Towards Integrated Supply Chain Management for the Enterprise Sustainability

Thesis extended abstract

J. M. Laínez-Aguirre

1 Introduction

The chemical industry is a sector making a significant contribution to the European Union (EU) economy. The EU has the second largest chemical industry in the world accounting in 2010 for 21%, worth 494 billion €, of the total global chemical sales. In addition, the chemical industry is a key supplier of practically every sector of the European economy. Indeed, it is considered that one job in the chemical industry creates two jobs outside of it[1]. Owing to this, it is claimed that the competitiveness of all other sectors is partially dependent on the efficient supply of chemical products. Nevertheless, the EU chemical industry has lost during the last years its traditional first place in the world ranking in favor of Asia. This has caused its customer base to erode as chemicals large users relocate their production to lower labor cost countries. To remain competitive and persist as a vital sector in the economy, the European Chemical Industry Council and the European Petrochemical Association have recognized that enterprises producing chemicals must continue improving their operations and reducing their costs. As the scope for further reductions related to equipment technology is limited provided the size and age of European plants, opportunities for performance improvement should come from an enhanced Supply Chain Management[2] (SCM). From another standpoint, the Process System Engineering (PSE) community also recognizes that an optimum management of the Supply Chain (SC) offers a key opportunity for preserving and improving firm's value[3].

SCM can be defined as the management of material, information and financial flows through a set of organizations that aim at producing and delivering goods or services to consumers[4]. The main objectives are to achieve the desired consumