuracy of closed-loop feed-back policy embedded within robust MPC depends on how precise the uncertainty representation is. If the scenario tree describes the evolution of the uncertainty perfectly, it computes an optimal feed-back policy; otherwise, it generates an approximate closed-loop response and the approximation depends on its closeness to actual uncertainty unfolding characteristic. For a better approximation of stagewise uncertainty unfolding in the decision-making process, the two-stage stochastic formulation can be extended to a multi-stage formulation. In multistage stochastic programming, the decisions are segregated into multiple sets rather than being limited to only two sets. The first-stage decisions are made before uncertainty is realized, and decisions correspond to the rest of the stages ($2\ldots n$) are postponed until next round of uncertainty realization (i.e., second stage) occurs. The process continues till it reaches the $n^{th}-$stage. Moreover, the control actions at the nodes which have same parent node need to be equal because the real-time decisions can not anticipate the future realization of uncertainty (*non-anticipativity nature*). The multi-stage stochastic robust MPC problem, denoted as

RMF (robust multistage formulation), is given by,

$$\min_{\Gamma} \quad \mathbb{E}[\mathfrak{J}^*] := \sum_s \rho_s \mathfrak{J}_s^* \tag{4.37a}$$

$$\text{s.t.} \quad f(x^{opt}, u^{opt}, h^{opt}, c_1) \leq 0 \tag{4.37b}$$

$$g(x^{opt}, u^{opt}, c_2) = 0 \tag{4.37c}$$

$$A_u \ u^{opt} = 0 \tag{4.37d}$$

$$A_h \ h^{opt} = 0 \tag{4.37e}$$

$$x_l \leq x^{opt} \leq x_u \tag{4.37f}$$

$$u_l \leq u^{opt} \leq u_u \tag{4.37g}$$

$$x^{opt} \in \mathbb{R}^{n_x \times n_s} \tag{4.37h}$$

$$u^{opt} \in \mathbb{R}^{n_u \times n_s} \tag{4.37i}$$

$$h^{opt} \in \{0, 1\}^{n_h \times n_s} \tag{4.37j}$$

For brevity of representation, $x^{opt}, u^{opt},$ and h^{opt} denote the augmented vector of states, continuous decisions, and binary decision variables respectively. That is,

$$x^{opt} = [\ x_{t,s}^{(1)}, \ldots, x_{t,s}^{(n)}\ ]; \quad u^{opt} = [\ u_{t,s}^{(1)}, \ldots, u_{t,s}^{(n)}\ ]; \quad h^{opt} = [\ h_{t,s}^{(1)}, \ldots, h_{t,s}^{(n)}\ ]$$

where superscript (n) denotes a nth stage variable. The non-anticipativity constraints (4.37d) and (4.37e) force the decision variables to take the same value across stages that have the same uncertainty output characterization. The constraints (4.37f) and (4.37g) represent the upper and lower limits on state and control variables respectively. For ease of explanation, it is assumed that the scenario tree is uniform, i.e., the tree has the same number of branches at all nodes. However, it is apparent that the framework is flexible enough to consider all possible kinds of uncertainty evolution structures. Consider Figure 4.4, which depicts one of many possible non-uniform scenario tree structure, where each branch takes varying values of uncertainty realizations and the number of branches at each stage and/or at each parent node are different. The weights of each scenario can also be changed to reflect the real-time uncertainty behavior.

It is evident that the number of scenarios quickly increases with the number of stages and number of discrete realizations considered at each stage. For a uniform branching structure, the number of scenarios is given by $N_r^{N_t}$, where N_r is the number discrete realizations at each node and N_t is the number of stages. Therefore, the size of resulting optimization problem grows exponentially with the number of stages (i.e. number of time periods). The presence of binary decision variables further increases the computation

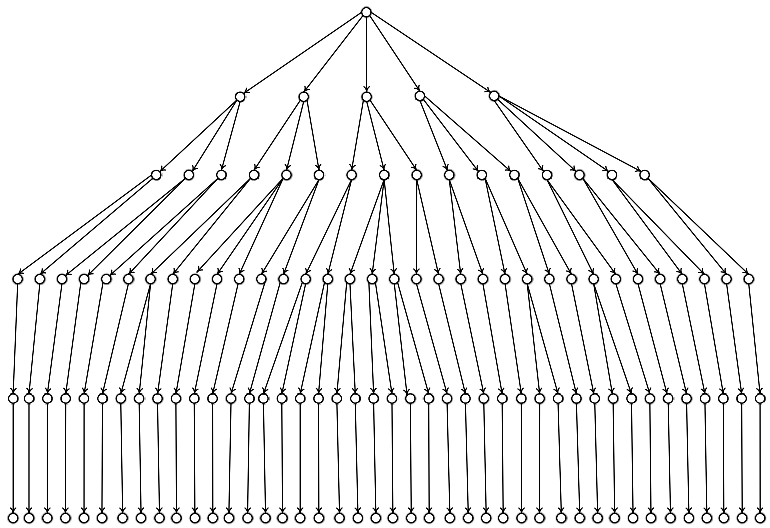

Figure 4.4: Multistage scenario tree structure. One of many possible structures of a multistage scenario tree with 6 time stages

time rapidly. With a specific end goal of reducing the computational burden, (Lucia, Finkler, and Engell, 2013) consider tree branching only up to a certain stage, which they termed as *robust control horizon*[1], and thereafter a constant uncertainty characterization is considered until the end of the prediction horizon (see Figure 4.5). The *robust control horizon* concept follows a similar idea of using a control horizon shorter than the prediction horizon in systems engineering applications for reducing the computation burden. Nonetheless, multi-stage stochastic optimization problem has a very special structure that can be exploited to devise decomposition methodologies to speed up the computation (see Gupta and Maranas, 2003), but this not within the scope of the present work.

Interestingly, the multi-stage stochastic controller formulation given by Equations (4.37a) to (4.37j) is a general framework and can be cast into nominal MPC, open-loop ROF, or two-stage RCF approach. The multi-stage RMF controller translates to the two-stage stochastic RCF controller by setting *robust control horizon* (r^c) to 2. In this case, the tree branching stops at time period $t = 2$, and scenarios become independent after second stage (see Figure 4.6). In other words, the definition of non-anticipativity constrains classifies decision sets into two, *first* and *second* stage decisions. ROF also uses same scenario tree structure as in two-stage RCF approach (see Figure 4.6). Therefore, a multistage stochastic formulation with r^c equal to 2 and restricting decision variables to take same values across different scenarios at each time period t transforms to an *open-loop* ROF controller. In other words, the requirement of generating a single control

[1]Please refer Lucia, Finkler, and Engell (2013) for detailed discussion on robust control horizon.

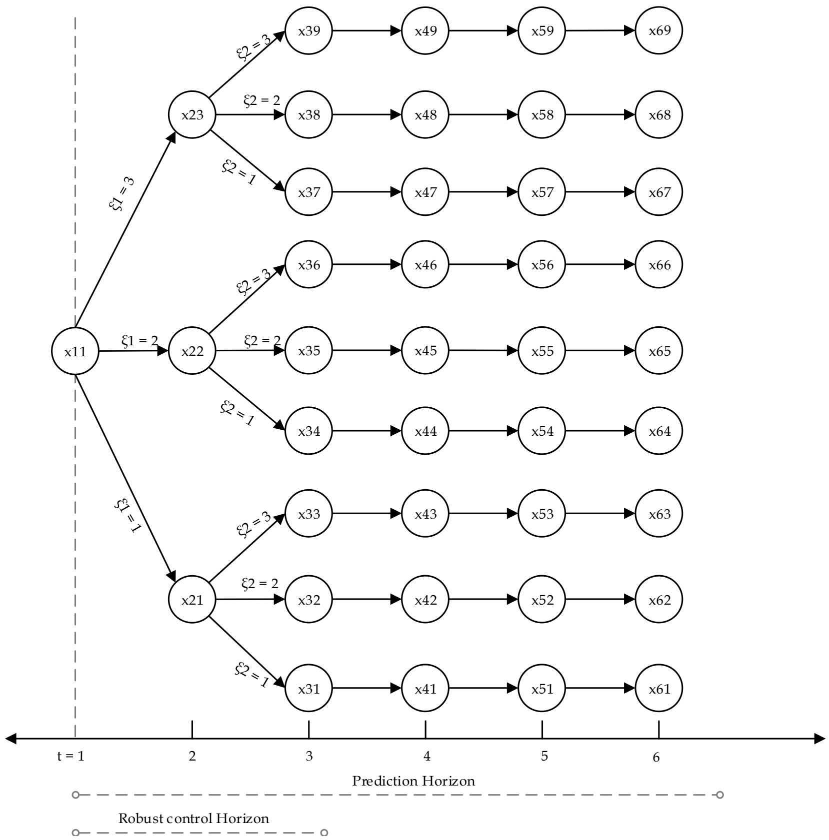

Figure 4.5: Illustration of robust control horizon concept for multi-stage stochastic robust MPC. Robust control horizon is taken as 3 for prediction horizon of length 6

trajectory for each decision variables in ROF can be accomplished by writing extra non-anticipativity constraints at each time period across all scenarios. On a similar note, nominal MPC can be thought of as having a *robust horizon* equal to 1 for the multi-stage stochastic controller. Since $r^c = 1$, no branching will be performed which restricts the number of scenarios to 1. If the future uncertainty characterization is represented by the nominal value of the uncertain parameter for entire prediction horizon, it essentially represents a nominal MPC controller.

4.5.6 Closed-Loop Implementation

Figure 4.7 shows the closed-loop implementation of the MPC framework on a supply chain system. At the first stage, an uncertainty description is generated in the form of yield and demand scenarios as discussed in Section 4.4 and applied within the SC optimizer. At the second stage, an SCO problem is solved to calculate control moves, which are

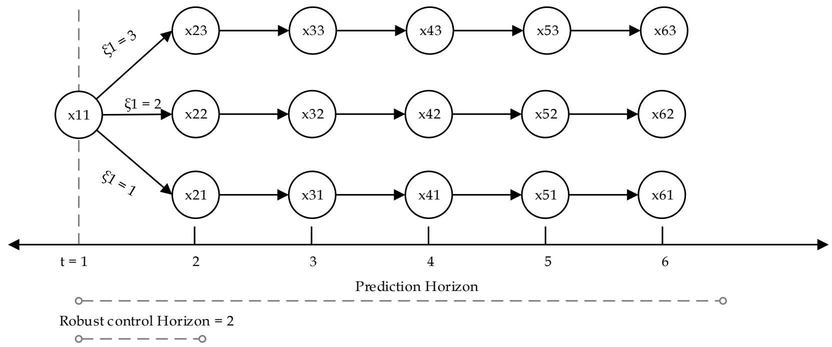

Figure 4.6: Scenario tree representation of uncertainty evolution for multi-stage stochastic controller with robust control horizon of 2

then implemented on the process SC or simulation model. Finally, at next sampling period, state information is updated using feedback information received from the process (or simulation model) and, scenarios (demand and yield) are regenerated. The process continues till it reaches at the end of simulation time horizon. In the implementation, we have taken the sampling time of ΔT (i.e. the same as the model discretization) for the MPC controller; however, this assumption can be readily relaxed.

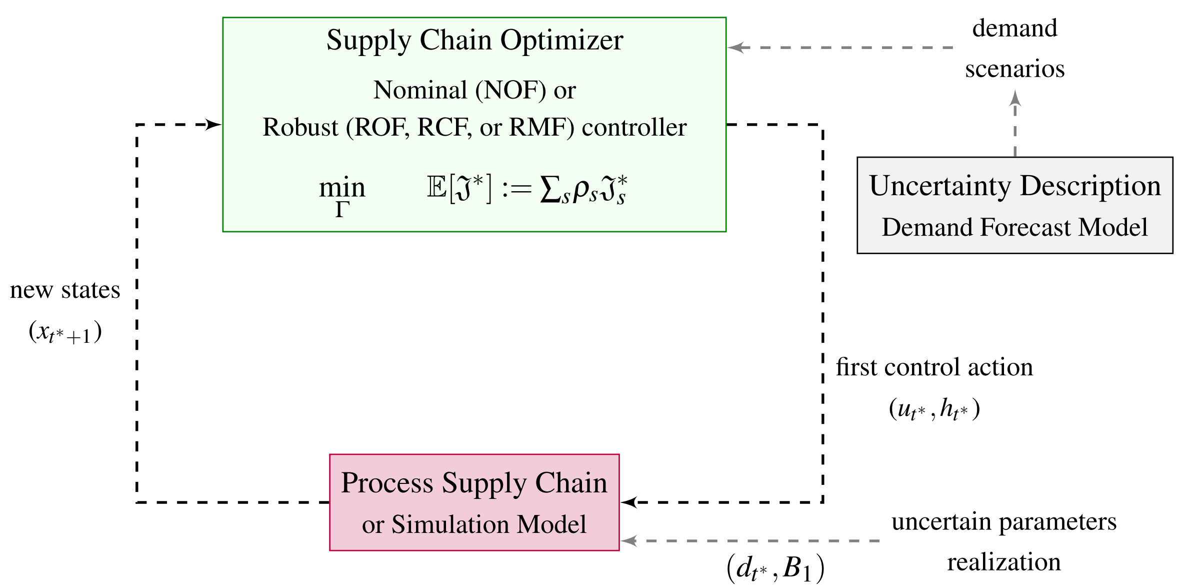

Figure 4.7: Closed loop implementation of robust MPC strategy

4.6 CASE STUDY

To analyze the robust stochastic MPC approaches presented in the previous section, we consider a multi-echelon supply chain case study, and compare the performance of nominal MPC and robust MPC formulations (ROF, RCF, and RMF). A Pareto analysis of economics and customer service is also presented, and the effect of disturbance and model uncertainty is explored. Further, the comparison of closed-loop performance between two multi-stage stochastic formulations is presented.

Case Study Description

The case study illustrates the application of robust control approaches to a multi-product, multi-echelon supply chain comprising of two suppliers ($\mathrm{LS}_1, \mathrm{LS}_2$), two plant sites ($\mathrm{M}_1, \mathrm{M}_2$), and two distribution sites ($\mathrm{DC}_1, \mathrm{DC}_2$). There are total 4 production schemes ($\mathrm{PS}_1, \ldots, \mathrm{PS}_4$) available to produce two final products E and G from two raw materials A and B. Materials C, D, and F are intermediate products. Production schemes PS_1 and PS_3 are available at the intermediate production facility while production schemes PS_2 and PS_4 are available at the final production facility. An intermediate product E is a final product, and therefore it is allowed to be shipped to the distribution center through the warehouse. Plant site M_2 requires the intermediate product D as one of the raw materials for the production scheme PS_3, and thus it can not start the production until it receives the material D from plant site M_1. Case study data are summarized in Tables 4.1 to 4.7. The production schemes installed at plant sites are presented in Figure 4.8 in which the stochiometry of the reaction schemes is also represented. We restrict the inter-plant shipments to originate from the intermediate product or final product storage locations, and to terminate at the raw material or intermediate product storage locations.

Table 4.1: Simulation parameter values for robust MPC study

Parameter	Value	Parameter	Value
n (days)	15	No. of scenarios	50
θ	0.1	Simulation length (days)	40
σ^2 of a	9	Range of yield parameters	$0.45 - 0.95$
Range of D_F	$0 - 50$	ΔT (days)	1

We compare the performance of the ROF and RCF schemes to the performance of a nominal MPC implementation, denoted by NOF (nominal open-loop formulation), that does not

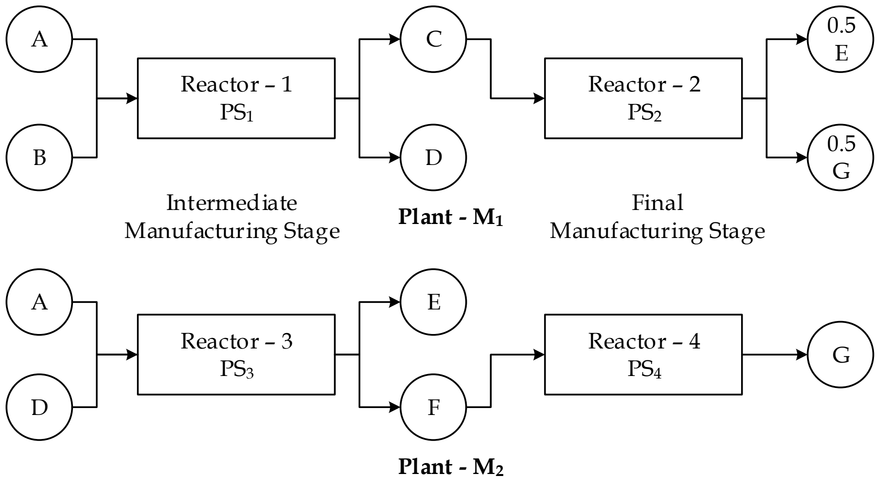

Figure 4.8: Production network consists of total four production schemes. Schemes PS_1 and PS_2 are installed at plant site M_1 and PS_3 and PS_4 are installed at plant site M_2

Table 4.2: Shipment and production cost parameters for the robust MPC case study

	Shipment Cost of F^P in C_u		Shipment Cost of F^F in C_u		Production Cost of P^I in C_u		Production Cost of P^F in C_u	
Plant site	Plant site		Distribution site		Production Task			
	M_1	M_2	D_1	D_2	PS_1	PS_3	PS_2	PS_4
M_1	–	4	2.7	2.8	1.25	1	–	–
M_2	4	–	2.8	2.5	–	–	1.3	1.5

Note: The shipment costs are the same for all chemicals within each shipment category.

Table 4.3: Material purchase cost for the robust MPC case study ($/unit)

Raw material	Suppliers	
	LS_1	LS_2
A	1	1.2
B	1.4	1.7

Table 4.4: Product back-order cost for the robust MPC case study ($/unit)

	Material	
	E	G
Cost ($/unit)	1.4	1.7

explicitly account for uncertainty. In the NOF, uncertain model parameters are assigned average values, and the demand forecast within the prediction horizon is conisdered as the demand resolved at the previous time period. In the ROF and RCF algorithms, uncertainties in customer demand and process yield are considered and characterized by 50 independent scenarios having an equal probability of occurrence. Demand scenarios

Table 4.5: Inventory parameter values for the robust MPC case study

Parameter	Plant site		Distribution site	
C_x	M_1	M_2	D_1	D_2
Cost of I^R	0.8	0.7	–	–
Cost of I^I	0.9	1.1	–	–
Cost of I^F	1.4	1.1	–	–
Cost of I^S	–	–	1.5	1.25
storage capacity Ω^R/ Ω^I/ Ω^F_E/ Ω^F_G/ Ω^S_E/ Ω^S_E	500	500	–	–

Note: The inventory costs are the same for each chemical within each inventory category.

Table 4.6: Production parameter values for the robust MPC case study

Parameter	Plant site	Production Scheme PS_1	PS_3	PS_2	PS_4
γ^{M^u} : production batch size					
	M_1	120	300	–	–
	M_2	–	–	120	150
γ^{M^l} : production batch size					
	M_1	25	60	–	–
	M_2	–	–	25	25
δ^M_{ps} : production delay (day)	–	1	2	2	1
μ of β^P_{PS}	–	0.8	0.7	0.8	0.7
σ^2 of β^P_{PS}	–	0.0025	0.0025	0.0025	0.0025

Table 4.7: Transportation parameter values for the robust MPC case study

Plant site	Supplier LS_1	LS_2	Distribution site D_1	D_2	Plant site M_1	M_2
transportation delay	δ^R		δ^S		δ^P	
M_1	3	3	3	4	0	2
M_2	2	2	4	2	2	0
transportation quantity	λ^R		λ^S		λ^P	
M_1	120	120	100	100	0	100
M_2	120	120	100	100	100	0

are generated using the method presented in Section 4.4.1. The “actual” supply chain system is represented by a simulation model that reflects a particular outcome of the uncertain model parameters. Furthermore, a demand trajectory is computed from the forecast model which represents the “actual” demand resolved. Each closed-loop case is simulated, as depicted in Figure 4.7, for a 40 day period. The performance of the closed-loop simulation is compared in terms of the supply chain metrics in the objective function of the supply chain optimization (i.e. operating cost and summation of back orders), as well as an alterative metric of customer service, which indicates the percentage of demand filled immediately, denoted as fill rate (FR) (Beamon, 1999).

The SCO problem is modeled with `AMPL` and solved using `CPLEX 12.5` to a 1% optimality gap. Simulations are performed on a 3.4 GHz Intel®Core^{TM} i7 machine with 8 GB of RAM, running Windows 7 Professional 64-bit. Table 4.8 summarizes the model size of each optimization framework. It is evident from Table 4.8 that, number of continuous and binary variables are significantly higher in RCF than in ROF and NOF, since second stage decision variables are dependent on the number of scenarios considered.

Table 4.8: Size of supply chain optimization formulation for the robust MPC case study

Framework	Continuous Variables	Discrete Variables
NOF	956	58
ROF	16,789	58
RCF	38,321	2,753

4.6.1 Pareto Analysis

Because a tradeoff exists between customer satisfaction and economics, the optimal solution generates a frontier denoted as a Pareto curve, which is shown in Figure 4.9 (o : $\mathfrak{J}_1$ *vs.* $\mathfrak{J}_2$). The two-objectives are weighted by weighting parameters (ω_1 and ω_2), the ratio $\kappa := \omega_1/\omega_2$ is been considered as a tuning parameter in the SC optimization problem. Essentially, a high value of κ depicts a scenario with more weight on satisfying customer orders against optimizing cost, while a low value translates to giving more weight to optimizing operating cost. A number of ROF closed loop simulations are performed with different values of κ. The values of objective function components $\mathfrak{J}_1$ and $\mathfrak{J}_2$ are calculated and plotted in Figure 4.9. Each data point shows the average performance over 20 independent simulations runs, having a distinct realization of demand and process yield uncertainty in each of the 20 simulation runs.

The Pareto curve shows a decreasing exponential relationship between cost and customer satisfaction. Lower customer satisfaction (high backorder cost) results in low cost as less safety stock is held to hedge against uncertainty. The customer service increases (i.e back order $\mathfrak{J}_1$ decreases) rapidly with a minimal increase in cost until location (1). However, for the region to the right of location (1) on the Pareto curve, the operating cost increases rapidly with a minimal increase in the customer service (minimal decrease in back orders, $\mathfrak{J}_1$). Therefore, from the cost perspective, it is preferable to operate the supply chain at the point (1) on the pareto curve than at (2). Thus, it is clear that κ has a strong influence on the controller action and therefore it is considered as tuning parameter in the MPC implementation.

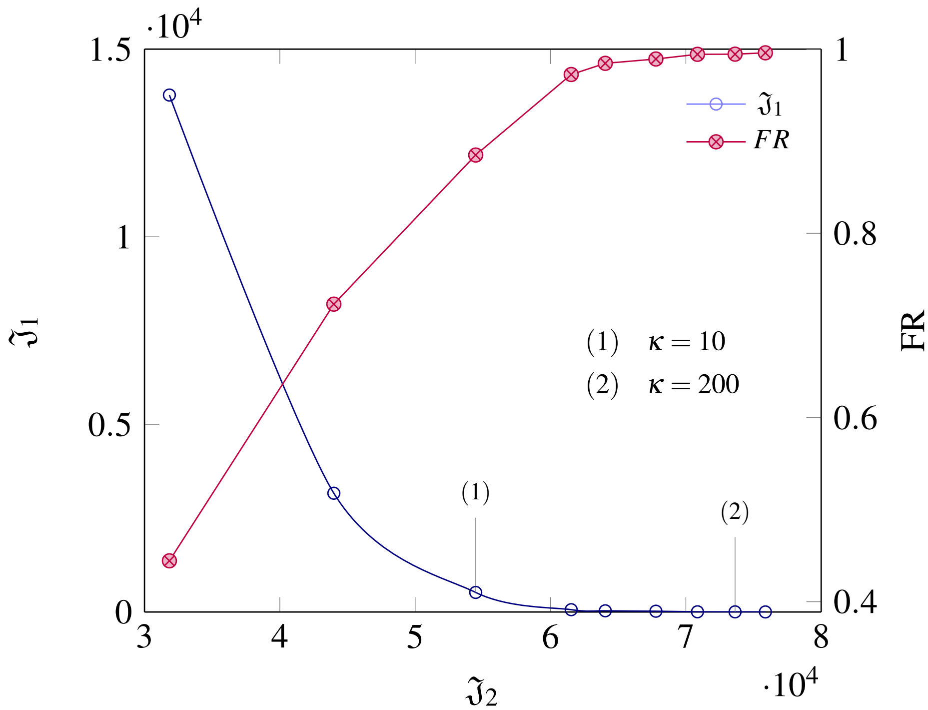

Figure 4.9: Pareto relationship between operating cost ($\mathfrak{J}_2$) and customer service ($\mathfrak{J}_1$) with ROF (Each data mark corresponds to average performance for 20 independent closed-loop simulations)

The relation between fill rate (FR) and economics ($\mathfrak{J}_2$) is shown by a blue dotted line (• - FR *vs.* $\mathfrak{J}_2$) in Figure 4.9. It shows that the fill rate improves with increase in cost, in other words the trend of fill rate corresponds to the trend of customer service. The points (1) and (2) indicate the increase in fill rate from 88% to 99% with the correspond increment in the cost from 54473 to 73637 monetary units (an increment of 35%). In conclusion, the Pareto curve provides an analytical tool to determine the optimal value of tuning parameter κ in the optimization problem. The Pareto curve for different supply chain environments are different and controller tuning needs to be selected based on operational preferences of a given supply chain.

4.6.2 Closed-Loop Performance Comparison with RCF, ROF, and NOF

Graphical comparison for single outcome

Figures 4.10 to 4.12 show the performance of closed-loop simulations with the RCF, ROF, and NOF control approaches for the same outcome of demand and yield uncertainties. Due to space limitations, only representative trajectories are included. All the cases are run with a κ value of 100. Figure 4.10 illustrates the closed-loop result with the NOF. A large amount of product back orders occurs for product E after day 15 as shown by the back order trajectories, B (DC_1), in Figure 4.10. Inventory of final product E at both distribution sites is driven to zero and thus results in insufficient stock to fulfill customer demand. The back order amount for the product G is comparatively lower than product E; however the inventory quickly vanishes to zero and therefore a back order situation arises after day 12. In the plots, the terms in parentheses indicate one or a combination of chemical, distribution center, manufacturing facility, production scheme, and demand. For example, P^I(A-PS_1-M_1) in subplot (2,2) in Figure 4.10 represents the consumption amount of material A in production scheme PS_1 at plant site M_1.

Figure 4.11 shows the closed-loop result for the ROF approach. As it considers uncertainty information at each controller execution, adequate safety stocks for all materials are maintained throughout the supply chain to meet varying demand. We can observe from Figure 4.11 that it does not create a stockout condition for either product throughout the simulation run, shown by the trajectory of back orders (B), with the ROF, as compared to the NOF.

Figure 4.12 illustrates the closed-loop result with the RCF. From the plot, it can be seen that it generates less conservative actions as it includes the effect of future control actions. The operating cost for the RCF is 8.5% less than the ROF approach with same customer satisfaction level. Analogous to the ROF approach, it chooses to maintain safety stock to hedge against uncertainty and therefore it does not show any back orders for the entire simulation run. It should be noted that for certain demand uncertainty realizations, the NOF simulation encounters a problem of insufficient storage capacity as it does not consider the demand uncertainty. Therefore, the storage capacity constraints in the NOF simulations are implemented as soft constraints with a large penalty.

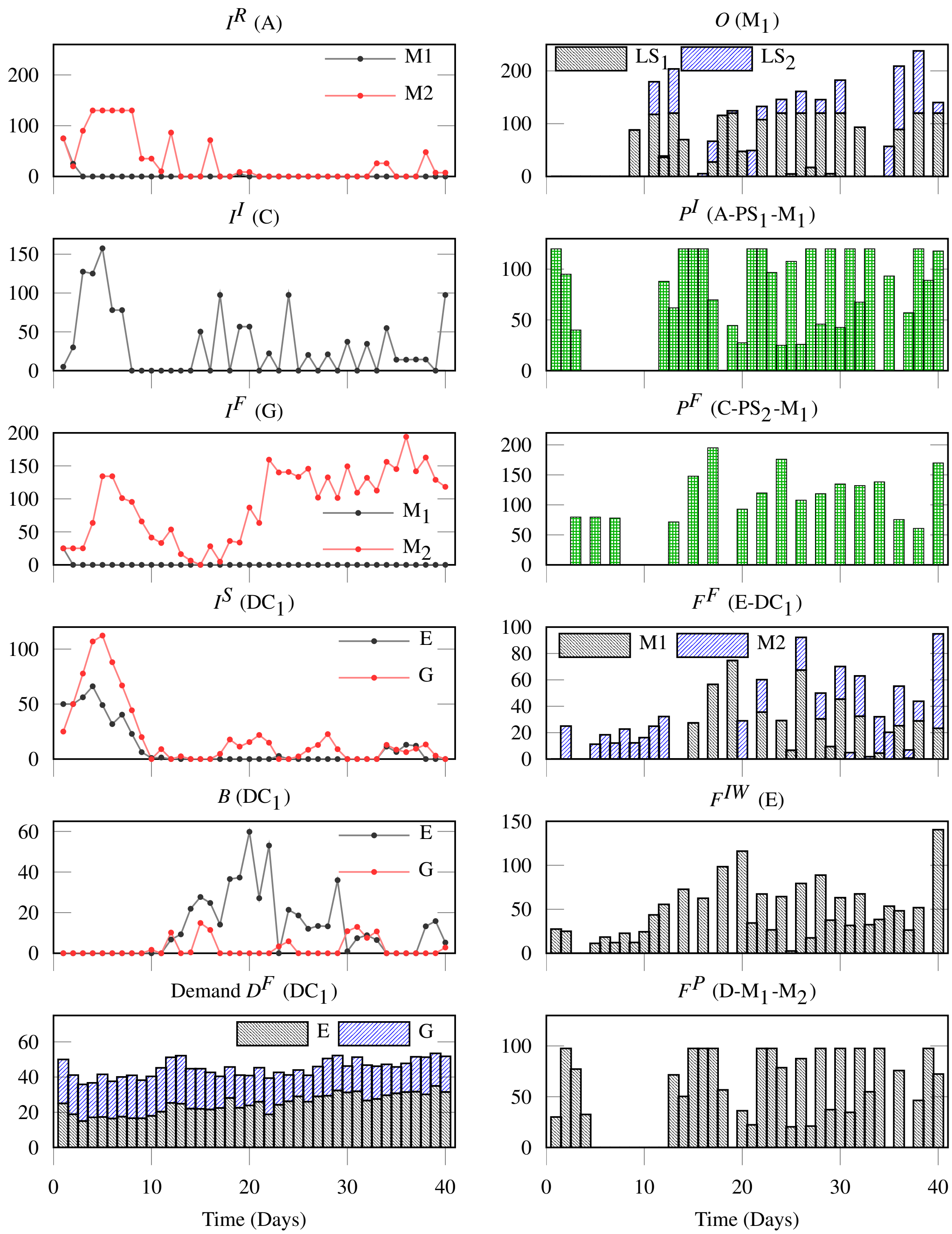

Figure 4.10: Representative inventory, production, and shipment profiles generated with NOF controller

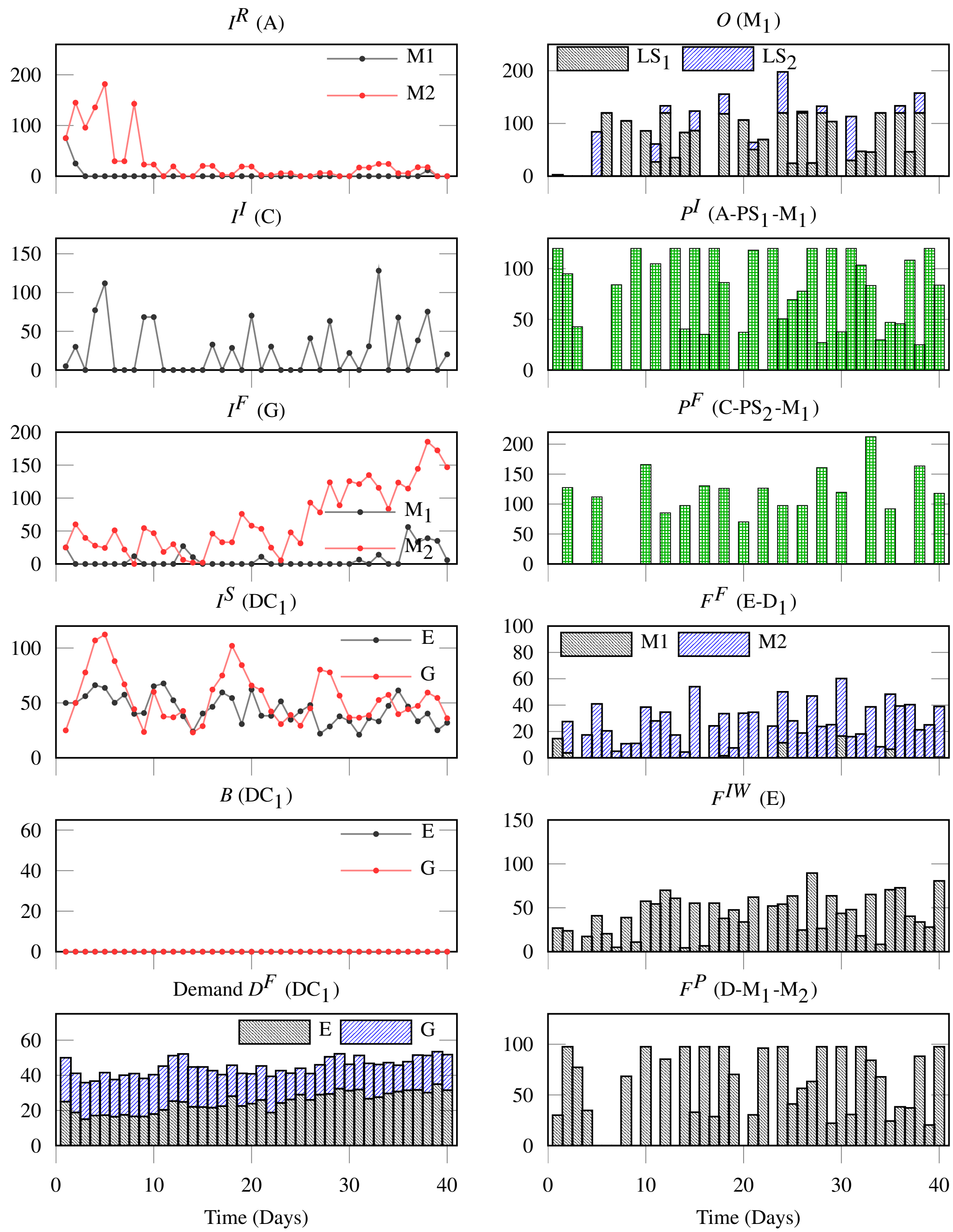

Figure 4.11: Representative inventory, production, and shipment profiles generated with ROF controller

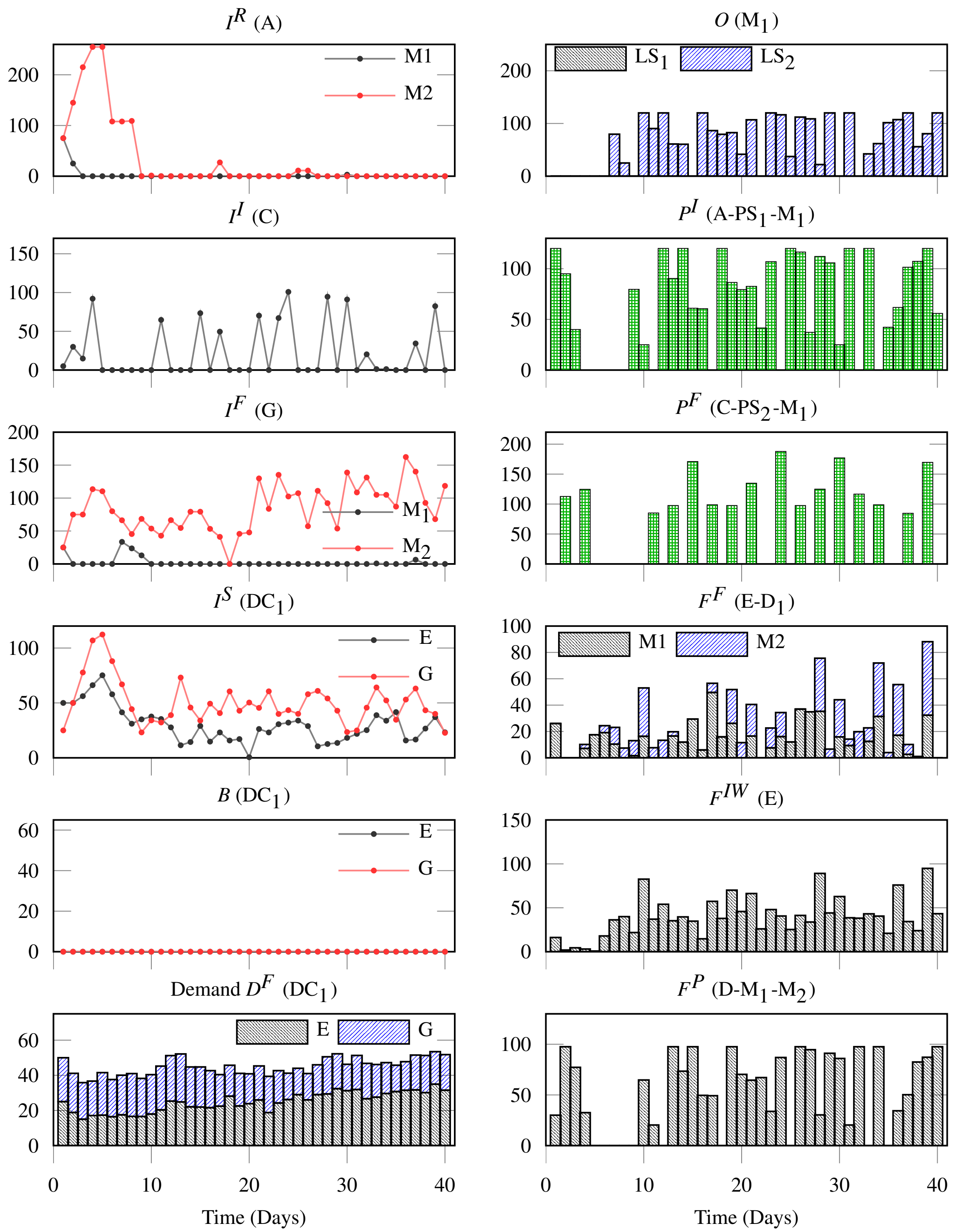

Figure 4.12: Representative inventory, production, and shipment profiles generated with RCF controller

Comparison between multiple simulations

Table 4.9: Size of supply chain optimization formulation

Framework	Case (κ)	Continuous Variables	Discrete Variables	$\mathfrak{J}_1$	$\mathfrak{J}_2 \times 10^{-4}$	FR	CPU (s)
NOF	− (100)	956	58	948.9	5.619	0.665	0.14
ROF	B (100)	16,789	58	8.3	6.972	0.992	6.8
RCF	B (100)	38,321	2,753	38.9	6.292	0.980	73.7

Note: Results correspond to the average performance over 20 independent closed-loop simulations.
B: Both uncertain demand and yield (50 scenarios applied to capture uncertainty in robust MPC frameworks)

In order to check in-depth behavior of the system dynamics with implementing ROF, RCF, and NOF, we performed a number of closed loop simulation runs. The performance is reported with the average values obtained by running 20 independent simulation runs with a κ value of 100. The simulation results are summarized in Table 4.9. The tabulated result shows that a significant improvement in performance is achieved with robust frameworks in compare with nominal framework. The amount of back orders for the RCF and ROF approach is relatively low compared to NOF approach, which indicates a large improvement in customer service level ($\mathfrak{J}_1$). The average fill rate with the NOF is 0.65 as compared to 0.98 with the RCF and 0.992 with the ROF.

The improvement in customer service for the RCF and ROF approaches are achieved at the expense of higher operating cost. The ROF and RCF approach maintained sufficient levels of safety stock of all materials in the supply chain to hedge against the demand and yield uncertainty and therefore they give rise to a higher operating cost. However, the robust frameworks maintain the right amount of safety stock to trade against the customer service and therefore the increase in operating cost is lower in comparison to a sharp improvement in the customer service level. As expected, RCF outperforms ROF in terms of the operating cost. RCF achieved similar level of customer satisfaction (drop of only 1.2%) as ROF at lesser cost (10.82%) as the presence of predicted feedback information in RCF helps it to not take overly conservative actions. Table 4.9 indicates the average computation time for one controller execution. The average computation time for the RCF and ROF is larger than the NOF but it still very modest considering the SCM sampling time of one day.

4.6.3 Effect of Fine Tuning Parameter κ

It should be noted from the previous simulation results (see Table 4.9) that κ has a significant influence on performance and same value of κ generates different control actions with the ROF and RCF. To further investigate the effect of fine tuning of parameter κ, several simulations are run with ROF and RCF at different value of κ and pareto curves are generated. The Pareto curves generated with the ROF and RCF are illustrated in Figure 4.13.

The pareto curve generated with RCF lies left to the curve generated with the ROF which indicates that an equivalent customer service level can be achieved with lower operating cost in the case of RCF than in ROF. Similarly, the point (1) is generated with a κ value of 3 with RCF while (2) is generated with a value of 5 with ROF, which illustrates that comparable customer service level can be achieved in RCF and ROF using different values of κ. In the case of points (1) and (2), the cost with ROF is 43991 monetary units, 16% more than RCF case (37886 units), while the customer service level is 5% higher. The spacing between two curves are not same at all levels and the percentage saving varies across the length of pareto curve. At high levels of customer service, the Pareto curves converge; however, a small percentage increment in economics results in a large dollar value in the SC network case.

Next, we consider the sensitivity of changing the κ value on the supply chain performance. Plot 4.14 depicts the sensitivity curve with the RCF and ROF. The acceptable customer service level is illustrated by a shaded region. The region outside the acceptable region is conservative (below) or non-robust (above). The “acceptable region" is depends on SC operating procedure and management principles. The ROF curve takes an exponential shape and is more sensitive to the ratio, while the RCF curve is linear and its performance is therefore less sensitive than ROF. Consequently, the range of κ for the customer service to stay in the acceptable region is significantly larger with RCF ($\varphi_1 > \varphi_2$), which in turn can be used to adjust the performance on a longer range.

4.6.4 Comparing Closed-Loop Performance with RMF and RCF

In this section, we compare the performance of two robust closed loop frameworks, multistage formulation (RMF) and two-stage formulation (RCF). In RMF, we consider 3-stage stochastic programming.

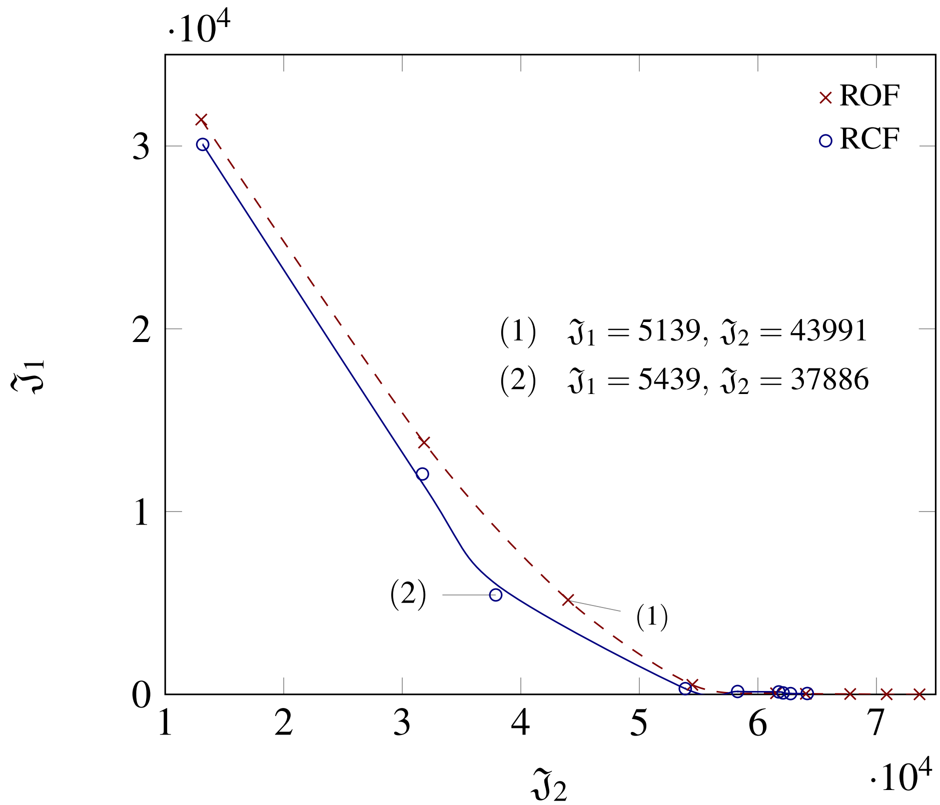

Figure 4.13: Pareto curve generated with ROF and RCF (Each data mark corresponds to average performance for 20 independent closed-loop simulations)

Graphical comparison for single outcome

The closed-loop performance with RCF and a 3-stage RMF controller is shown in Figures 4.15 and 4.16 for the same outcome of demand and yield uncertainty. A κ value of 5 is used to generate the closed-loop trajectories. The RMF case systematically responds to the demand uncertainty in three stages compared to only two stages in RCF and keeps the optimal amount of inventory. Therefore it results in lower back order amount than in RCF (please refer subplot (4,2) in Figures 4.15 and 4.16). The title of subplot (2,2) P^I(A-PS$_1$-M$_1$) can be read as the consumption amount of material A in production scheme PS$_1$ at plant site M$_1$.

Comparison between multiple simulations

A number of closed-loop simulations are performed with the RCF ($2-$stage) and 3-stage RMF controller. The performance is reported with the average values obtained by running 30 independent simulation runs with a κ value of 5. We consider 6 possible events at

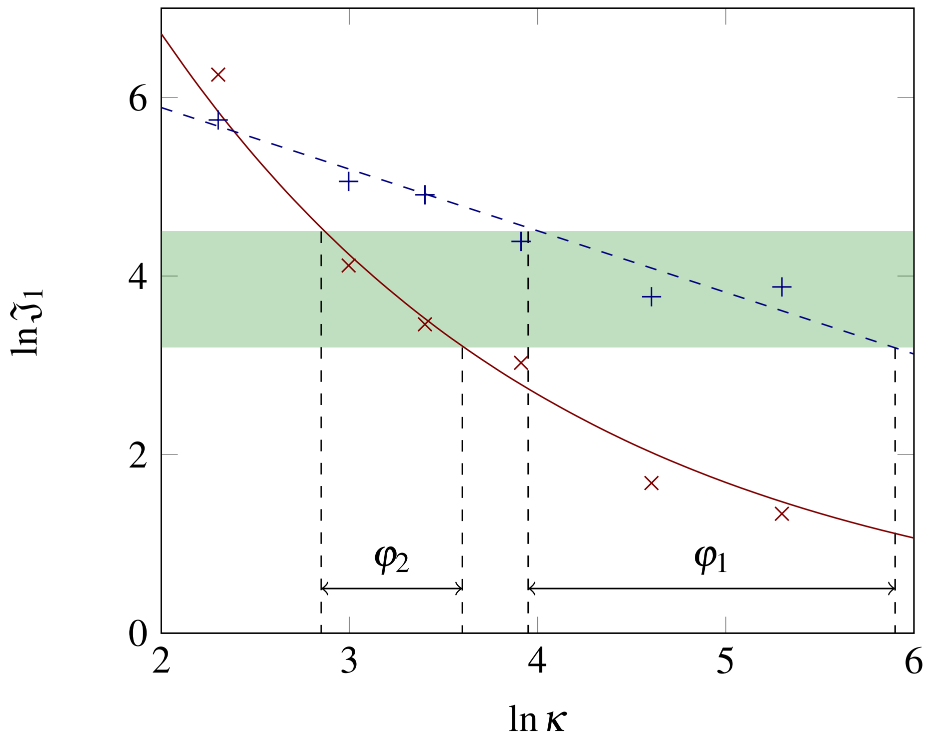

Figure 4.14: Comparing the sensitivity of the ratio between weighting parameter (κ) to the closed-loop customer service performance with ROF and RCF (× — ROF ; + - - RCF) (Each data mark corresponds to average performance for 20 independent closed-loop simulations)

each stage (see Figure 4.2) to represent demand uncertainty that translates to 6 demand scenarios for RCF and 36 demand scenarios for 3-stage RMF at each controller execution. The simulation results are summarized in Table 4.10. The result indicates that the 3-stage RMF controller yields low amount of back-orders compared to RCF, i.e. an improvement in customer service level ($\mathfrak{J}_1$). The average fill rate with the RCF is 0.937 as compared to 0.992 with the 3-stage RMF.

Table 4.10: Size of supply chain optimization formulation (6 uncertain events at each stage in robust MPC frameworks)

Framework	Case (κ)	# scenarios	Continuous Variables	Discrete Variables	$\mathfrak{J}_1$	$\mathfrak{J}_2 \times 10^{-4}$	FR	CPU time (sec)
RCF	B (5)	6	1980	330	108.6	5.9788	0.937	1.87
3-stage RMF	B (5)	36	27577	4645	2.7	6.4375	0.994	77.26

Note: Results correspond to the average performance over 30 independent closed-loop simulations.
B: Both uncertain demand and yield

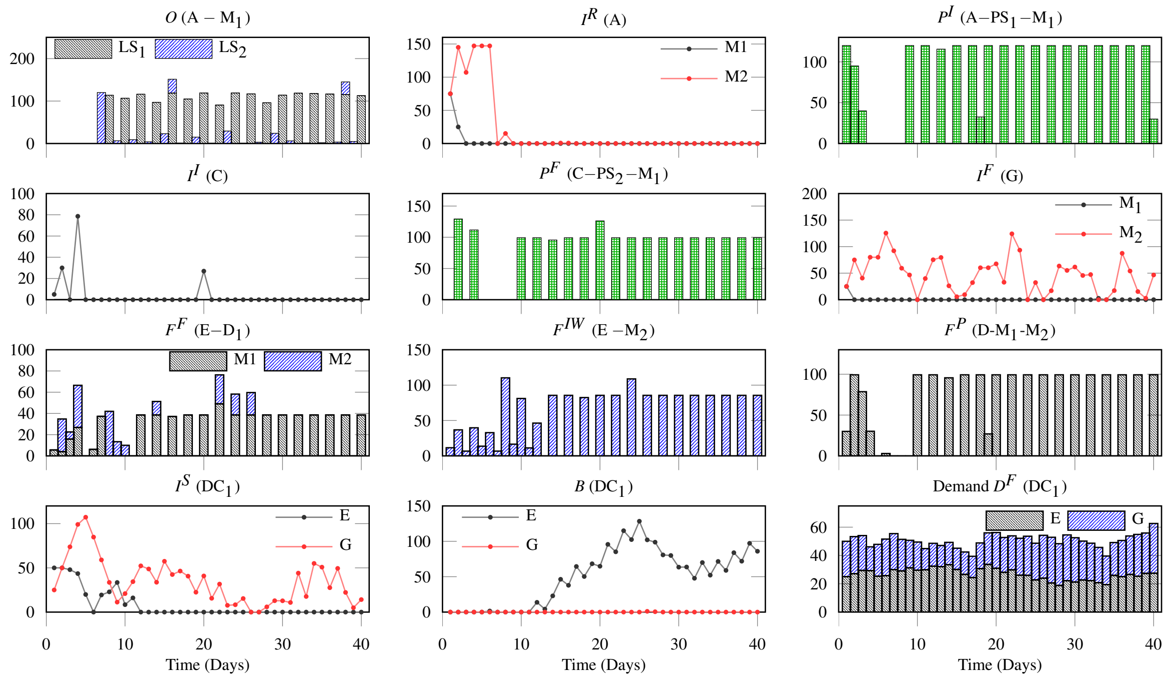

Figure 4.15: Closed-loop result with RCF. 6 discrete realizations at each stage which is equivalent to considering 6 demand scenarios at each controller execution.

It is interesting to note that unlike in ROF-RCF comparison, a higher customer satisfaction is accompanied with a higher operating cost for 3-stage RMF. However, the increase in operating cost is 7.67% which is considered relatively moderate against the improvement in customer service from 93.7% to 99.2%. The average computation time for controller execution is given in the last row (CPU time) of Table 4.10. The average computation time for the 3-stage RMF is quite a bit larger than the RCF but it still considerably less than the SCM sampling time. However, the computation time increases rapidly with the number of uncertain event considered at each stage and hence efforts should be invested to reduce the computation time.

4.6.5 Effect of Fine Tuning Parameter κ

To investigate the effect of the tuning parameter κ on RMF, several simulations were run with RCF and 3-stage RMF at different values of κ and the Pareto curves are generated. 6 uncertain events are considered at each stage within robust MPC controller. The Pareto curves generated with the RCF and 3-stage RMF are illustrated in Figure 4.17 and show similar behavior observed in the case of ROF−RCF.

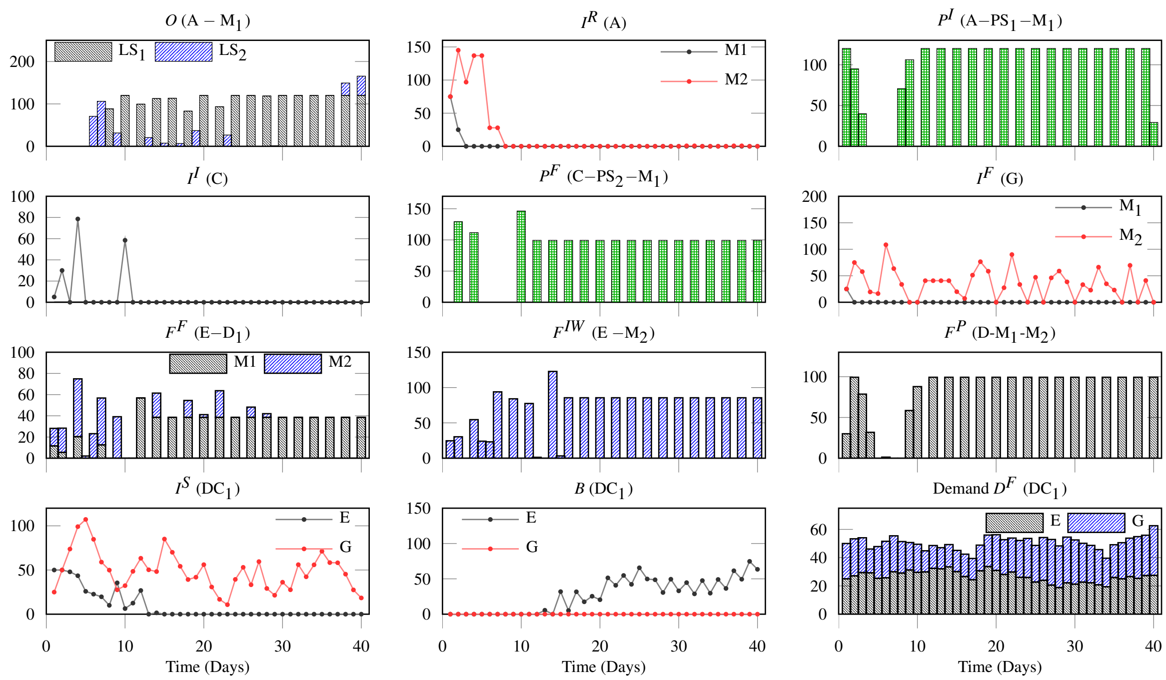

Figure 4.16: Closed-loop result with RCF. 6 discrete realizations at each stage which is equivalent to considering 6 demand scenarios at each controller execution.

The relative left placement of the 3-stage RMF curve to the RCF curve suggests that multistage stochastic controller generates more optimal control actions compared to the two-stage stochastic controller. The points (1) and (2) are generated with a κ value of 5. The cost with RCF−point (2) is 45860 units, 2.69% more than 3-stage RMF (44659 units), while the customer service level is 3.55% higher. The percentage spacing varies across the length of the Pareto curve. The comparison results indicate that the increased number of stages results in improved system performance with the Pareto curve shifting to the left.

4.7 CONCLUSIONS

In this work, we presented a robust decision making tool for SCM, which addresses uncertainty in demand and model parameters explicitly. Through closed-loop simulation, it was shown that the robust formulation substantially reduces the occurrence of back orders, as compared to a nominal MPC formulation, by maintaining a sufficient level of safety stock within inventory echelons. Of significance is that the robust framework maintains an appropriate level of safety stock dependent on the uncertainty characterization, which is

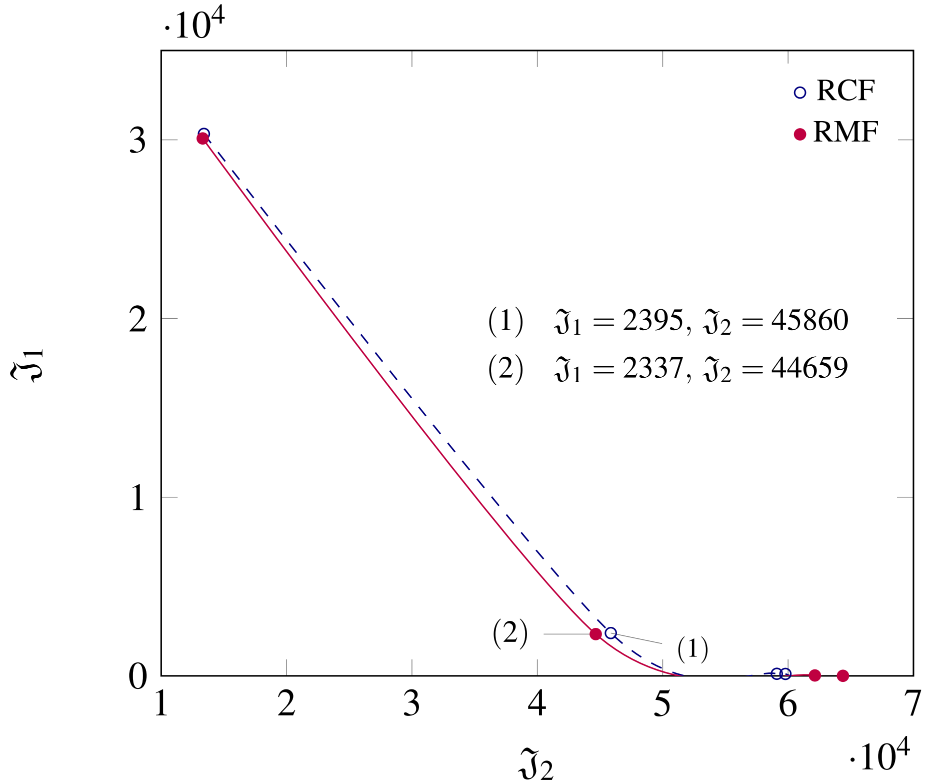

Figure 4.17: Pareto curve generated with RCF and RMF. Each data mark corresponds to average performance for 30 independent closed-loop simulations

a better technique than fixing safety stock levels on the basis of past data and experience. In this paper, we consider both *open-loop* and *closed-loop* predictions of uncertainty propagation. The *closed-loop* formulation explicitly considers the likelihood of responding to the future uncertainty realizations, and it mitigates the overly conservative nature of the open-loop robust MPC. Simulation results provide favorable evidence to suggest that the robust closed-loop formulation provides an equivalent level of customer service at a reduced operating cost. Furthermore, this approach provides performance which is significantly less sensitive to the objective function weighting. In the closed-loop multistage stochastic controller formulation, the system performance improves with the number of stages because of its increased flexibility in responding to future realizations of uncertainty. The main disadvantage of a multi-stage stochastic controller is that the size of resulting problem grows rapidly with number of stages. In this chapter, uncertainty in demand and process yield was considered. However, the method could be extended to include uncertainty in transportation delay. This could be a useful avenue for further study.

Nomenclature

Indicies/Sets

$d \in D$	distribution site
$e, e' \in E$	plant site inventory echelon
$j \in J$	material (chemical)
$ls \in LS$	raw material supplier
$m, m' \in M$	plant site
$ps \in PS$	production scheme
$s \in S$	scenario
$t, t' \in T$	time period (in supply chain model)
$t^* \in T^*$	actual time period
J^P	set of final products
J^{PF}_m	set of products for FPM at plant site m
J^{PI}_m	set of products for IPM at plant site m
J^R	set of raw materials
J^{RF}_m	set of raw materials for FPM at plant site m
J^{RI}_m	set of raw materials for IPM at plant site m
PS^I_m	set of production schemes available at IPM at plant site m
PS^F_m	set of production schemes available at FPM at plant site m

Binary Variables

$u^I_{m,ps,t}$	1 if the IPM process unit in plant site m begins a production scheme ps at time period t; and 0 otherwise
$u^F_{m,ps,t}$	1 if the FPM process unit in plant site m begins a production scheme ps at time period t; and 0 otherwise

Continuous Variables

$B_{j,d,t}$	quantity of back orders of final product j in distribution site d at time period t
$F^F_{j,m,d,t}$	quantity of final product j shipped from plant site m to distribution site d at time period t
$F^{IW}_{j,m,t}$	quantity of material transferred from intermediate product storage facility to warehouse in plant site m at time period t

$F^{P}_{j,e,e',m,m',t}$	quantity of material shipped from storage echelon e at plant site m to storage echelon e' at plant site m' in time period t
$F^{S}_{j,d,t}$	quantity of final product j shipped from distribution site d to fulfil customer demand and back orders at time period t
$I^{F}_{j,m,t}$	inventory of final product j at warehouse in plant site m at time period t
$I^{I}_{j,m,t}$	inventory of intermediate product j at intermediate product storage facility in plant site m at time period t
$I^{R}_{j,m,t}$	inventory of raw material j at raw material storage facility in plant site m at time period t
$I^{S}_{j,d,t}$	quantity of final product j inventory in distribution site d at time period t
$P^{F}_{ps,m,t}$	quantity of main raw material j which begins to undergo production to final product in plant site m at time period t (batch size)
$P^{I}_{ps,m,t}$	quantity of main raw material j which begins to undergo production to intermediate product in plant site m at time period t (batch size)
$O_{j,ls,m,t}$	purchase quantity of raw material j to supplier ls from plant site m at time period t

Parameters

n	length of prediction horizon (days)
r^{c}	length of robust control horizon
$D^{F}_{j,d,t}$	customer demand of final product j at distribution site d at time period t
β^{P}_{ps}	process yield of product produced per unit of raw material consumed in production scheme ps
$\gamma^{M^u}_{m,ps}$	maximum batch size for production scheme ps in plant site m
$\gamma^{M^l}_{m,ps}$	minimum batch size for production scheme ps in plant site m
δ^{M}_{ps}	manufacturing delay for production scheme ps (days)
$\delta^{P}_{m,m'}$	shipping delay between plant site m and m' (days)
$\delta^{R}_{ls,m}$	delivery delay of procured material between supplier ls and plant site m (days)
$\delta^{S}_{m,d}$	shipping delay between plant site m and distribution site d (days)
κ	ratio between weighting parameters (ω_1/ω_2)
$\lambda^{R}_{ls,m}$	maximum quantity of raw material which can be ordered from supplier j during a time period
$\lambda^{F}_{m,d}$	maximum transportation capacity from plant site m to distribution site d during a time period
$\lambda^{P}_{m,m'}$	maximum transportation capacity from plant site m to m' during a time period

$\mu_{j,ps}$	mass balance coefficient of material j in production scheme ps
ρ_s	probability of the occurrence of scenario s
ω_1	weighting parameter attributed to customer service ($\mathfrak{J}_1$)
ω_2	weighting parameter attributed to operating cost ($\mathfrak{J}_2$)
Ω_m^R	maximum storage capacity of raw material in plant site m
Ω_m^I	maximum storage capacity of intermediate product inventory in plant site m
$\Omega_{j,m}^F$	maximum storage capacity of final product j in plant site m
$\Omega_{j,d}^S$	maximum storage capacity of final product j in distribution site d (units)
ΔT	execution frequency of model predictive controller (days)

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CHAPTER 5

Integrated Medium and Short-term Planning Framework for Process Supply Chains

The set of results in this chapter are set to appear in or have been published in:

JOURNAL PAPER

Shailesh Patel and Christopher L.E. Swartz (2016). “Integrated planning framework for model-based rolling horizon supply chain operation”. In: *Computers & Chemical Engineering* -.-, To be submitted

CONFERENCE PAPER

Shailesh Patel and Christopher L.E. Swartz (2015). “Integrated planning framework for model-based rolling horizon supply chain operation”. In: *65th Canadian Chemical Engineering Conference, Calgary*

5.1 INTRODUCTION

A supply chain (SC) system is a production and distribution network with an objective of procuring the right quantity of raw materials from suppliers to process them into high-value products in their manufacturing facilities and selling them to customers through a distribution channel. In today's fast and dynamic market, maintaining an efficient and adaptable supply chain is very critical for survival, particularly given the uncertainties in the business environment and shifting focus towards increasing customer satisfaction. Each node performs a distinct role, and it is important to synchronize these node activities to attain a resonance between different SC partners. Supply chain planning is a set of activities to integrate production and distribution network in an optimized manner to achieve desired customer satisfaction at minimum cost.

In chemical production networks, the manufacturing often spans over a large geographical region to lower the operating cost by optimizing raw material, production and transportation cost. However, planning of such a global manufacturing network is a complex task, making it difficult to estimate the true production and transportation capacity of the network and utilize them efficiently. Accurate representation of system capacity helps to improve financial aspects in terms of optimally using the production and transportation capacity to reduce the operating cost and increase customer satisfaction. Being a complex and involved procedure, supply chain planning (SCP) is carried out in a hierarchical framework where increasingly detailed information are considered as it moves from the upper to lower decision stage for scheduling production and transportation operations. This exercise divides the modeling and computational complexity of the planning procedure and makes it manageable. Based on the time frame of involved planning activities, it can be partitioned into *strategic* (long-term), *tactical* (medium-term), and *operational* (short-term) planning. Strategic or long-term planning aim to decide the location and size of production and storage facilities, and shipment quantities within the network over a relatively large time frame ranging from few months to several years. These are the decisions which affect the long-term performance of a supply chain. The targets set by the strategic planning are communicated to a lower decision-making layer, midterm tactical planning. It refines the production levels, inventory levels and shipment quantities on a finer time scale than into strategic planning to optimize the system performance by including more detailed system information. The short-term operational planning comes at the bottom, and allocates available resources to operational tasks to fulfill the requirements by considering more precise process details such as resource availability (production units, machines, personnel), production and transportation time and cost, production change-over time and cost, and makes detailed plan for production and material shipment within the network. As the decisions of operational planning are implemented on the system, it considers finer process details, and therefore to limit the problem complexity, operational planning is typically carried out for individual units (i.e. nodes), e.g. production scheduling takes care of production activities within manufacturing sites, logistic planning takes care of material flows of a distribution channel. The midterm planning incorporates some features from both the strategic and operational models. For example, it considers key resource limitations in a similar fashion as in operational models. Similarly, much like strategic planning, they account for interactions between different facilities in an abstract way to layout the production and distribution plan. Due to consideration of varying levels of information at each stage, the plan created at upper layer may not remain feasible at the bottom level. For example, strategic planning uses a simpler representation of a process due to a large time horizon and to limit the model complexity. It represents production and logistic activities in an aggregated way in comparison to a detailed production planning model. Further, infeasibility may be introduced because of system disturbances, like uncertainty in demand and production yield, maintenance activities, and planned or unplanned plant shutdown. The planned maintenance activities can be taken into account by careful planning, but model complexity restricts the accommodation of all known plant dynamics at the upper level. To make this framework more efficient, there is a need to develop a mechanism to ensure that feasible targets are passed from the upper layers, and causes of any infeasible production plan should be fed back to the upper level in some way to reduce the occurrence of infeasibility. In other words, information should flow in both directions. This constitutes the main focus of our work.

Sousa, Shah, and Papageorgiou (2008) present a multilevel planning approach for a chemical supply chain and discuss the need for integration between planning levels. They cite that due to aggregated information utilized at the upper level and ignoring task sequencing produce the occurrences of under-utilization of resources at lower level and results in sub-optimal production and distribution plans. They investigate different integration methodologies, such as restricting resource availability, working towards effectively utilizing bottleneck resources, coordinating different planning layers, and analyzing the system efficiency by comparing planning metrics. In these methodologies, information collected at bottom level is used to improve the upper-level planning. Bose and Pekny (2000) integrate multi-level planning and devise a framework to schedule detailed planning activities for a consumer goods supply chain network.

Production planning is a part of company-wide production and distribution network. Considering its prime importance within process supply industries, production planning and scheduling gathered major attention in the systems engineering community. Kallrath (2002a) discusses the importance of combining strategic and operational planning in a production network, and states that analyzing strategic and operational planning simultaneously can greatly improve the system performance. He mentions that production bottlenecks can be easily removed if the appropriate information is incorporated at the upper level. Further, he cites that organization structure and company culture also play a vital role in implementing integration approaches. Kallrath (2002b) provides a thorough discussion on planning and scheduling models and algorithms. He cites that integration between strategic and operational planning is one of the emerging research focus areas in the chemical process industries. Maravelias and Sung (2009) have written an excellent review on medium-term production planning and scheduling and discussed the benefits of integrating these two layers.

Early work on integrating scheduling decisions in a campaign planning problem for parallel continuous batch plants is addressed by Papageorgiou, and Pantelides (1996). A cyclic production schedule is considered within each campaign, and a decomposition based approach is presented to solve an integrated campaign planning and scheduling problem. Susarla and Karimi (2011) present a planning tool to study the effects of resource allocation such as maintenance, limited resource availability, new product introduction and delivery delays on the production schedules and system performance. Within each campaign planning period, production sequencing is enabled where production changeover time has been included. Bhatnagar, Mehta, and Teo (2011) integrate shipment planning and scheduling in multi-mode transportation networks by iteratively using the shipment scheduling information in a planning problem. They use a more responsive but costly air shipment route in place of a less expensive sea shipment route to offset demand uncertainty. Verderame and Floudas (2008) achieve an integration effect by formulating discrete time operational planning with a production disaggregation model which generates daily production targets for the underlying scheduling level. They use an iterative framework to compute production scheduling decisions in a staged manner. In the first iteration, the operational planning model computes the targets for the entire horizon, and the scheduling model lays out production activities to satisfy the target for the first time period. In the next iteration, the planning problem is resolved with the known planning targets for the first time period and adjusted demand targets.

Another approach to handling the integration between planning and scheduling is to include a surrogate model which defines abstract scheduling information within the planning model. One such way is to include the feasibility information of a scheduling model by a set of constraints. Li and Ierapetritou (2009) develop convex underestimation of the production cost of the scheduling model and incorporate it into the planning problem, and solve the integrated problem in an iterative fashion. Sung and Maravelias (2007) present an offline approach to estimate the convex region of feasible production targets and convex underestimation of production cost in terms of linear constraints involving only planning variables. These linear constraints are then added in the planning problem to integrate the effect of production scheduling at the planning level. Stefansson, Shah, and Jensson (2006) study the problem of multiscale production planning and scheduling for the pharmaceutical industry. They incorporate a bidirectional information exchange in the form of feasibility constraints which are derived based on the lower level's information. In some cases, the computation of surrogate models becomes too complex and can be replaced by a simple interaction parameter/factor. Wu and Ierapetritou (2007) derive a factor (which they termed as a *sequence factor*) to include the effect of production sequencing in a planning model, and used it in an iterative framework to solve a hierarchical production planning and scheduling problem. The factor is calculated from objective function values of the planning and scheduling problem, and updated in each iteration.

In its simplest form, the integration can be accomplished by inserting scheduling constraints into the planning problem. Although the exercise is straightforward, the resulting problem becomes large and complex to manage. An alternate way to solve such a complex problem is to decompose it based on the system knowledge or mathematical structure. In the PSE literature, Lagrangian decomposition and its variants are widely used to solve such types of problems. The decisions that appear in both problems can be decoupled by creating a copy of these variables and linked through so called the *linking* constraints. These linking constraints are then relaxed with the use of a Lagrangian relaxation method. Shah and Ierapetritou (2012) use an augmented Lagrangian decomposition algorithm to handle the large scale integrated planning and scheduling problem. Further, to reduce the algorithm complexity, they use a diagonal quadratic approximation to handle the quadratic penalty term appearing in the objective function. Heever and Grossmann (2003) propose an integration framework for a hydrogen production network, where they include detailed scheduling decisions only for a subset of the entire planning horizon. However, to handle the problem complexity of a nonlinear mixed integer model, they use a Lagrangian decomposition based heuristic algorithm to break the integrated problem. Erdirik-Dogan and Grossmann (2006) formulate an integrated production planning and scheduling problem and decompose it to create master planning problem and slave scheduling problem. An iterative framework is used, and cuts (integer cuts and logical) are added to speed up the computation. Erdirik-Dogan and Grossmann (2008) extend it to include the cyclic production sequencing constraints, formulated using an asymmetric traveling salesman problem, in the upper-level problem. This work is further extended for multi-site continuous production and distribution networks by Terrazas-Moreno and Grossmann (2011). The problem complexity is handled using a bilevel and a spatial Lagrangian decomposition method. In the area of refinery planning, Mouret, Grossmann, and Pestiaux (2011) use a Lagrangian decomposition method to solve an integrated production planning & crude oil scheduling problem.

As an alternative to keep the problem complexity minimal, Kopanos, Puigjaner, and Maravelias (2011) present a multi-model approach for a continuous production facility. They utilize a discrete time approach for inventory and product delivery for production planning, immediate precedence based approach for aggregated production sequencing, and lot-sizing based continuous time approach for production scheduling. This hybrid model incorporates a scheduling model within each planning period and a discrete time planning model across composite time periods. Figueira et al. (2015) present a slot based scheduling modeling approach embedded within a discrete time planning model to integrate production planning with scheduling of an integrated paper and pulp mill. The integration is further tightened by using aggregated production sequence set up information at the planning level.

The advanced process control technique, model predictive control (MPC) which is widely used in systems engineering, provides a systematic approach to generate a decision policy for supply chain planning (Wang and Rivera, 2008; Tzafestas, Kapsiotis, and Kyriannakis, 1997; Seferlis and Giannelos, 2004), and offers an advantage of improving performance in the presence of supply and demand variability. Bose and Pekny (2000) use an MPC framework for SC planning and scheduling. They study three different control structures namely, (1) centralized, (2) decentralized, and (3) distributed MPC; and use an integrated model to derive a detailed production schedule for the first time period and capacity planning for the rest of the time periods. Munawar and Gudi (2005) achieve the integration effects using a control theoretic framework, with cascade and receding horizon control techniques. Using a control framework, they ensure that disturbances are handled at local levels. The information from the lower level is fed back to the upper level regarding shortfall or overproduction. To ensure the robustness of upper-level decisions, the planning constraints are posed conservatively by adding a sloping loss terms. Additionally, to improve the flexibility of the solution, the objective function is devised to push for a tighter production schedule for the initial periods. For semiconductor manufacturing, Wang, Rivera, and Kempf (2007) use an MPC based control framework for tactical and inventory planning which receives the targets from a strategic planning module. Through a simulation study, they conclude that the MPC controller improves customer service levels in the presence of high stochasticity in the manufacturing process.

It is apparent from the above literature review that most of the approaches presented for integrated planning & scheduling target only a single facility, production. In the present work, we consider tactical and operational planning of a supply chain network which includes multiple production and distribution facilities. To tackle the problem of infeasibility and lack of coordination faced in the traditional hierarchical framework, we combine midterm tactical planning and short-term operational planning in one model. In the proposed modeling framework, a few initial time periods are modeled with detailed planning activities and remaining periods with a medium-term planning model. Further, we use MPC-based tools to calculate the planning decisions in a rolling horizon fashion. Because of the inherent feedback mechanism embedded in the MPC framework, the approach partially offsets the effects of model inconsistency and system disturbances.

The rest of the chapter is organized as follows. A modeling framework for supply chain planning and scheduling is presented in the next section. This includes an optimization based decision framework (Section 5.2.5). In Section 5.3, the proposed method is implemented on a simulation case study and the results are presented. The conclusion and remarks are noted down in section 5.6.

5.2 INTEGRATED PLANNING

We consider a supply chain system illustrated in Figure 5.1. It consists of parallel suppliers, multiple production facilities, and distribution centers. A plant site places an order for raw material to suppliers. We assume that there is an upper limit on the purchase quantity that can be ordered from suppliers. Purchased raw materials are stored at the plant site. Each production site (facility) houses batch reactors that operate in parallel. Batch reactors are used to produce intermediate and final products. Some final products are produced in a single stage, and the remaining final products are produced in a multi-stage fashion through intermediates. Final and intermediate products are stored at the plant site. After receiving an order, the plant site ships the final products to the distribution center where it is stored and shipped to the customer upon receiving the customer order. Each batch reactor can run multiple production schemes and produce different products. We assume that the data is given for what products can be produced at each reactor, their minimum and maximum production capacity and processing time. Sequence-dependent change-over time and cost are given. The changeover and production time are considered as an integral number of time discretization period of the short-term planning (STP) model. We further assume that the cleaning time between two different production runs is limited by the minimum discretization period. The maximum storage capacity of each storage echelon is given. Further, the transportation quantity between two SC nodes is governed by the shipping capacity of the lanes, capacity of the production facility and/or the customer demand. We assume that the transportation amount must be at least as large as minimum capacity to use that route. All decisions related to the raw material purchase, production and transportation occur at the beginning of the discrete time intervals. The storage location can not store more than its design capacity. Customer orders are delivered at the end of each time period. All non-satisfied orders are accumulated as back-orders and carried forward to the next time period. Back-orders are fulfilled before a new demand request can be met.

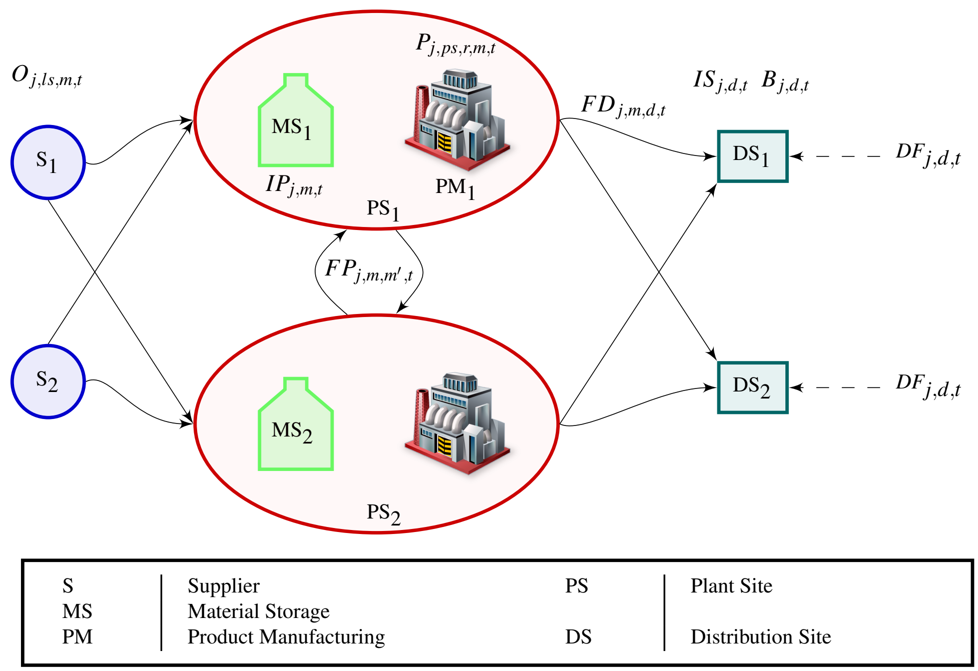

Figure 5.1: Schematic of a process supply chain system for integrated planning study

The integrated model involves two time scale models, a short-term planning and medium-term planning (MTP) model. The MTP (tactical model) makes the decisions pertaining to the order amount placed at suppliers, transportation quantities for shipping lanes, production amount of each product, start and end time of production runs (production tasks) and cleaning operations, and inventory levels of storage locations over large time periods (e.g. week). The STP (operational) model uses a finer time scale and makes the production scheduling decisions such as assignment of production task to a reactor, production sequencing, start and end time of cleaning operations, production amount of each product, transportation quantities between nodes of the network, inventory levels at plant storage sites and distribution centers, and order quantities to suppliers. The integrated model derives these decisions by optimizing the operating cost of the supply chain.

An integrated hybrid-time process supply chain model

In this section, we present an integrated planning model. We use a discrete time formulation for the mathematical description of SC planning activities. The discrete time model divides the time horizon into a finite number of discrete time intervals and defines planning constraints at these discrete time points, which simplifies problem definition and model structure (Méndez et al., 2006). The integrated model, presented in this section, incorporates two different time buckets - a finer time grid for operational planning constraints and a coarser time grid for tactical planning constraints. In the coming sections, we interchangeably refer the tactical model as medium-term planning model (MTP) and operational model as short-term planning model (STP) due to their associated time scale. The integrated planning model describes initial periods with detailed planning operation as more accurate system information, and demand forecast are available, while later time periods are modeled using a coarse representation due to growing uncertainty in both system information and demand forecast. The combination of STP and MTP model provides following benefits, (1) the integration exercise eliminates the infeasibility issue encountered in the hierarchical framework, (2) it allows scheduling operational activities for a long horizon due to a relatively moderate computing resources requirement, which facilitates inclusion of any planned maintenance activities, and/or shutdown if any, and therefore their impact can be better managed, (3) decisions derived from an integrated model can be implemented directly on the system as detailed planning activities are determined for the initial time periods, and (4) aggregation in the later time periods facilitates the handling of not so known distant demand prediction with aggregate decisions. Along with these benefits, it comes with the disadvantage of a complex problem formulation due to the involvement of a non-uniform time discretization. Figure (5.2) shows the time discretization of the integrated modeling framework. N^S is the total number of STP (operational) time periods, and N^P is the total number of planning periods for the integrated model. The time index t represents the time period of the integrated model, which combines both the operational and tactical planning models. The operational planning model use a time index t_s, which runs from 1 to N^S, while the tactical model time index t_m runs from $N^S + 1$ to N^P. Please note that the superscripts S and M

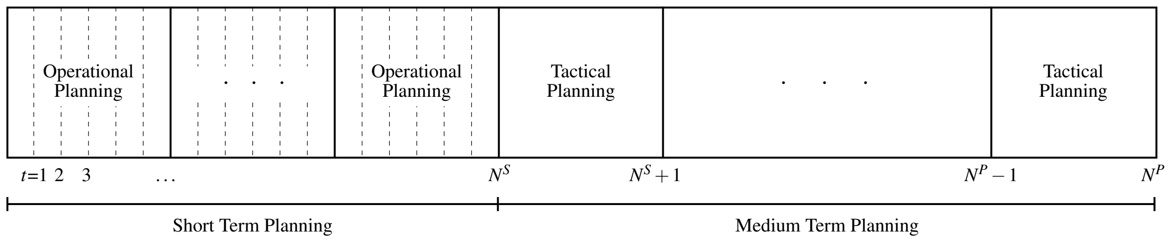

Figure 5.2: Schematic diagram showing time index map of the integrated model

indicate variables corresponding to the STP and MTP model respectively. For a better representation of model constraints, we divide them in three subsections; (i) operational planning constraints, (ii) tactical planning constraints, and (iii) interface constraints.

5.2.1 Operational (Short-term) Planning Constraints

The operational planning constraints characterize the short-term dynamic behavior of material and information flow within a supply chain. It uses time discretization of length ΔT_s, where each STP period is indexed by t_s. A discrete-time representation facilitates the inclusion of time delays (lags). Further, we assume that decision-making occurs at the beginning of each time period. The operational constraints include material balances around each echelon, production and storage capacity constraints, production sequencing constraints, and change-over constraints. The operational planning constraints presented here are an extension of the hybrid time model by Mastragostino, Patel, and Swartz (2014) and Chapter 4, modified to change the production network representation and to include production sequencing.

The decisions that we are considering for operational planning are, (i) allocation of production task ps to batch production unit r at time period t_s, U_{ps,r,t_s}; (ii) production sequencing and detailed timings of production and cleaning tasks, (iii) amount of material j processed in production unit r at plant site m at time period t_s, P^S_{j,ps,r,m,t_s}; (iv) quantity of material j ordered from supplier ls for plant site m at time period t_s, O^S_{j,ls,m,t_s}; (iv) inventory level of material j at plant site m at time period t_s, IP^S_{j,m,t_s}; and at distribution center d at time period t_s, (IS^S_{j,d,t_s}); (v) shipment quantity between two plant site m and m' at time period t_s, FP^S_{j,m,m',t_s}; and from plant site m to distribution center d at time period t_s, FD^S_{j,m,d,t_s}; and (vi) amount of final product j delivered to customers at time period t_s, FS^S_{j,d,t_s}.

Mass balance at plant site

We define J_{ps}^{R} and J_{ps}^{P} as the set of raw materials and products for a production task ps respectively. Set $PS_{r,m}$ is the set of production tasks that can be performed on unit r at plant site m. The material set J_R contains the raw materials that need to be ordered from suppliers, J includes all materials, and J_m is the set of materials involved at plant site m.

The mass balance of material j around the storage echelon at plant site m is given by Equation (5.1). The inventory level of material j at plant site m at the start of time period t_s+1, IP_{j,m,t_s+1}^{S} equals the inventory present at the start of time period t_s minus (i) the quantity consumed at plant site m, P_{j,ps,r,m,t_s}^{S}, (ii) the amount shipped to other plants FP_{j,m,m',t_s}^{S} and distribution centers FD_{j,m,d,t_s}^{S}, plus (i) the amount produced at plant site m, (ii) the amount received from suppliers and other plants.

$$\begin{aligned} IP_{j,m,t_s+1}^{S} = IP_{j,m,t_s}^{S} &+ \sum_{ls:j\in J^R} O_{j,ls,m,t_s-(\delta_{ls,m}^{R}/\Delta T_s)}^{S} - \sum_{d:j\in J^P} FD_{j,m,d,t_s}^{S} \\ &+ \sum_{r}\sum_{ps\in PS_{r,m}:j\in J_{ps}^{P}} P_{j,ps,r,m,t_s-(\sigma_{ps}/\Delta T_s)}^{S} - \sum_{r}\sum_{ps\in PS_{r,m}:j\in J_{ps}^{R}} P_{j,ps,r,m,t_s}^{S} \\ &+ \sum_{m':j\in J/J^R} FP_{j,m',m,t_s-(\delta_{m',m}^{P}/\Delta T_s)}^{S} - \sum_{m':j\in J/J^R} FP_{j,m,m',t_s}^{S} \quad \forall\, j\in J_m, m, t_s \end{aligned} \tag{5.1}$$

where, $\delta_{ls,m}^{R}$ is the shipment delay between when an order for raw material j is made to a supplier ls ($O_{j,ls,m,t}$) to the corresponding delivery. Similarly, $\delta_{m,m'}^{P}$ is the transportation delay for an inter-plant shipment. σ_{ps} is the batch time of production scheme ps.

The consumption amount of raw material j is expressed in terms of the consumption amount of main raw material of the corresponding production scheme. Similarly, the production amount of material j produced in production scheme ps is also expressed in terms of its main raw material consumption.

$$P_{j,ps,r,m,t_s}^{S} = \mu_{j,ps}\, P_{j',ps,r,m,t_s}^{S} \qquad \forall\, j\in J_{ps}^{R}, j'\in J_{ps}^{MR}, ps\in PS_{r,m}, r, m, t_s \tag{5.2}$$

$$P_{j,ps,r,m,t_s}^{S} = \beta_{ps}\, \mu_{j,ps}\, P_{j',ps,r,m,t_s}^{S} \qquad \forall\, j\in J_{ps}^{P}, j'\in J_{ps}^{MR}, ps\in PS_{r,m}, r, m, t_s \tag{5.3}$$

The mass balance coefficient of chemical j in production scheme ps is denoted as $\mu_{j,ps}$, and β_{ps} is the process yield of production scheme ps.

Capacity constraints

The inventory of material j at plant site m is restricted to a maximum storage capacity of Ω^R_m.

$$IP^S_{j,m,t_s} \leq \Omega^R_{j,m} \qquad \forall\, j \in J_m, m, t_s \tag{5.4}$$

Equation (5.5) represents the maximum order which can be made to supplier ls for raw material j ($\lambda^R_{ls,m}$) during a time period. Similarly, constraint (5.6) restricts the inter-plant shipment quantity to a maximum quantity of $\lambda^P_{m,m'}$ during a time period. Similarly, the shipment amount of products from plant site m to distribution site d is restricted by $\lambda^F_{m,d}$ during a time period and given by Equation (5.7).

$$O^S_{j,ls,m,t_s} \leq \lambda^R_{ls,m} \qquad \forall\, j \in J^R, ls, m, t_s \tag{5.5}$$

$$\sum_{j \in J/J^R} FP^S_{j,m,m',t_s} \leq \lambda^P_{m,m'} \qquad \forall\, m, m', t_s \tag{5.6}$$

$$\sum_{j \in J^P} FD^S_{j,m,d,t_s} \leq \lambda^F_{m,d} \qquad \forall\, m, d, t_s \tag{5.7}$$

Equation (5.8) restricts the consumption amount of main raw material P^S_{j,ps,r,m,t_s} to lie between a lower ($\gamma^l_{ps,m}$) and upper ($\gamma^u_{ps,m}$) bound. The binary variable $U_{ps,r,t}$ is introduced to model a disjunction in the continuous variable P^S_{j,ps,r,m,t_s}. $U_{ps,r,t}$ is 1 if processing unit r at plant site m begins production task ps at time period t_s; and 0 otherwise.

$$\gamma^l_{ps,m}\, U_{ps,r,t_s} \leq P^S_{j,ps,r,m,t_s} \leq \gamma^u_{ps,m}\, U_{ps,r,t_s} \qquad \forall\, j \in J^{MR}_{ps}, ps \in PS_{r,m}, r, m, t_s \tag{5.8}$$

Production sequencing

Production assignment constraints allocate a production task to a production unit. At any given time, a production unit can be associated with only one task. Further, allotment of another task can not be initiated until the current task is finished. Equation (5.9) is a *full backward* constraint that restricts the start of another production task ps at the processing unit r at time period t_s, if a task has already begun within the backward time interval $[t_s - (\sigma_{ps}/\Delta T) + 1, t_s]$. σ_{ps} represents the processing time of production task ps. CL_{r,t_s} represents the existence of a cleaning operation at unit r. CL_{r,t_s} is 1 if cleaning operation is initiated; and 0 otherwise.

$$\sum_{ps} \sum_{t'=t_s-(\sigma_{ps}/\Delta T_s)+1}^{t_s} U_{ps,r,t'} + CL_{r,t_s} \leq 1 \qquad \forall\, r, t_s \tag{5.9}$$

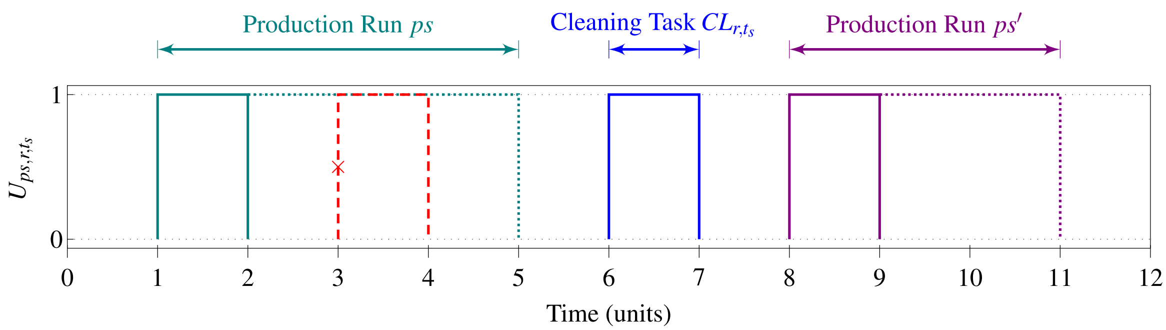

Figure 5.3: Production sequencing and cleaning operation placement. Production run ps (green) starts at time $t_s = 1$ which lasts for 4 time periods, so another production run (red) can not be started. Cleaning task has to be scheduled before running other production run ps' (violet)

Sequence-dependent change-over

In most batch production operation environments, a production unit needs cleaning or some kind of preparation before another production scheme can run on the same unit. The cleaning constraints are adapted from Kondili, Pantelides, and Sargent (1993) and are represented in a *backward-time* format. Equation (5.10) is the cleaning constraint, which states that a cleaning operation (CL_{r,t_s}) is required, if a production task ps is performed at processing unit r at time t_s, and another task ps' is performed in the same unit within the time interval $[t'_s,\ t_s]$ and no other task is performed in-between. Figure 5.3 illustrates production sequencing and the placement of a cleaning operation.

$$UT_{ps,r,t_s} + \sum_{ps' \in PS_r : ps' \neq ps} UT_{ps',r,t'_s} - \sum_{t=t'_s+1}^{t_s-1} \sum_{ps' \in PS_r} UT_{ps',r,t} - 1 \leq \sum_{t=t'_s+1}^{t_s-1} CL_{r,t_s} \qquad \forall\ ps \in PS_r, r, t_s, t'_s < t_s \qquad (5.10)$$

$$UT_{ps,r,ts} = \sum_{t'=t_s-(\sigma_{ps}/\Delta T_s)+1}^{t_s} U_{ps,r,t'} \qquad \forall\ ps \in PS_r, r, t_s \qquad (5.11)$$

The auxiliary variables UT_{ps,r,t_s} records the occupancy of unit r by production scheme ps at time period t_s and is derived from the binary decision variable $U_{ps,r,t}$ which represents the start time of a production scheme ps. UT_{ps,r,t_s} take the value 1 if task is running, otherwise 0. The formulation ensures the integrality of the continuous variables CL and UT. In the case where two different processing tasks (ps and ps') take place in adjacent time periods (i.e. $t'_s = t_s - 1$), the first and second term take the value 1 in expression (5.10), while the summation term $\sum_{t=t'_s+1}^{t_s-1} [\cdot]$ becomes zero and therefore the left hand side takes the value $1+1-0-1=1$ and right hand side becomes 0, and thus it prevents such situation from occurring.

Mass balance at distribution site

The mass balance of final product j in distribution site d is given by Equation (5.12), where $\delta^F_{m,d}$ is the transportation delay between plant site m and distribution site d, and $FS^S_{j,d,t}$ is the quantity of final product j delivered from distribution center d at time period t_s to satisfy customer demand and accumulated back orders.

$$IS^S_{j,d,t_s+1} = IS^S_{j,d,t_s} + \sum_m FD^S_{j,m,d,t_s-(\delta^F_{m,d}/\Delta T_s)} - FS^S_{j,d,t_s} \qquad \forall\, j \in J^P, d, t_s \tag{5.12}$$

$$IS^S_{j,d,t_s} \leq \Omega^S_{j,d} \qquad \forall\, j \in J^P, d, t_s \tag{5.13}$$

The total maximum amount of inventory of material j that can be stored at distribution site d is $\Omega^S_{j,d}$.

Back-order balance

If sufficient inventory of final product j is present, the full customer order will be satisfied; otherwise only a partial order will be shipped. The unsatisfied demand will be recorded as back orders and will be shipped at a future time. Equation (5.14) represents the back order balance for final product j at distribution site d,

$$B^S_{j,d,t_s+1} = B^S_{j,d,t_s} - FS^S_{j,d,t_s} + DF_{j,d,t_s} \qquad \forall\, j \in J^P, d, t_s \tag{5.14}$$

Here, DF_{j,d,t_s} is the demand of final product j at distribution site d at time period t_s.

The amount of final product j (FS^S_{j,d,t_s}) delivered from distribution site d at time period t_s to satisfy customer demand and accumulated back orders is given by,

$$FS^S_{j,d,t_s} = \begin{cases} DF_{j,d,t_s} + B^S_{j,d,t_s}, & \text{if } IS^S_{j,d,t_s} \geq DF_{j,d,t_s} + B^S_{j,d,t_s} \\ IS^S_{j,d,t_s}, & \text{if } IS^S_{j,d,t_s} < DF_{j,d,t_s} + B^S_{j,d,t_s} \end{cases} \qquad \forall\, j \in J^P, d, t_s \tag{5.15}$$

IS^S_{j,d,t_s} is the inventory of final product j at distribution site d at time period t_s. The above disjunction function can be formulated using a binary variable. To circumvent the need to add new binary variables, the variable FS^S_{j,d,t_s} is eliminated by introducing an auxiliary variable $IS^{*S}_{j,d,t_s} = IS^S_{j,d,t_s} - B^S_{j,d,t_s}$ as given in Mastragostino, Patel, and Swartz (2014). Equations (5.12) and (5.14) are then translated into Equation (5.16), where IS^{*S}_{j,d,t_s} is positive if sufficient inventory exists and negative in the case where sufficient inventory is not present and therefore results in a back-order.

$$IS^{*S}_{j,d,t_s+1} = IS^{*S}_{j,d,t_s} + \sum_{m} FD^{S}_{j,m,d,t_s-(\delta^{F}_{m,d}/\Delta T_s)} - DF_{j,d,t_s} \qquad \forall\, j \in J^P, d, t_s \tag{5.16}$$

In the plant simulation model, the storage capacity constraints (5.4) and (5.13) are modified as,

$$IP^{S}_{j,m,t_s} \leq \Omega^{R}_{m} + SIP^{S}_{m,t_s}$$
$$IS^{S}_{j,d,t_s} \leq \Omega^{S}_{j,d} + SIS^{S}_{j,d,t_s}$$

where, SIP^{S}_{m,t_s} and SIS^{S}_{j,d,t_s} are slack variables to avoid problem infeasibility issues arising due to demand uncertainty in plant simulations.

Since, Equation (5.14) is replaced by Equation (5.16), the amount of back-order is given using the following constraint (5.17).

$$-IS^{S^*}_{j,d,t_s} \leq B^{S}_{j,d,t_s} \leq IS^{S}_{j,d,t_s} - IS^{S^*}_{j,d,t_s} \qquad \forall\, j \in J^P, d, t_s \tag{5.17}$$

Minimizing back-order quantity B^{S}_{j,d,t_s} and inventory amount IS^{S}_{j,d,t_s} in the objective function ensures that, Equation (5.17) sets $B^{S}_{j,d,t_s} = -IS^{S^*}_{j,d,t_s}$ and $IS^{S}_{j,d,t_s} = 0$ when $IS^{S^*}_{j,d,t_s}$ is negative, and $B^{S}_{j,d,t_s} = 0$ and $IS^{S}_{j,d,t_s} = IS^{S^*}_{j,d,t_s}$ if $IS^{S^*}_{j,d,t_s}$ is positive.

Bounds on variables

$$IP^{S}_{j,m,t_s},\ IS^{S}_{j,d,t_s},\ B^{S}_{j,d,t_s} \geq 0 \qquad \forall\, j, m, d, t_s$$
$$O^{S}_{j,ls,m,t_s},\ P^{S}_{ps,r,m,t_s},\ FP^{S}_{j,m,m',t_s},\ FD^{S}_{j,m,d,t_s} \ \geq\ 0 \qquad \forall\, j, ls, ps, r, m, m', d, t_s$$
$$U_{ps,r,t_s} \in \{0,1\} \qquad \forall\, ps \in PS_r, r, t_s$$
$$CL_{r,t_s},\ UT_{ps,r,t_s} \in [0,1] \qquad \forall\, r, ps, t_s$$

5.2.2 Medium-term Planning Constraints

The MTP constraints are an aggregated version of STP constraints. They use time index of ΔT_m ($> \Delta T_s$) and determine production, inventory, and shipment amounts over a coarser time scale. The MTP model ignores the detailed production and cleaning timing constraints, however it approximates them using cyclic scheduling constraints. The goal of MTP is to determine the optimal production and transportation quantity over a long time horizon (months) considering raw material availability, storage capacity, production capacity, and cost of materials, storage and transportation. Along with aggregated decisions of the operational planning, the decisions that we are addressing for tactical planning operation are, (i) allotment of production task ps to unit r at each time period t_m, YP_{ps,r,t_m}; (ii) number of batches for each production task ps at unit r, NB_{ps,r,t_m}; (iii) first (YF_{ps,r,t_m}) and last task (YL_{ps,r,t_m}) of the production sequence at each time period t_m, (iv) precedence of a production task ps in the production sequence at each time period t_m, XP_{ps,ps',r,t_m}; (iv) production link between scheme ps and ps' to be broken to generate production sequence from a cyclic schedule at unit r at each time period t_m, XB_{ps,ps',r,t_m}; (v) change-over variable to make the cleaning decision between two different production schemes across planning time periods, XC_{ps,ps',r,t_m}.; and (vi) total production change-over time at each time period t_m, TC_{r,t_m}. The superscript M denotes a MTP model variable.

Material storage at plant site - Mass balance

The inventory balance for MTP time period can be written in a similar way as for STP period. The inventory level of material j, IP^M_{j,m,t_m+1} at the start of time period t_m+1 is the inventory present at the start of time period t_m plus (i) the amount received from suppliers O^M_{j,ls,m,t_m} and other plant sites FP^M_{j,m',m,t_m}, (ii) the amount produced P^M_{j,ps,r,m,t_m}, minus (i) the quantity consumed at plant site m, and (ii) the shipment quantity to distribution centers FD^M_{j,m,d,t_s} and other plant sites FP^M_{j,m',m,t_s}.

Raw material procurement orders, production batch runs, and shipment orders, that are initiated during operational planning periods and still in-transit (or in-process) at the interface point ($t = N^S$), is received during the first time period of tactical model and hence these quantities are added in the inventory balance for time $t_m = N^S + 1$ Equation (5.18). For example, the term $\sum_{t'=N^S-(\delta^R_{ls,m}/\Delta T_s)+1}^{N^S} O^S_{j,ls,m,t'}$ represents the raw material procurement order that is placed during STP time periods $t = N^S - (\delta^R_{ls,m}/\Delta T_s) + 1$ to N^S and is received at MTP time period $t = N^S + 1$, hence the quantity is added in the balance Equation (5.18).

$$
\begin{aligned}
IP^M_{j,m,t_m+1} = IP^M_{j,m,t_m} &+ \sum_{ls\,:\,j\in J^R} \left(O^M_{j,ls,m,t_m} + \sum_{t'=N^S-(\delta^R_{ls,m}/\Delta T_s)+1}^{N^S} O^S_{j,ls,m,t'} \right) \\
&+ \sum_{r} \sum_{ps\in PS_{r,m}\,:j\in J^P_{ps}} \left(P^M_{j,ps,r,m,t_m} + \sum_{t'=N^S-\sigma^{ps}_{ls,m}+1}^{N^S} P^M_{j,ps,r,m,t'} \right)
\end{aligned}
$$

$$+ \sum_{m':\, j \in J/J^R} \left(FP^M_{j,m',m,t_m} + \sum_{t'=N^S-(\delta^P_{m',m}/\Delta T_s)+1}^{N^S} FP^S_{j,m',m,t'} \right)$$
$$- \sum_{r} \sum_{ps \in PS_{r,m}\ : j \in J^R_{ps}} P^M_{j,ps,r,m,t_m} - \sum_{m':j \in J/J^R} FP^M_{j,m,m',t_m} - \sum_{d:j \in J^P} FD^M_{j,m,d,t_m}$$
$$\forall\ j \in J^R_m, m, t_m = N^S + 1 \qquad (5.18)$$

The following material balance (5.19) appears for the subsequent time periods.

$$IP^M_{j,m,t_m+1} = IP^M_{j,m,t_m} + \sum_{ls\ :\ j \in J^R} O^M_{j,ls,m,t_m} - \sum_{d:j \in J^P} FD^M_{j,m,d,t_m}$$
$$+ \sum_{r} \sum_{ps \in PS_{r,m}\ : j \in J^P_{ps}} P^M_{j,ps,r,m,t_m} - \sum_{r} \sum_{ps \in PS_{r,m}\ : j \in J^R_{ps}} P^M_{j,ps,r,m,t_m}$$
$$+ \sum_{m':\, j \in J/J^R} FP^M_{j,m',m,t_m} - \sum_{m':j \in J/J^R} FP^M_{j,m,m',t_m}$$
$$\forall\ j \in J^R_m, m, t_m = N^S + 2, \ldots, N^P \qquad (5.19)$$

Similar to the operational planning, the consumption and production amount of material j involved in task ps are expressed as,

$$P^M_{j,ps,r,m,t_m} = \mu_{j,ps}\ P^M_{j',ps,r,m,t_m} \qquad \forall\ j \in J^R_{ps}, j' \in J^{MR}_{ps}, ps \in PS_{r,m}, r, m, t_m \qquad (5.20)$$
$$P^M_{j,ps,r,m,t_m} = \beta_{ps}\ \mu_{j,ps}\ P^M_{j',ps,r,m,t_m} \qquad \forall\ j \in J^P_{ps}, j' \in J^{MR}_{ps},\ ps \in PS_{r,m}, r, m, t_m \qquad (5.21)$$

Capacity constraints

The inventory of material j at plant site m is restricted to its maximum storage capacity Ω^R_m in a similar fashion as it is described in the operational planning.

$$IP^M_{j,m,t_m} \leq \Omega^R_{j,m} \qquad \forall\ j \in J_m, m, t_m \qquad (5.22)$$

The total order quantity of raw material j, O^M_{j,ls,m,t_m} from supplier ls during time period t_m is restricted by $\lambda^R_{ls,m}$ times H, where H is number of operational planning periods that can be fit within one tactical planning period. For example, if the time bucket of operational model is 1 day and tactical model is 1 week (7 days), H takes the value 7.

$$O^M_{j,ls,m,t_m} \leq H\ \lambda^R_{ls,m} \qquad \forall\ j \in J^R, ls, m, t_m \qquad (5.23)$$
$$\sum_{j \in J^P} FD^M_{j,m,d,t_m} \leq H\ \lambda^F_{m,d} \qquad \forall\ m, d, t_m \qquad (5.24)$$

$$\sum_{j \in J/J^R} FP^M_{j,m,m',t_m} \leq H\ \lambda^P_{m,m'} \qquad \forall\ m, m', t_m \tag{5.25}$$

Similarly, the shipment amounts of product j from plant site m to distribution site d (FD^M_{j,m,d,t_m}) and from plant site m to another plant site m' (FP^M_{j,m,m',t_m}) are restricted by their respective design capacities as given by Equations (5.24) and (5.25).

Because of the larger time grid, the production capacity constraint is described by an aggregated version of the capacity constraint introduced in the STP model. The aggregated total production amount from production unit r during time period t_m from all production schemes that can run on unit r is expressed in terms of the production amount of main material of those production schemes and their relative production capacity coefficients η_{ps}, and should not exceed the design capacity of unit r (Γ^u_r). Constraint (5.27) states that if production scheme ps is allocated at time period t_m (i.e. $YP_{ps,r,t_m} = 1$), the production amount on unit r should be greater than its allowable minimum design capacity ($\gamma^l_{ps,m}$).

$$\sum_{ps \in PS_{r,m}} \eta_{ps}\ P^M_{j,ps,r,m,tm} \leq (H - TC_{r,t_m}/\Delta T_s)\ \Gamma^u_r \qquad \forall\ j \in J^{MR}_{ps}, r, m, tm \tag{5.26}$$

$$\gamma^l_{ps,m}\ YP_{ps,r,t_m} \leq P^M_{j,ps,r,m,t_m} \qquad \forall\ j \in J^{MR}_{ps}, ps \in PS_{r,m}, r, m, t_m \tag{5.27}$$

$$P^M_{j,ps,r,m,t_m} \leq (H - TC_{r,t_m}/\Delta T_s)\ \gamma^u_{ps,m}\ YP_{ps,r,t_m} \quad \forall\ j \in J^{MR}_{ps},\ ps \in PS_{r,m}, r, m, t_m \tag{5.28}$$

TC_{r,t_m} is the production changeover time during time period t_m, and is an aggregate version of cleaning variable CL_{r,t_s}. As explained earlier, the change-over represents cleaning or other set up activities required between two different production runs and hence the unit is not available for production. The term $H - TC_{r,t_m}$ represents the total time available for production within time period t_m. The production changeover time is defined in the cyclic scheduling section. Constraint (5.28) sets the production amount to zero when scheme ps is not allocated during time period t_m. Since, the aggregated production amount is constrained by Equation (5.26), the term $(H - TC_{r,t_m})$ in Equation (5.28) can be changed to H without any loss to remove the bi-linearity.

$$P^M_{j,ps,r,m,t_m} \leq H\ \gamma^u_{ps,m}\ YP_{ps,r,t_m} \qquad \forall\ j \in J^{MR}_{ps}, ps \in PS_{r,m}, r, m, t_m \tag{5.29}$$

Cyclic scheduling constraints

To account for production sequencing, the MTP model incorporates cyclic scheduling constraints without considering actual timings of production schemes. The cyclic scheduling is formulated using a travelling salesman problem (TSP). These constraints generate a cyclic production schedule in a way that minimizes production change-over time and cost.

The production cycle is then converted to an optimal production sequence by breaking a production link having highest change-over time. These constraints are adapted from Erdirik-Dogan and Grossmann (2007) and modified to include the scenario where no production is running on a unit.

(a) Number of batches for each production scheme

$$NB_{ps,r,tm} = P^{M}_{j,ps,r,m,t_m} \ / \ \gamma^{u}_{ps,m} \qquad \forall\ j \in J^{MR}_{ps}, ps \in PS_{r,m}, r, m, t_m \tag{5.30}$$

Constraint (5.30) calculates the total number of batches of each production scheme at processing unit r. $NB_{ps,r,tm}$ is treated as an integer variable in the formulation.

(b) Changeover time - within time period

The following constraints generate a cyclic schedule of assigned products and breaks the link having highest changeover time to calculate the minimum changeover time in each time period.

$$YP_{ps,r,t_m} = \sum_{ps' \in PS_r} XP_{ps,ps',r,t_m} \qquad \forall\ ps \in PS_r, r, t_m \tag{5.31}$$

$$YP_{ps',r,t_m} = \sum_{ps \in PS_r} XP_{ps,ps',r,t_m} \qquad \forall\ ps' \in PS_r, r, t_m \tag{5.32}$$

Constraints (5.31) and (5.32) state that if production scheme ps is allocated to unit r during time period t_m ($YP_{ps,r,t_m} = 1$), two production transitions, one from scheme ps to ps' and second from scheme ps' to ps, must occur during time period t_m. XP_{ps,ps',r,t_m} indicates the transition from production scheme ps to ps' at unit r during time period t_m.

It is worth mentioning that, in constraints (5.31) and (5.32), production task (or scheme) ps and ps' may represent the same production task. If ps and ps' are restricted to be different, it results in an infeasible schedule for a single production task allotment case. On the contrary, permitting $ps = ps'$ generates a schedule with self-loops (a cycle consisting one production scheme repeating multiple times) due to zero change-over time. To permit the self-loop only for the single production scenario, the following set of constraints (5.33) − (5.35) are included. Expression (5.35) states that, if production scheme ps is running in unit r at time period t_m (i.e. $YP_{ps,r,t_m} = 1$), and no other production scheme ps' different than ps is assigned in the same unit at same time period (i.e. $\sum_{ps' \in PS_r : ps' \neq ps} YP_{ps',r,t_m} = 0$), then only the production scheme ps can be followed by scheme ps (XP_{ps,ps,r,t_m} can take value 1), and vice versa.

$$YP_{ps,r,t_m} \geq XP_{ps,ps,r,tm} \qquad \forall\, ps \in PS_r, r, t_m \qquad (5.33)$$

$$YP_{ps',r,t_m} + XP_{ps,ps,r,t_m} \leq 1 \qquad \forall\, ps, ps' \in PS_r, ps' \neq ps, r, t_m \qquad (5.34)$$

$$YP_{ps,r,t_m} - \sum_{ps' \in PS_r : ps' \neq ps} YP_{ps',r,t_m} \leq XP_{ps,ps,r,t_m} \qquad \forall\, ps \in PS_r, r, t_m \qquad (5.35)$$

The optimal production schedule is determined by breaking exactly one link of a generated cyclic schedule. The binary variable XB_{ps,ps',r,t_m} represents the pair (link) to be broken in constraint (5.36).

$$\sum_{ps \in PS_r} \sum_{ps' \in PS_r} XB_{ps,ps',r,t_m} = 1 \qquad \forall\, r, t_m \qquad (5.36)$$

In the cases where no production task is allocated to the unit due to insufficient inventory of raw material or maintenance shutdown, there is no requirement for scheduling production activities during that time period. However, constraint (5.36) demands to break exactly one production link, which implicitly requires running at least one production scheme irrespective of raw material or production equipment availability. To accommodate a no-production case constraints (5.37) - (5.39) are formulated which state that if no production scheme is running at unit r at time period t_m, the transition variable XB_{ps,ps',r,t_m} takes the value zero, otherwise exactly one transition is allowed. Defining an indicator variable DD_{r,t_m} for recording whether any production task is running on unit r at time period t_m, the Equations (5.37) - (5.38) state that the variable DD_{r,t_m} takes the value one if at least one production task ps is assigned to unit r.

$$DD_{r,t_m} \geq YP_{ps,r,t_m} \qquad \forall\, r,\ ps \in PS_r, t_m \qquad (5.37)$$

$$DD_{r,t_m} \leq \sum_{ps \in PS_r} YP_{ps,r,t_m} \qquad \forall\, r, t_m \qquad (5.38)$$

$$\sum_{ps \in PS_r} \sum_{ps' \in PS_r} XB_{ps,ps',r,t_m} = DD_{r,t_m} \qquad \forall\, r, t_m \qquad (5.39)$$

$$0 \leq DD_{r,t_m} \leq 1$$

If the pair is not selected in the cycle, the corresponding transition link takes the value zero, enforced by constraint (5.40) :

$$XB_{ps,ps',r,t_m} \ \leq \ XP_{ps,ps',r,t_m} \qquad \forall\, ps, ps' \in PS_r, r, t_m \qquad (5.40)$$

The total changeover time (TC_{r,t_m}) in each time period is the summation of the changeover time corresponding to each selected pair minus the changeover time of broken link.

$$TC_{r,t_m} = \sum_{ps \in PS_r} \sum_{ps' \in PS_r} \tau_{ps,ps'} \; XP_{ps,ps',r,t_m} - \sum_{ps \in PS_r} \sum_{ps' \in PS_r} \tau_{ps,ps'} \; XB_{ps,ps',r,t_m} \qquad \forall r, t_m \quad (5.41)$$

$\tau_{ps,ps'}$ is the production change-over time from scheme ps to ps'.

(c) Changeover time - across time period

To determine the changeover time between adjacent time periods, one need to know the first and last production scheme running at each time period.

$$YF_{ps',r,t_m} \geq \sum_{ps \in PS_r} XB_{ps,ps',r,t_m} \qquad \forall ps' \in PS_r, r, t_m \quad (5.42)$$

$$YL_{ps,r,t_m} \geq \sum_{ps' \in PS_r} XB_{ps,ps',r,t_m} \qquad \forall ps \in PS_r, r, t_m \quad (5.43)$$

If the link between production scheme ps and ps' is broken, then scheme ps becomes the last scheme ($YL_{ps,r,t_m} = 1$) and ps' becomes the first scheme ($YF_{ps',r,t_m} = 1$) to be run in the optimal production sequence for unit r during time period t_m. Moreover, exactly one production scheme can be run as the first production scheme and one scheme can be run as the last production scheme, as indicated by (5.44) and (5.45).

$$\sum_{ps \in PS_r} YF_{ps,r,t_m} = 1 \qquad \forall r, t_m \quad (5.44)$$

$$\sum_{ps \in PS_r} YL_{ps,r,t_m} = 1 \qquad \forall r, t_m \quad (5.45)$$

The changeover variable between two adjacent time periods (XC_{ps,ps',r,t_m}) becomes 1, if production scheme ps is running at time period t_m and scheme ps' at time period $t_m + 1$. According to constraint (5.46), exactly one changeover happens from scheme ps, if and only if scheme ps is the last production run at time period t_m. Similarly, exactly one changeover happens to scheme ps', if and only if scheme ps' is run the first at time period $t_m + 1$.

$$\sum_{ps' \in PS_r} XC_{ps,ps',r,t_m} = YL_{ps,r,t_m} \qquad \forall ps \in PS_r, r, t_m \quad (5.46)$$

$$\sum_{ps \in PS_r} XC_{ps,ps',r,t_m} = YF_{ps',r,t_m+1} \qquad \forall ps' \in PS_r, r, t_m \in 1..NMT-1 \quad (5.47)$$

(d) Time balance

The summation of changeover times and the production times within each time period should be less than the length of tactical planning period ($\Delta T_m = H\ \Delta T_s$).

$$\sum_{ps \in PS_r} NB_{ps,r,t_m}\ \sigma_{ps} + TC_{r,t_m} + \sum_{ps \in PS_r} \sum_{ps' \in PS_r} XC_{ps,ps',r,t_m}\ \tau_{ps,ps'}\ \le\ H\ \Delta T_s \quad \forall r, t_m \tag{5.48}$$

Distribution site - Mass balance

The inventory balance of material j at distribution site d is given by mass balance (5.49) for time $t_m = N^S + 1$, and (5.50) for the subsequent time periods. Equation (5.49) includes the effect of transportation and production delay as explained earlier. The inventory level of material j (IS^M_{j,d,t_m}) increases by the amount FD^M_{j,m,d,t_m} received from plant sites and decreases by the amount FS^M_{j,d,t_m} shipped to customers at time period t_m.

$$IS^M_{j,d,t_m+1} = IS^M_{j,d,t_m} + \sum_m \left(FD^M_{j,m,d,t_m} + \sum_{t'=N^S-(\delta^F_{m,d}/\Delta T_s)}^{N^S} FD^M_{j,m,d,t'} \right) - FS^M_{j,d,t_m}$$

$$\forall\ j \in J^P_m \cup J^P, d, t_m = N^S + 1 \tag{5.49}$$

$$IS^M_{j,d,t_m+1} = IS^M_{j,d,t_m} + \sum_m\ FD^M_{j,m,d,t_m} - FS^M_{j,d,t_m}$$

$$\forall\ j \in J^P_m \cup J^P, d, t_m = N^S + 2, \ldots, N^P \tag{5.50}$$

$$IS^M_{j,d,t_m} \le \Omega^S_{j,d} \qquad \forall\ j \in J^P, d, t_m \tag{5.51}$$

$\Omega^S_{j,d}$ represents the maximum storage capacity for material j at distribution site d.

Back-order balance

Similar to the operational planning model, the back order balance is given by Equation (5.52).

$$B^M_{j,d,t_m+1} = B^M_{j,d,t_m} - FS^M_{j,d,t_m} + DF_{j,d,t_m} \qquad \forall\ j \in J^P, d, t_m \tag{5.52}$$

The amount of final product j (FS^M_{j,d,t_m}) delivered from distribution site d at time period t_m to satisfy customer demand and accumulated back orders is given by,

$$FS^M_{j,d,t_m} = \begin{cases} DF_{j,d,t_m} + B^M_{j,d,t_m}, & \text{if } IS^M_{j,d,t_m} \ge DF_{j,d,t_m} + B^M_{j,d,t_m} \\ IS^M_{j,d,t_m}, & \text{if } IS^M_{j,d,t_m} < DF_{j,d,t_m} + B^M_{j,d,t_m} \end{cases} \qquad \forall\ j \in J^P, d, t_m \tag{5.53}$$

A similar reformulation as done in the short term planning model gives,

$$IS^{M*}_{j,d,t_m+1} = IS^{M*}_{j,d,t_m} + \sum_{m} \left(FD^{M}_{j,m,d,t_m} + \sum_{t'=N^S-(\delta^F_{m,d}/\Delta T_s)}^{N^S} FD^{S}_{j,m,d,t'} \right) - DF_{j,d,t_m}$$
$$\forall\, j \in J^P, d, t_m = N^S + 1 \quad (5.54)$$

$$IS^{M*}_{j,d,t_m+1} = IS^{M*}_{j,d,t_m} + \sum_{m} FD^{M}_{j,m,d,t_m} - DF_{j,d,t_m} \;\; \forall\, j \in J^P, d, t_m = N^S + 2, \ldots, N^P \quad (5.55)$$

where DF_{j,d,t_m} is the demand of final product j at distribution site d at time period t_m.

Bounds on variables

$$IP^{M}_{j,m,t_m},\; IS^{M}_{j,d,t_m},\; B^{M}_{j,d,t_m} \geq 0 \qquad \forall\, j, m, d, t_m$$
$$B^{M}_{j,d,t_m} \geq -IS^{M*}_{j,d,t_m} \qquad \forall\, j \in J^P, d, t_m$$
$$IS^{M}_{j,d,t_m} \geq IS^{M*}_{j,d,t_m} + B^{M}_{j,d,t_m} \qquad \forall\, j \in J^P, d, t_m$$
$$XP_{ps,ps',r,t_m}, XB_{ps,ps',r,t_m}, XC_{ps,ps',r,t_m} \in \{0,1\} \qquad \forall\, ps, ps' \in PS_r, r, t_m$$
$$YP_{ps,r,t_m}, YF_{ps,r,t_m}, YL_{ps,r,t_m} \in \{0,1\} \qquad \forall\, ps \in PS_r, r, t_m$$

5.2.3 Interface Constraints

In an effort to simplify the model representation, the operational and tactical model constraints were represented separately. However, they form part of a single overall model. An adjustment is made to material balances in the first time period of the tactical model to account for delays in the operational model. To complete the connection between the two models, we equate the inventory levels at the interface point $t = N^S$.

The inventory levels of material j at the end of the operational model (i.e $t = N^S + 1$) is equal to the inventory level at the start of tactical planning period (i.e. $t = N^S + 1$).

$$IP^{M}_{j,m,N^S+1} = IP^{S}_{j,m,N^S+1} \qquad \forall\, j, m \quad (5.56)$$
$$IS^{*,M}_{j,d,N^S+1} = IS^{*S}_{j,d,N^S+1} \qquad \forall\, j, d \quad (5.57)$$

5.2.4 MPC Optimization Problem Representation

The MPC optimization problem optimizes the objective function respecting system constraints and system dynamics.

Integrated model

The model can be represented in the following form to simplify the MPC optimization problem.

$$x^s_{t+1} = A^s_1 x^s_t + B^s_1 u^s_t + \ldots + B^s_v u^s_{t-v} + G^s w^s_t + c_1 \qquad t = 1, \ldots, N^S \tag{5.58}$$

$$x^m_{t+1} = A^m_1 x^m_t + B^m_1 u^m_t + E^m_1 u^s_{N^S} + \ldots + E^m_v u^s_{N^S - v} + G^m_1 w^m_t \qquad t = N^S + 1 \tag{5.59}$$

$$x^m_{t+1} = A^m_2 x^m_t + B^m_2 u^m_t + G^m_2 w^m_t \qquad t = N^S + 2, \ldots, N^P \tag{5.60}$$

$$A_1 x^s_t + A_2 p^s_t + B_1 u^s_t + B_2 q^s_t + G_1 w^s_t + c_2 \leq 0 \qquad t = 1, \ldots, N^S \tag{5.61}$$

$$A_3 x^m_t + A_4 p^m_t + B_3 u^m_t + B_4 q^m_t + B_5 h^m_t + G_2 w^m_t + c_3 \leq 0 \qquad t = N^S, \ldots, N^P \tag{5.62}$$

$$x^m_{N^S+1} = x^s_{N^S+1} \tag{5.63}$$

where, superscripts s and m denote the vector of variables for operational and tactical model respectively. $x, p, u, q, h,$ and w are the vectors of state variables, auxiliary state variables, continuous decisions variables, binary decision variables, integer decision variables, and disturbance parameters. $c_1, c_2,$ and c_3 are the vector of constants. The parameter v represents the maximum value of production and transportation delay, that is $v = \left[\max\{\delta^F_{M,D},\ \delta^P_{M,M},\ \delta^R_{LS,M}\} - 1\right]$.

Some of the decisions variables in Equation (5.58) reflects the decisions in the past when the time period t is less than or equal to v. These decisions variables are treated as parameters and are captured through the vector of constants c_1. Equations (5.58) to (5.60) are inventory balance equations, where Equation (5.58) represents the set of constraints (5.1) and (5.16), Equation (5.59) represents constraints (5.18) and (5.49), and Equation (5.60) represents constraints (5.19) and (5.50). Equation (5.61) represents the set of constraints (5.2)−(5.11), (5.13), and (5.17). Equation (5.62) represents the set of constraints (5.20)−(5.27), (5.29)−(5.32),(5.37)−(5.48) and (5.51). Equation (5.63) describes the equality constraints (5.56) and (5.57).

$$x^s \equiv \left[\ IP^S_{J_m,M},\ IS^{*S}_{J^P,D}\ \right]$$
$$x^m \equiv \left[\ IP^M_{J_m,M},\ IS^{*,M}_{J^P,D}\ \right]$$
$$p^s \equiv \left[\ B^S_{J^P,D},\ IS^S_{J^P,D}\ \right]$$

$$
\begin{aligned}
p^m &\equiv \left[\; B^M_{J^P,D},\; IS^M_{J^P,D} \;\right] \\
u^s &\equiv \left[\; O^S_{J^R,LS,M},\; P^S_{J,PS,R,M},\; FP^S_{J/J^R,M,M},\; FD^S_{J^P,M,D} \right] \\
u^m &\equiv \left[\; O^M_{J^R,LS,M},\; P^M_{J,PS,R,M},\; FP^M_{J/J^R,M,M},\; FD^M_{J^P,M,D}, \right] \\
q^s &\equiv [\; U_{PS,R}, CL_R,\; UT_{PS,R} \;] \\
q^m &\equiv \left[\; YP_{PS^R,R},\; XB_{PS^R,PS^R,R},\; YF_{PS^R,R},\; YL_{PS^R,R},\; XP_{PS^R,PS^R,R},\; XC_{PS^R,PS^R,R},\; DD_R, \right. \\
&\quad \left. TC_R \;\right] \\
h^m &\equiv [\; NB_{PS,R} \;] \\
w^s &\equiv \left[\; DF^S_{J^P,D} \;\right] \\
w^m &\equiv \left[\; DF^M_{J^P,D} \;\right]
\end{aligned}
$$

The variables indices shown above indicate their maximum dimensions and would be defined over the sets described in the model formulation section using the notation,

$$
IP^S_{J_m,M} := \left\{ IP^S_{j,m}, \quad \forall\, m \in M, j \in J_m \right\}
$$

defined similarly for the other variables. Conveniently, the state and decision variables for operational and tactical planning models can be combined together and represented as, $x_t = [x^s_t \;\; x^m_t]$, $p_t = [p^s_t \;\; p^m_t]$, $u_t = [u^s_t \;\; u^m_t]$, and $q_t = [q^s_t \;\; q^m_t]$

Performance function

The performance of supply chain systems is quantified by various criteria. Neely, Gregory, and Platts (1995) categorize SC performance metrics into four classes; quality, time, cost, and flexibility. Beamon (1999) provides an overview of SC performance measures and their evaluation, and presents a framework for the selection of performance measures for SCs. We use a bi-criterion objective function consisting of quality and cost in the MPC optimization problem. In our analysis, customer satisfaction is considered as a quality measure for the supply chain operation and economics is measured in terms of the total operating cost of running the supply chain. The customer satisfaction level is measured in terms of total number of back-orders and is given by the following expression.

$$
\mathcal{J}_1 := \sum_{j,d} \left[\sum_{t_s=1}^{N^S-1} B^S_{j,d,t_s+1} + \sum_{t_m=N^S}^{N^P-1} B^M_{j,d,t_m+1} \right] \tag{5.64}
$$

The economic performance is measured by the total operating cost of running the supply chain.

$$\mathcal{J}_2 := \sum_{t=1}^{N^P-1} \left[C_x^{\mathsf{T}} x_{t+1} + C_p^{\mathsf{T}} p_{t+1} + C_u^{\mathsf{T}} u_t \right] \tag{5.65}$$

where C_x is a cost vector for the state variables x_t, C_p is a cost vector for the auxiliary variables p_t (states that are dependent on other independent state variables), and C_u is a cost vector for the decision variables u_t.

The multi-objective function for the integrated planning problem is given by weighted sum of customer satisfaction ($\mathcal{J}_1$) and operating cost ($\mathcal{J}_2$), where ω_1 and ω_2 are the weighting parameters.

$$\mathcal{J}^* := \omega_1 \mathcal{J}_1 + \omega_2 \mathcal{J}_2 \tag{5.66}$$

Remarks

1. As it was stated earlier, the model can accommodate transportation delays by setting non-zero values to the delay parameters. However due to discrete-time formulation, it (delay value) should be an integral of the STP discretization period.

2. It is assumed that the change-over cost is directly proportional to change-over time and therefore breaking the production link having highest change-over time to generate production schedule from a cyclic schedule will ensure minimum operating cost.

3. It is assumed that cleaning operation ($CL_{r,t}$) takes exactly one STP time period for all processing units.

4. For the instances where no production task is allocated to a unit during any time period, the production scheduling is not required. In this case, the constraints set (5.37)−(5.39) sets the value of production indicator variable DD_{r,t_m} to zero.

5. The TSP constraints (5.30) to (5.48) for cyclic scheduling start the production scheme, only if the involved raw materials are available or going to be produced during that time period. So in the cases where one production scheme uses intermediate products of another production scheme as raw materials, and no intermediate product is available at the start of the time period, it will allocate both production schemes in one time period. However, the precedence of production schemes is selected in a way that only minimizes the change-over time and neglects the necessity of starting a production scheme that yields intermediate products for another scheme. In this scenario, the solution obtained at the tactical planning may differ

from the operational model although no subcycle exists. By contrast, the operational model uses a smaller time grid and checks for the raw material availability before allocating any production scheme to a unit.

6. The back-order and inventory amounts are accumulated at each time period and penalized in the objective function. Due to the big time bucket ($\Delta T_m > \Delta T_s$) of tactical model, the intermediate dynamics present in these variables is simply lost, and hence is not considered in the cost calculation. Therefore, the tactical model is expected to underestimate the back-order and inventory cost of the operational model.

5.2.5 Model Predictive Control (MPC) Framework

In the MPC framework, the controller solves a dynamic optimization problem spanning the time horizon of interest and uses a process model to determine the optimal input moves in accordance with a specified objective. Figure 5.4 shows a single layer decision framework proposed in the current work. The MPC optimization problem calculates the decisions using the hybrid time model discussed in the previous section. Only the first input moves are implemented on the process. The system dynamics included in the model may not exactly represent the real process behavior. Moreover the prediction of demand and process yield are also not precise and therefore the implemented decisions will generate process outputs that are different than the model predicted outputs. The mismatch information is fed back to the controller at the next time increment. The time horizon is advanced and the system is re-optimized with this new information. The feedback essentially includes the effect of plant-model mismatch and system disturbances. Since

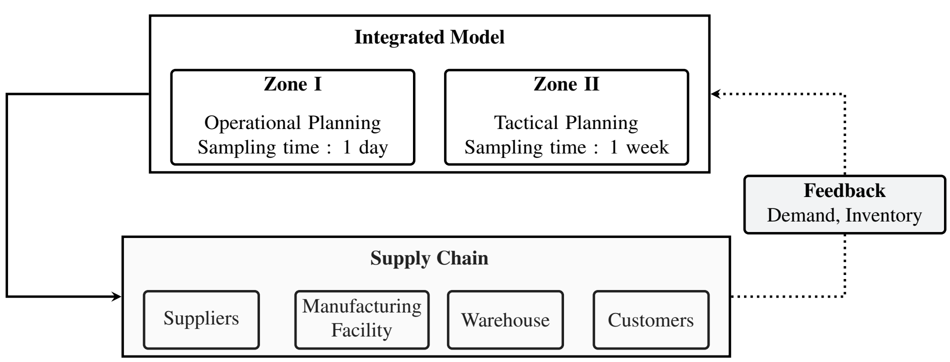

Figure 5.4: Schematic representation of the proposed integrated planning decision framework

the integrated model incorporates a non-uniform time grid, the advancement of the time horizon is achieved in a block manner that synchronizes the time grid of STP and MTP models. Figure 5.5 shows a schematic diagram of the horizon advancement framework. In the current approach, the time horizon is not extended until it reaches at the end of the first large time bucket (ΔT_m). Let's consider a time snap shot at $t = 4$. At this point, the decisions for time $t = 1, 2,$ and 3 are known, therefore the MPC optimization problem at $t = 4$ treats these variables as parameters and re-calculates the control trajectories. The time synchronization of both models occurs at the end of large-bucket time period (here, at $t = 7$). At this time instant, the time horizon is advanced by one large-bucket time period as illustrated in the figure, and the past time periods are dropped.

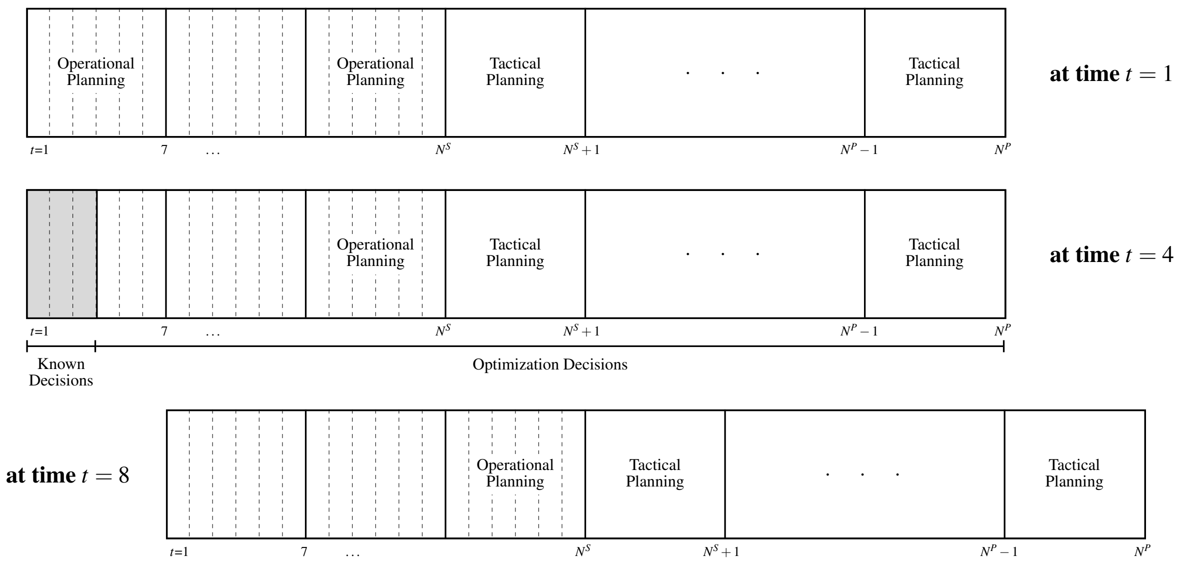

Figure 5.5: A rolling horizon strategy for MPC implementation. The time horizon advances when it reaches at the end of a large time bucket (ΔT_m).

5.3 CASE STUDY

The implementation of the proposed integrated modeling approach in a rolling horizon MPC framework is demonstrated on a simulation case study of a multi-product, multi-echelon supply chain. It comprises of two suppliers ($\mathrm{LS}_1, \mathrm{LS}_2$), two plant sites ($\mathrm{M}_1, \mathrm{M}_2$), four reactors ($\mathrm{R}_1, \ldots, \mathrm{R}_4$) that can run five production schemes ($\mathrm{PS}_1, \ldots, \mathrm{PS}_5$), and two distribution sites ($\mathrm{DC}_1, \mathrm{DC}_2$). The manufacturing facility has multiple reactors that can run in parallel. Each reactor can run only subset of production schemes. As shown in Figure 5.6, total 5 production schemes are available to produce two final products E and G from two main raw materials A and B. Materials C, D, and F are intermediate products. Plant site M_1 has two reactors R_1 and R_2. Reactor R_1 can run the production scheme PS_1 and

PS_2, and the production scheme PS_3 can be run on reactor R_2. The plant site M_2 houses two reactors R_3 and R_4. The production scheme PS_4 and PS_5 can be run on reactor R_3 and R_4 respectively. Plant site M_2 uses intermediate product D as one of its raw materials for the production scheme PS_4, and thus it can not start production until it receives it from plant site M_1. The mass balance coefficients of the reaction scheme are represented in Figure 5.6. Customer demand and process yield are considered as input disturbances in

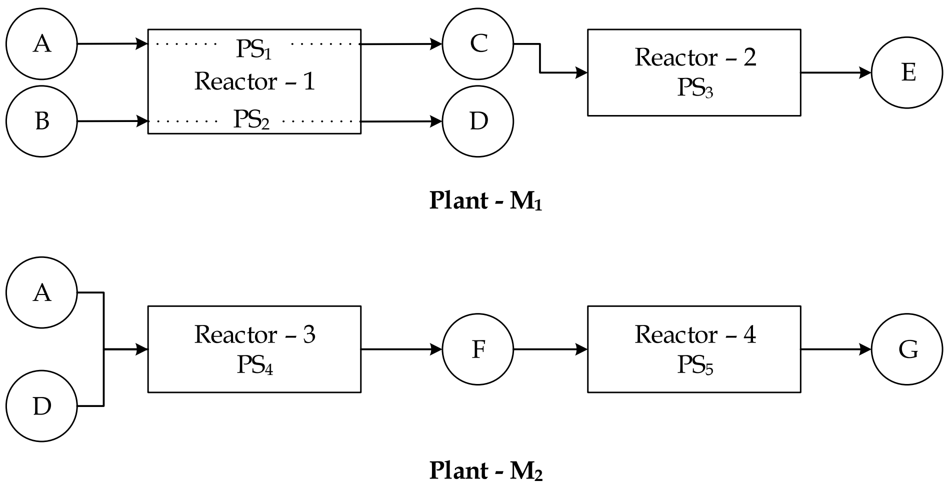

Figure 5.6: Production network of a integrated planning case study. Reactor 1 is a multipurpose batch production unit, and all other plants are dedicated plants.

the MPC framework. In the analysis, the customer service level is weighted 15 times the process economics. To check the computation and economic efficiency of an integrated model, we compare it against a full-sized detailed planning (DP) model. In the DP, the entire planning horizon is formulated using the operational planning model. Because of the inclusion of detailed dynamics, the DP provides a more accurate representation of the system and is expected to yield an upper bound in terms of system performance. Total operating cost and customer satisfaction are used as solution statistics to compare the performance. The production change-over time ($\tau_{ps,ps'}$) is taken as 1 day for all production switches. The aggregated production capacity (Γ_r^u) for unit R_1, R_2, R_3 and R_4 is taken as 200 units. The case study data are summarized in Tables 5.1 to 5.8.

Table 5.1: Simulation parameter values for integrated planning case study

Parameter	Value	Parameter	Value
Simulation length	100 days	ω_1/ω_2	15
ΔT_s	1 day	ΔT_m	1 week

Table 5.2: Raw material cost for the integrated planning case study ($/unit)

Raw material	Supplier	
	LS_1	LS_2
A	1	1.2
B	1.4	1.7

Table 5.3: Product back-order cost for the integrated planning case study ($/unit)

	Material	
	E	G
Cost ($/unit)	5	5

Table 5.4: Cost parameter values for the integrated planning case study

Plant site	Shipment Cost of FP in C_u		Shipment Cost of FF in C_u		Production Cost of P^S/ P^M in C_u				
	Plant site		Distribution site		Production Task				
	M_1	M_2	D_1	D_2	PS_1	PS_3	PS_2	PS_4	PS_5
M_1	–	1.05	2.7	2.8	1.25	1	1	–	–
M_2	1.05	–	2.8	2.5	–	–	–	1	1

Note: The shipment costs are the same for all chemicals within each shipment category.

Table 5.5: Inventory parameter values for the integrated planning case study

Parameter	Plant site		Distribution site	
C_x ($/unit)	M_1	M_2	D_1	D_2
Cost of IP	0.8	0.7	–	–
Cost of IS	–	–	1.5	1.25
Storage capacity				
Ω^R	150	150	–	–
Ω^F_E/ Ω^F_G	100	100	–	–

Note: The inventory costs are the same for each chemical within each storage site.

The optimization problem is modeled with `AMPL` and solved using `CPLEX 12.6`. Simulations are performed on a 3.4 GHz Intel® Core^{TM} i7 machine with 8 GB of RAM to a 0.01% optimality gap, running Windows® 7 Professional 64-bit.

5.3.1 Nominal Case

In this section, we investigate the system performance using the integrated modeling based MPC framework. The STP model uses a time discretization period of 1 day and the

Table 5.6: Production parameter values for the integrated planning case study

Parameter	Plant site	Production Scheme				
		PS_1	PS_3	PS_2	PS_4	PS_5
γ^u : production batch size						
	M_1	200	200	200	–	–
	M_2	–	–	–	200	200
γ^l : production batch size						
	M_1	25	25	25	–	–
	M_2	–	–	–	25	25
σ_{ps} : production delay (day)	–	2	1	1	1	2
β^P_{ps} : process yield	–	0.8	0.8	0.8	0.8	0.8
η_{ps} : relative production Coef.	–	1	1	1	1	1

Table 5.7: Maximum transportation quantity for the integrated planning case study

	λ^R (units)		λ^F (units)		λ^P (units)	
	Supplier		Distribution site		Plant site	
Plant site	LS_1	LS_2	D_1	D_2	M_1	M_2
M_1	150	150	100	100	–	100
M_2	150	150	100	100	100	–

Table 5.8: Mass balance coefficients of production schemes for the integrated planning case study

Production scheme	Material						
	A	B	C	D	E	F	G
PS_1	1^*	–	1	–	–	–	–
PS_2	–	1^*	–	1	–	–	–
PS_3	–	–	1^*	–	1	–	–
PS_4	1^*	–	–	1	–	1	–
PS_5	–	–	–	–	–	1^*	1

Note: * denotes the main raw material for the corresponding production scheme

MTP model uses a 1 week discretization time. The sampling time of each MPC run is 1 day. The performance is reported with the values obtained by running the MPC framework for 100 days. All simulation cases are run with weighting parameters, $w_1 = 15$ and $w_2 = 1$ and subjected to the same demand realization.

Integrated model accuracy

Here, we check the modeling accuracy of the integrated model against the detailed operational model by running different simulations with varying combinations of operational and tactical planning horizons. The DP model is considered as the base case for the comparison. We aim to analyze the degradation in performance and thereby choosing the optimal horizon for the integrated model.

System performance comparison

Different simulations are run with an MPC prediction horizon of 49 days with the assumption that operational model exhibits true process dynamics, that is no plant model mismatch. Each run uses a different combination of small and composite time periods; (1) 14 days + 5 weeks, (2) 21 days + 4 weeks, (3) 28 days + 3 weeks, (4) 35 days + 2 weeks, (5) 42 days + 1 week and (6) 49 days (base case - operational planning). The performance value is reported by running each case for 100 simulation days. The x-tickmark *14d+5w* denotes an MPC planning horizon of 7 weeks; 14 days (2 weeks) of operational planning and 5 weeks of tactical planning. Figure 5.7 shows the MPC controller performance of optimizing operating and back-order cost using the integrated model. In all simulation runs, same outcome of demand realization is considered.

The *49d+0w* case, which represents a detailed modeling approach, shows the highest level of customer satisfaction with minimum possible cost. As more and more time periods are filled with a tactical planning model, the economic performance degrades. This is due to the approximation of production and transportation capacity in the tactical planning periods. However, the customer satisfaction level is more or less same in all the cases, varying over a very narrow range from 91.15% to 91.56%. Another interesting observation is that the rate of increase in economic performance (i.e. decrease in operating plus back-order cost) diminishes as the number of operational planing blocks increases. The system performance improves at a steep rate initially until 5 weeks of operational planning period (*35d+2w*) but then it flattens off. Therefore, it can be inferred from the results that for a prediction horizon of 49 days (7 weeks), the integrated model with 35 days of operational and 2 weeks tactical planning horizon achieves comparable performance with the detailed operational model (*49d+0w*). The total cost is 1.1495 $\times 10^5$ units and 1.1589 $\times 10^5$ units with the cases *49d+0w* and *35d+2w* respectively.

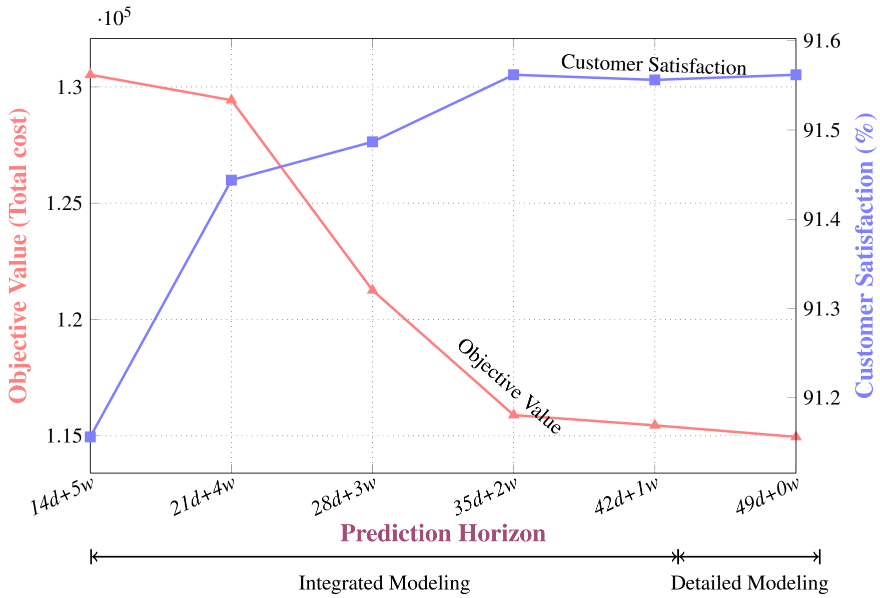

Figure 5.7: Performance comparison between integrated and detailed modeling approach (without transportation delay)

Computation time

Figure (5.8) shows the computational performance of the integrated modeling framework. The plot indicates that the computation time increases with increasing slope as the time horizon of STP model increases. The computation time is reported as the average time required to solve one MPC optimization problem by running each simulation case for a simulation horizon of 100 days. The number of binary and continuous variables increases with the number STP blocks and hence the computation load goes up. Due to the high number of decision variables for the detailed planning case, the computation load is the highest among all. It is worthwhile to mention that the operational model (*49D+0W*) yields superior performance (0.80 % against the case *35d+2w*) but at the same time the computation time is 6 times higher than the case *35d+2w*. The analysis suggests if the computation time of 11.1 sec is acceptable, operating the supply chain with an MPC prediction horizon of 35 days + 2 weeks is superior to 49 days + 0 week, as comparable economics performance is achieved at a significantly lower computation burden.

Similar comparison analysis is performed where transportation delay is considered in the operational model, and results are summarized in Figure 5.9. The transportation delay parameters are tabulated in Table 5.9. The performance gap quickly diminishes as more and more number of time periods are filled with the operational model, and the case *35d+2w* generates very similar performance as detailed modeling case *49d+0w*. It

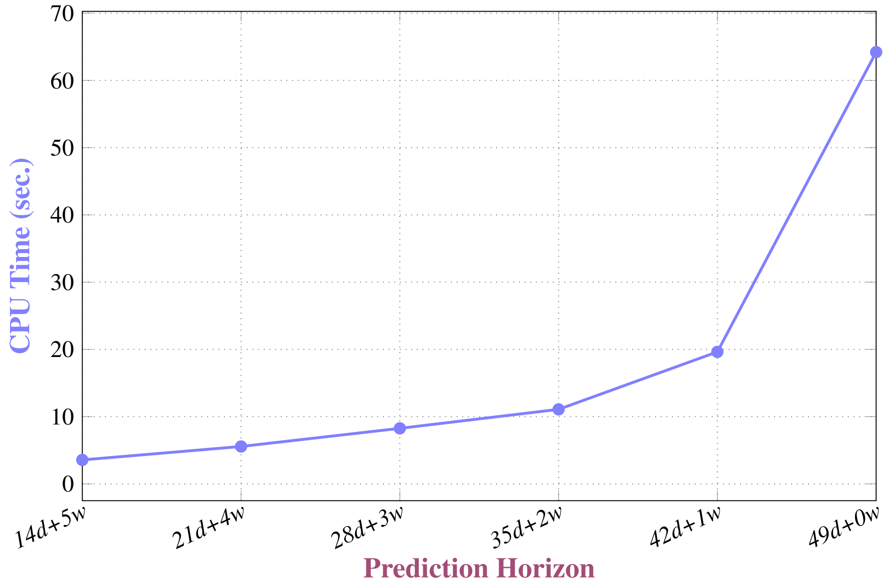

Figure 5.8: Computational performance comparison between integrated and detailed modeling approach (without transportation delay)

is significant to note that though the tactical model does not account for transportation delay, the performance degradation for the case *35d+2w* against *49d+0w* is quite minimal and we believe that the feedback effect present in the MPC framework helps to offset the losses. However, the total cost of operating a supply chain for the case *49d+0w* with delay has increased to 4.9849 $\times 10^5$ from the non-delay case 1.1495 $\times 10^5$, nearly 4 fold increase. It is our assessment that the back-order cost constitutes a major portion of the total cost. Delays in transporting materials across network causes delays in dispatching the first batch of products to customers and creates stock-out conditions. Moreover, because of the limited production capacity of the reactors, it takes longer to satisfy the accumulated customer orders, and therefore the stock-out condition lasts for a longer horizon. Further, this is compounded by the high weighting of the back-order cost. The effect of the transportation delay is clearly seen in the level of customer satisfaction; for the base case *49d+0w*, the level drops from 91.56 % to 76.82 %. However, unlike the case with no transportation delay, the customer satisfaction level increases from 61.55 % to 76.81 % as the operational planning horizon increases from 14 days (*14d+5w*) to 49 days (*49d+0w*).

Table 5.9: Transportation delays for the integrated planning case study

Plant site	Supplier		Distribution site		Plant site	
	LS_1	LS_2	D_1	D_2	M_1	M_2
transportation delay	δ^R		δ^F		δ^P	
M_1	3	3	3	4	0	2
M_2	2	2	4	2	2	0

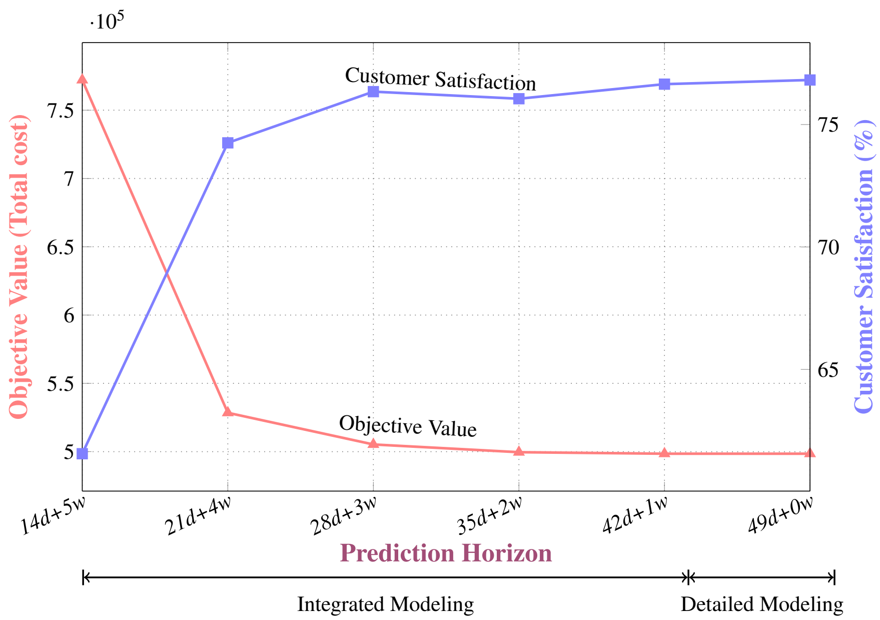

Figure 5.9: Performance comparison between integrated and detailed modeling approach (with transportation delay)

5.4 PLANNED MAINTENANCE SHUTDOWN

The MPC employs a feedback mechanism to mitigate the effect of disturbances and uncertainty on the system performance. In this section, we investigate the system performance under planned maintenance shutdown. We first discuss phenomena involving shutdown modeling for the integrated planning. The presence of a non-uniform time grid needs to be considered while formulating the shutdown model. For ease of explanation, first we narrate how we model plant shutdown dynamics for a single time grid and then extend it to for a hybrid time grid.

Shutdown formulation

The plant shutdown restricts the availability of an individual processing unit. In the STP model, we represent this conditions by incorporating the following constraint (Chong, 2012) that makes the production unit unavailable by setting the value of a variable UT_{ps,r,t_s} to zero. UT_{ps,r,t_s} as defined in Section 5.2.1, takes the value 1 if production task is assigned to unit r at time t_s.

$$UT_{ps,r,t_s} \leq 1 - \alpha^{shut}_{r,t_s} \qquad \forall\; ps, r, t_s \tag{5.67}$$

where $\alpha^{shut}_{r,t_s} \in \{0, 1\}$ is an indicator variable that shows the status of processing unit r at time period t_s. It takes the value 1 when the unit is shut down and 0 for normal operation. For instance, if we wish to induce a manual plant shutdown, we can explicitly impose the following constraint by setting the value of $\alpha^{shut}_{r,t}$ as follows,

$$\alpha^{shut}_{r,t} = \begin{cases} 1 & t = t_{start}, \ldots, t_{end},\ r \in R \\ 0 & \text{elsewhere} \end{cases} \tag{5.68}$$

where t_{start} is shutdown start time and t_{end} is shutdown end time. While α^{shut}_{r,t_s} is a binary variable, the explicit fixing of variables results in no net increment of binary variables in the optimization problem and hence the computational complexity does not increase.

The above formulation is applicable if the shutdown period covers only STP time horizon, as production unit availability UT_{ps,r,t_s} is not defined for the MTP period. If a plant shutdown event covers both STP and MTP time periods, additional constraints need to be imposed to restrict the production activities in the MTP period. Shutdown activities may not cover the whole MTP period due to the relatively large time bucket of the MTP model which therefore makes the extension a non-trivial exercise. To model the plant shutdown phenomena for the MTP horizon, we introduce a production capacity factor $\nu_{r,tm}$ for unit r at time period t_m into the MTP model. It is defined as the percentage of MTP period available for production that is a non-shutdown time. By definition, the available production time is the duration of a MTP period ($H\ \Delta T_m$) less the shutdown time. We further assume that the shutdown period is in multiple of the STP discretization time.

To facilitate the calculation of the plant shutdown time for a MTP period, we extend the definition of the shutdown variable $\alpha^{shut}_{r,t}$ to cover the whole planning horizon rather than restricting it to the STP time horizon. The shutdown indicator variable uses a STP discretization time index over the whole planning horizon, i.e. the time index of $\alpha^{shut}_{r,t}$

takes value from $t = 1$ to $t = N^S + (N^P - N^S)H$, similar to considering a detailed planning time grid over the entire horizon. The new definition of the shutdown indicator variables is therefore given by,

$$\alpha^{shut}_{r,t} \in \{0,1\} \qquad \forall\, r, t \in 1, \ldots, N^S + (N^P - N^S)H$$

Naturally, it increases the number of binary variables; however it makes the shutdown formulation easier to extend from a single time grid to the hybrid time grid. The shutdown time (γ_{t_m}) for a MTP period t_m is now calculated simply from shutdown variable $\alpha^{shut}_{r,t}$ as follows,

$$\gamma_{t_m} = \sum_{t=N^S+(t_m-1)H+1}^{N^S+t_m H} \alpha^{shut}_{r,t} \qquad \forall\, r, t_m \tag{5.69}$$

Having defined the shutdown period, the production capacity factor is given as follows,

$$\nu_{r,t_m} = 1 - \frac{\gamma_{t_m}}{H} = 1 - \frac{\sum\limits_{t=N^S+(t_m-1)H+1}^{N^S+t_m H} \alpha^{shut}_{r,t}}{H} \qquad \forall\, r, t \tag{5.70}$$

The production capacity factor scales down the production capacity during shutdown. Depending on the fraction of time period t_m covered by shutdown activities, the summation term in the denominator takes the value between 0 and H, which sets the value of the production capacity factor between 0 and 1.

Adjustment of the production capacity for a shut down period requires modification of the constraints (5.26) and (5.29) as follows,

$$\sum_{ps \in PS_{r,m}} \eta_{ps}\, P^M_{j,ps,r,m,tm} \leq (H - TC_{r,t_m}/\Delta T_s)\, \nu_{r,t_m}\, \Gamma^u_r \qquad \forall\, j \in J^{MR}_{ps}, r, m, t_m \tag{5.71}$$

$$P^M_{j,ps,r,m,t_m} \leq H\, \gamma^u_{ps,m}\, \nu_{r,tm}\, YP_{ps,r,t_m} \qquad \forall\, j \in J^{MR}_{ps},\ ps \in PS_{r,m}, r, m, t_m \tag{5.72}$$

In the case of complete shutdown during time period t_m, the right side of constraints (5.71) and (5.72) becomes zero (as $\nu_{r,tm} = 0$), while they reduce to Equations (5.26) and (5.29) respectively when no shutdown activities are scheduled. In simulation, $\alpha^{shut}_{r,t}$ and $\nu_{r,tm}$ are specified as parameters and hence the problem remains a mixed-integer linear programming problem (MILP).

As plant shut-down restricts the plant availability for production, the time balance equation

(5.48) needs to change to account for shutdown activities.

$$\sum_{ps \in PS_r} NB_{ps,r,t_m} \sigma_{ps} + TC_{r,t_m} + \sum_{ps \in PS_r} \sum_{ps' \in PS_r} XC_{ps,ps',r,t_m} \, \tau_{ps,ps'} + \gamma_{t_m} \, \Delta T_s \, \leq \, H \, \Delta T_s \quad \forall r, \, t_m \quad (5.73)$$

The constraint (5.73) states that the summation of changeover time, shutdown time ($\gamma_{t_m} \, \Delta T_s$) and production time within each time period should be less than the length of each MTP time period $H \, \Delta T_s$. All other model equations are kept the same as presented in Section 5.2.

To simulate a manually triggered shutdown scenario, the shutdown indicator variable is set to one for the shutdown period and $\nu_{r,tm}$ is calculated before running each instance of an MPC optimization. At the end of a large-bucket time period, the MPC horizon is advanced by a MTP period; $\alpha_{r,t}^{shut}$ and $\nu_{r,tm}$ are re-calculated to match the actual shutdown period with a new MPC prediction horizon, and control inputs are updated.

For the simulation case study, we manually introduce shutdowns in units 1 and 3 from time period 53 to 66, while unit 2 and 4 undergo shutdown from time period 67 to 80 (time markers and performance results are depicted in Figure 5.10). The MPC controller sees the future plant shutdown condition and changes production planning in order to minimize the impact of the plant shutdown and maximize the customer service level. The integrated planning activities are scheduled with a prediction horizon of length varying from *28d+1w* (28+1×7 = 35 days) to *28d+6w* (28+6×7 = 70 days). In all simulation runs, same outcome of demand realization is considered. The longer the prediction horizon, the MPC controller starts acting early and hence it gets more time to reschedule the production activities. The customer service level increase steadily with the prediction horizon and the improvement tapers off after a sufficiently long prediction horizon is employed in the MPC controller. In the current study, it is achieved at *28d+5w* (28+5×7= 63 days). Similarly, the operating cost decreases with the prediction horizon.

The schedule of maintenance activities naturally decreases the availability of production resources, and hence the customer satisfaction level drops from 91.48% (no maintenance case with *28d+3w*) to 57.84 % (maintenance case with *28d+3w*).

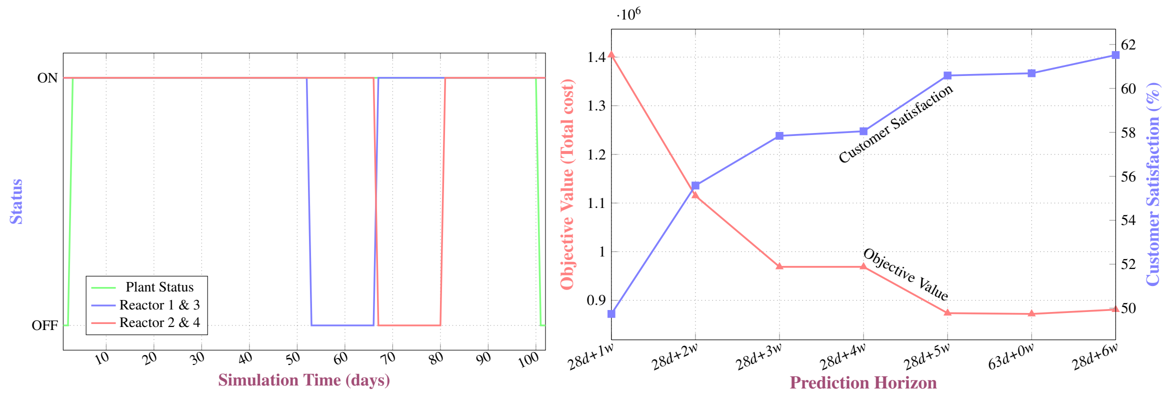

Figure 5.10: (a) Operational status of reactors 1−4; (b) Performance results for integrated planning with STP period of 28 days and MTP period varies from 1 week to 6 week

5.5 MAINTENANCE SHUTDOWN PERIOD OPTIMIZATION

In this section, we consider planned maintenance activities in which a time frame is specified over which it can be completed. In this scenario, the maintenance activities should be scheduled at a time point where it has minimal impact on the system performance. In other words, the start and finish time of plant shutdown period should be optimized without jeopardizing plant safety.

Optimal shutdown formulation

We formulate an optimal shutdown model to decide the best time to initiate the plant shutdown within a given time frame [$t_p^{start} - t_p^{end}$], where t_p^{start} is the earliest time by which shutdown event can be initiated and t_p^{end} is the latest time by which shutdown process should be completed.

In the earlier section, the shutdown period was given a priori and hence $\alpha_{r,t}^{shut}$ and $\nu_{r,tm}$ are treated as parameters; however in the case of maintenance period optimization, they are unknown and need to be determined within the optimization framework. Being a discrete decision variable, $\alpha_{r,t}^{shut}$ increases the total count of binary variables and hence computational burden, however it makes the extension of the single time scale shutdown formulation for the hybrid time grid straightforward. Once a unit experiences shutdown, it remains in shutdown mode for predefined time. In order to mark the shutdown start and end time, we employ following constraint formulation from Kelly and Zyngier (2007) to calculate the time-markers. The advantage of these constraints is that it does not require the definition of any new binary variables and thus does not adversely affect the solution complexity.

$$\alpha_{r,t}^{shut} - \alpha_{r,t-1}^{shut} = DN_t - UP_t \qquad \forall\, t \in t_p^{start}, \ldots, t_p^{end} \tag{5.74}$$
$$\alpha_{r,t}^{shut} + \alpha_{r,t-1}^{shut} = DN_t + UP_t + 2QK_t \qquad \forall\, t \in t_p^{start}, \ldots, t_p^{end} \tag{5.75}$$
$$DN_t + UP_t + QK_t \le 1 \qquad \forall\, t \in t_p^{start}, \ldots, t_p^{end} \tag{5.76}$$
$$DN_t;\ UP_t;\ QK_t \in [0,1]$$

DN_t and UP_t shows the start ($DN_t = 1$) and end ($UP_t = 1$) time of a shutdown period respectively. QK_t takes the value 1 when plant is in shutdown mode except at the start and end time instant. The formulation defined by constraints (5.74) − (5.76) enforce the integrality of the the continuous variables $DN_t, UP_t,$ and QK_t.

When a unit undergoes maintenance, the plant stays offline for a specified contiguous duration. The following formulation is adapted from Chong (2012) to ensure that the shutdown event lasts for a specified duration TW.

$$SP_t = \sum_{t}^{t+TW-1} \alpha_{r,i}^{shut} \qquad \forall\, t = t_p^{start}, \ldots, t_p^{end} - TW \tag{5.77}$$
$$SP_t \ge TW\ DN_t \qquad \forall\, t = t_p^{start}, \ldots, t_p^{end} - TW \tag{5.78}$$
$$\sum_{t=t_p^{start}}^{t_p^{end}} DN_t = 1 \tag{5.79}$$
$$\sum_{t=t_p^{start}}^{t_p^{end}} \alpha_{r,t}^{shut} \le TW \tag{5.80}$$
$$DN_t = 0 \qquad \forall\, t = t_p^{end} - TW + 1, \ldots, t_p^{end} \tag{5.81}$$
$$\alpha_{r,t}^{shut} = 0 \qquad \forall\, t < t_p^{start} \tag{5.82}$$
$$\alpha_{r,t}^{shut} = 0 \qquad \forall\, t > t_p^{end} \tag{5.83}$$

Here TW is the length of shutdown period; SP_t is the TW step ahead summation of shutdown variable $\alpha_{r,t}^{shut}$. Note that TW is assumed to be an integral of the STP discretization time.

As some of the parameters of the shutdown formulation become variables, a few constraints need to be altered. Considering ν_{r,t_m} as a decision variable in shutdown period optimization problem introduces bilinearity. The term $(H - TC_{r,t_m}/\Delta T_s)\ \nu_{r,tm}$ in Equation (5.71) and $\nu_{r,t_m}\ YP_{ps,r,t_m}$ in Equation (5.72) become bi-linear, which transforms the plant shutdown formulation to a mixed-integer non-linear programming (MINLP) formulation. MINLP problems are difficult to solve, because of the combinatorial nature and non-convexity. In an effort to keep the problem complexity minimal, we reformulate bilinear terms into linear forms so that optimality can be more readily guaranteed. Moreover, it also makes it easy to compare the system performance with different tuning parameters. If the bilinear term contains one continuous variable and one binary variable, exact linearization can be applied given the lower and upper bound of the continuous variable (FICO Xpress Optimization Suite, 2009). The exact linear re-formulation of Equation (5.72) can be given by the following set of equations.

$$AY_{ps,r,t_m} \leq YP_{ps,r,t_m} \qquad \forall\, ps \in PS_r, r, t_m \tag{5.84a}$$

$$0 \leq \nu_{r,t_m} - AY_{ps,r,t_m} \leq 1 - YP_{ps,r,t_m} \qquad \forall\, ps \in PS_r, r, t_m \tag{5.84b}$$

$$P^M_{j,ps,r,m,t_m} \leq H\ \gamma^u_{ps,m}\ AY_{ps,r,tm} \qquad \forall\, j \in J^{MR}_{ps}, ps \in PS_{r,m}, r, m, t_m \tag{5.84c}$$

Here, $AY_{ps,r,t_m} = \nu_{r,t_m}\ YP_{ps,r,t_m}$ is an auxiliary variable.

In Equation (5.71), the term representing available production time $(H - TC_{r,t_m}/\Delta T_s)\ \nu_{r,tm}$ is bi-linear. Instead of multiplying $(H - TC_{r,t_m}/\Delta T_s)$ by ν_{r,t_m}, we insert the definition of shutdown period and subtract it from $H - TC_{r,t_m}/\Delta T_s$ to calculate the available production time, which converts the Equation (5.71) to a linear form.

$$\sum_{ps \in PS_{r,m}} \eta_{ps}\ P^M_{j,ps,r,m,tm} \leq (H - TC_{r,t_m}/\Delta T_s - \gamma_{t_m})\ \Gamma^u_r \qquad \forall\, j \in J^{MR}_{ps}, r, m, tm \tag{5.85}$$

The model can be extended to optimize the shutdown time for each processing unit individually; for the simulation case study, we assume that all units experience shutdown at the same time. All other model equations are kept same as presented in Section 5.2. For the maintenance period optimization study, we run multiple open loop MPC simulations with two prediction horizon lengths, *21d+11w* and *35d+9w*, to schedule maintenance activities. The maintenance activities of 7 days has to be scheduled within specified time frame, which has a start time of day 20 to a end time varying from day 30 to day 85. A κ value of 0.5 is employed in the analysis. The maintenance period optimization results are summarized in Table 5.10.

The results show the controller objective function value for open loop simulations that is, running MPC controller only once at time $t = 1$ for the same outcome of demand realization. The case with maintenance time frame of day $20 - 35$ yields the highest cost (see Table 5.10). The cost gradually decreases with increasing maintenance time window. For the given case study data, the maintenance gets pushed to the end as we extend

Table 5.10: Maintenance period optimization results with a 7 day maintenance period and different MPC prediction horizons and maintenance time windows

Case	Maintenance Window	obj fn value (monetary units) MPC Prediction horizon			
	from − to (day)	*21d+11w*	Maintenance days	*35d+9w*	Maintenance days
1	20 − 30	438924 (0%)	24-30	408897 (0%)	24-30
2	20 − 40	428710 (2.3%)	33-39	399847 (2.2%)	34-40
3	20 − 50	416316 (5.2%)	43-49	373144 (8.7%)	43-49
4	20 − 60	403579 (8.1%)	54-60	359226 (12.1%)	54-60
5	20 − 70	395403 (9.9%)	64-70	351050 (14.1%)	63-69
6	20 − 85	394654 (10.1%)	67-73	347762 (15.6%)	75-81

the maintenance time window. The number in bracket shows the % improvement from the base case−1. For the prediction horizon *21d+11w*, case−6 (maintenance time frame from 20 to 85) shows a 10% improvement compared to case−1 (20−30). As discussed earlier, due to the mismatch in the discretization periods, the operating and back-order cost for the operational and tactical model yield different numbers and therefore the comparison between different combination of prediction horizon is not performed for open-loop simulation runs.

5.6 CONCLUSIONS

In this work, we presented an integrated modeling framework to combine operational and tactical planning activities into a single mathematical model and used model predictive control as a decision making tool. Through simulation, it was shown that the quality of the integrated modeling framework performance depends on how many detailed planning periods are used and it improves as more and more time periods are modeled with detailed scheduling activities. Further, a good quality solution can be achieved with low computation cost. We applied the proposed framework to a supply chain system having multiple suppliers, multi-stage production facilities, and multiple warehouses. Moreover, we studied the framework for maintenance shutdown cases and extended the formulation to schedule the shutdown event to optimize the cost and improve the customer satisfaction.

NOMENCLATURE

Indicies/Sets

$d \in D$	distribution site
$j \in J$	material (chemical)
$ls \in LS$	raw material supplier
$m \in M$	plant site
$ps \in PS$	production scheme
$r \in R$	production unit
$t_s \in T$	STP time period
$t_m \in T$	MTP time period
J_{ps}^{MR}	set of main raw-materials for production scheme ps
J^P	set of final products
J_m^P	set of products for plant site m
J^R	set of raw materials
J_m^R	set of raw materials for plant site m
PS_r	set of production schemes can be run at unit r
$PS_{r,m}$	set of production schemes can be run at unit r at site m
R_m	set of processing units installed at site m

Binary Variables

U_{ps,r,t_s}	1 if the processing unit r begins a production scheme ps at time period t_s; and 0 otherwise
XB_{ps,ps',r,t_m}	1 if the link between production schemes ps and ps' is to be broken; and 0 otherwise
XC_{ps,ps',r,t_m}	changeover variable between scheme ps and ps' across adjacent time periods t_m and $t_m + 1$
XP_{ps,ps',r,t_m}	1 if production scheme ps precedes scheme ps in unit r at time period t_m; and 0 otherwise
YF_{ps,r,t_m}	1 if the production scheme ps is running as first scheme at unit r at time period t_m; and 0 otherwise

YL_{ps,r,t_m}	1 if the production scheme ps is running as last scheme at unit r at time period t_m; and 0 otherwise
YP_{ps,r,t_m}	1 if the production scheme ps at unit r at time period t_m ; and 0 otherwise

Integer Variable

NB_{ps,r,t_m}	number of batches of production scheme ps in unit r during time period t_m

Continuous Variables

t_p^{end}	end time of shutdown event
t_p^{start}	start time of shutdown event
AY_{ps,r,t_m}	auxiliary variable represents multiplication of production factor ν_{r,t_m} and YP_{ps,r,t_m}
$B_{j,d,t}^{(\cdot)}$	back-order quantity of final product j in distribution site d at time period t
C_x	cost coefficients for inventory held at the plant
C_p	cost coefficients for inventory held at the distribution site
C_u	cost coefficients for decision variables (raw material procurement, production and transportation amount)
CL_{r,t_s}	1 if cleaning task begins at process unit r at time period t_s; and 0 otherwise
DN_t	1 if shutdown event starts at time period t; and 0 otherwise
$FD_{j,m,d,t}^{(\cdot)}$	quantity of final product j shipped from plant site m to distribution site d during time period t
$FP_{j,m,m',t}^{(\cdot)}$	quantity of material j shipped from plant site m to site m' during time period t
$FS_{j,d,t}^{(\cdot)}$	quantity of final product j shipped from distribution site d to fulfil customer demand and back orders during time period t
$IP_{j,m,t}^{(\cdot)}$	inventory of material j stored at plant site m during time period t
$IS_{j,d,t}^{(\cdot)}$	inventory of product j held at distribution site d at time period t
$IS_{j,d,t}^{*(\cdot)}$	auxiliary variable for inventory level of product j held at distribution site d at time period t

$O^{(\cdot)}_{j,ls,m,t}$	purchase quantity of raw material j to supplier ls from plant site m at time period t
$P^{(\cdot)}_{j,ps,r,m,t}$	quantity of material j begins to undergo production in unit r of plant site m at time period t (batch size)
QK_t	1 if plant is in shutdown mode except at start and end time; 0 otherwise
SP_t	TW step ahead summation of shutdown indicator variable $\alpha^{shut}_{r,t}$
TC_{r,t_m}	total changeover time of unit r in time period t_m
UT_{ps,r,t_s}	state of processing unit r for production scheme ps at time period t_s
UP_t	1 if shutdown event ends at time period t; 0 otherwise
$\alpha^{shut}_{r,t}$	shutdown indicator variable of processing unit r at time period t
γ_{t_m}	duration of shutdown event in multiple of STP concretization period at time period t_m
$\mathcal{J}^*$	overall objective function
$\mathcal{J}_1$	measure of customer satisfaction level
$\mathcal{J}_2$	measure of economic performance

Parameters

t_{end}	end time of planned maintenance shutdown event
t_{start}	start time of planned maintenance shutdown
v	maximum value of transportation and production delay parameters
$DF_{j,d,t}$	customer demand of final product j at distribution site d at time period t
H	number of operational planning periods that can be fit within one tactical planning period
N^S	number of STP time periods
N^P	length of prediction horizon for integrated planning model
ΔT_m	discretization time of MTP model
ΔT_s	discretization time of STP model
TW	length of shutdown event
σ_{ps}	processing time of production scheme ps
β^P_{ps}	yield of production scheme ps
$\gamma^u_{r,ps}$	maximum batch size for production scheme ps at processing unit r

$\gamma^l_{r,ps}$	minimum batch size for production scheme ps at processing unit r
$\delta^F_{m,d}$	shipment delay between plant site m and distribution site d
$\delta^P_{m,m'}$	shipment delay between plant site m and m'
$\delta^R_{ls,m}$	delivery delay of procured material between supplier ls and plant site m
η_{ps}	relative production capacity coefficient for production scheme ps
κ	ratio between weighting parameters (ω_1/ω_2)
$\lambda^F_{m,d}$	maximum transportation capacity from plant site m to distribution site d during a time period
$\lambda^P_{m,m'}$	maximum transportation capacity from plant site m to m' during a time period
$\lambda^R_{ls,m}$	maximum quantity of raw material which can be ordered from supplier j during a time period
$\mu_{j,ps}$	mass balance coefficient of material j in production scheme ps
ν_{r,t_m}	production capacity factor at time period t_m
ρ_s	probability of the occurrence of scenario s
$\tau_{ps,ps'}$	production change-over time from scheme ps to ps'
ω_1	weighting parameter assigned to customer service ($\mathcal{J}_1$)
ω_2	weighting parameter assigned to operating cost ($\mathcal{J}_2$)
Γ^u_r	aggregated production capacity of production unit r
Ω^R_m	maximum storage capacity of raw material in plant site m
$\Omega^S_{j,d}$	maximum storage capacity of final product j in distribution site d

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CHAPTER 6

Conclusions and Recommendations

In this chapter, we summarize the main contributions of the research work and discuss recommendations for the future work.

6.1 CONCLUSIONS

A supply chain system comprises a number of activities, and for a better and efficient management, it is generally decomposed in a hierarchical way. Within a hierarchical decision-making framework, the long-term strategic layer comes at the top where the design of supply chain network is finalized. After deciding the network structure, medium term planning activities are scheduled based on the demand forecast. At the bottom, the actual plant level operational decisions, such as production amount and sequencing are decided. In this research, we first developed a strategic design approach. Then in the second phase, we worked on a bottom operational decision level of a hierarchical control framework. In the last phase of our research, we devised an approach to combine midterm (tactical) and short-time (operational) planning. In the research work, we used various techniques such as mixed-integer model formulation, stochastic modeling, variants of the model predictive control (MPC) framework, and hybrid time scale modeling.

In the initial phase of research, discussed in Chapter 3, we considered the design of supply chains in the presence of demand uncertainty, with a particular focus on capturing the effects of time-limited transportation contracts in which specified minimum durations of transportation linkages must be adhered to. The network design plays a vital role in defining the optimum operation of a supply chain by dictating the optimum production and transportation capacity of the network. An optimization based design formulation was proposed, with flexibility in allowable node connections and direction of material flow. In the optimization formulation, the network superstructure was represented by a mathematical model with the use of two sets of constraints: network structure constraints, and operational planning constraints. All node connections were represented using binary variable definitions, which provided the flexibility to include the node connection by setting the value to one for the corresponding linkage. The time limited transportation contracts were modeled without introducing any new binary variables, which helped to minimize the computation burden in solving the MILP optimization problem. Demand uncertainty was handled using a two-stage stochastic programming approach in which the uncertain parameter space was discretized, with the design problem formulated as an MILP. The advantage of the proposed *flexible* and *time-varying* network approach was illustrated via an industrially based case study and the economic impact of taking time-limited contractual constraints into account in the supply chain design, where these exist, was demonstrated.

Next, in Chapter 4, we proposed an operational decision-making tool for a hybrid process supply chain using a model predictive control (MPC) technique. Model predictive control is an efficient control mechanism used in systems engineering to control chemical processes. We used it to control a process supply chain in the presence of demand uncertainty. In this work, we modeled the supply chain operational processes using a hybrid process model where decisions governed by logical conditions/rulesets were accommodated using binary variables. The uncertainty in demand and process yield were captured using a scenario-based approach and handled using a robust MPC strategy formed by combining stochastic programming with nominal MPC. Three variants of an uncertainty propagation mechanism were presented, an open-loop approach, an approximate closed-loop strategy, and a multi-stage closed-loop strategy. Multiple supply chain performance metrics, customer service, and economics, were included within an integrated optimization framework. The customer service (satisfaction level) and operating cost (economics) play against each other; a *Pareto* optimality curve was generated to guide the selection of the best optimum operating condition. The performance of the robust MPC framework was analyzed through its application to a multi-product, multi-echelon process supply chain case study. The proposed approach was shown to provide a substantial reduction in the occurrence of back orders when compared to a nominal MPC implementation.

Finally, we proposed a medium-term planning framework integrated with an operational planning model. Due to the use of different time scale models at each layer, challenges of coordination and infeasibility arise, which ultimately affects the supply chain efficiency. In this research, tactical and operational planning activities of a multiproduct, multi-stage, multi-echelon production and distribution network were described using an integrated hybrid time modeling approach in which first few planning periods were formulated using an operational planning model and the remaining time periods were modeled with a tactical planning model. The key features of this strategy were, (1) representation of two different time-scale planning activities in a single integrated model; (2) a general optimization framework for an integrated planning approach that simultaneously considered supply chain nodes such as suppliers, production network, transportation and storage network, and customers; and (3) a model predictive control (MPC) based rolling horizon formulation to update the optimal decisions to mitigate the effects of system disturbances. A comparison analysis was performed to check the accuracy of the integrated model and demonstrated that the proposed approach yields comparable performance with lower computational resources. Further, we extended the modeling framework to include planned maintenance and used it to optimize system economics in the case of plant maintenance. The formulation was again expanded to optimally decide the start time of the planned maintenance over a given time-frame.

6.2 RECOMMENDATIONS FOR FURTHER WORK

In this section, we identified several broad topics of future work.

- Decomposition strategy to speed up the computation
  For the supply chain design approach, including demand uncertainty is essential to obtain a robust design, however, the time to solve the resulting two-stage stochastic problem is very high. As the two-stage stochastic problem has a distinct mathematical structure, a decomposition strategy such as Bender's decomposition can be employed to decompose and speed up the computation. After separating a master problem containing only first stage decisions from the subproblems having only second-stage variables, it can be solved separately in an iterative fashion till convergence. The second-stage variables across scenarios are independent and hence parallel computation can be employed to reduce the computation time tremendously.

- Contract dependent pricing
  We included time-limited transportation contracts in the design formulation. An extension to this work would be incorporation of an optional transportation route

with no contract limitation but with a high shipping cost. However, a restriction can be imposed to connect two nodes with only one transportation route at any time period and implement switching fees from a time-limited contract option to a no-contract option to reflect the cost of managing the material shipment routes. The optimizer will then decide the optimal way to transport the materials across the network.

- **Time-limited transportation links in long-term planning**
  The supply chain design problem developed in Chapter 3, makes design decisions along with long-term planning decisions. Once the network structure is finalized, the model can be used to make and update strategic decisions. In the strategic planning problem, the decisions pertaining to design will be fixed, and the remaining decisions can be classified into the first stage and second stage decisions. The first stage decisions will correspond to the first time period decisions and the rest are second stage decisions. Thus, the problem decides one set of the transportation linkages for the first time period, and they would be same for all scenarios as those decisions have to be implemented. If the optimizer decides to set up the link in the first time period, then it will remain in service for minimum lock-in period irrespective of scenario. However, the linkages for second time period onwards can be selected based on the demand scenarios and can be different across scenarios. Similarly, production and transportation amounts will also be different for a different scenario. As time progresses, the problem will be solved to update these decisions.

- **Scenario reduction using a particle filtering approach**
  A large number of demand scenarios is required to characterize demand uncertainty. However, the problem size increases rapidly with the increase in scenario number, which exponentially increases computation load. Monte-Carlo sampling has been shown to be an effective method for reducing the number of scenarios required to characterize the demand uncertainty (Mastragostino, 2012). However, that also results in a relatively high number of discrete realizations when the number of uncertain parameters increases. A *particle filter* is a sequential Monte Carlo method based on point mass (or "particle") representations of probability densities. It is a generic framework of the sequential importance sampling (SIS) algorithm and works on the principle of survival of the fittest. Because of the presence of this dynamic sampling, the estimate of the true probability density function approaches the optimal Bayesian estimate. Future work could use a particle filtering technique to reduce the number of scenarios within multi-stage stochastic programming (Kostanjcar, Jeren, and Cerovec, 2009).

- **Including uncertainty in the integrated planning framework**
  Accurate prediction of demand is not possible. Moreover, processing yield changes due to different operating conditions, and thus there is uncertainty regarding production capacity too. Future plan is to include demand and system uncertainties in the integrated planning framework. Naturally, including uncertainty will increase the computation load and therefore alternative strategies to solve a stochastic MPC problem should be investigated.

- **Inclusion of continuous-time model within integrated planning framework**
  In the proposed integrated planning approach, it is assumed that the cleaning time is multiple of the discretization time of the operational model. In a scenario where the cleaning time is less than the sampling time, it results in underestimation of available production time. One alternative is to use separate time index for production sequencing or use of continuous time modeling approach. Further, there are other instances where continuous-time representation is more convenient, such as having processing time of production schemes that varies over wide time range. Questions regarding how to fuse these different time representation models into one have to be answered.

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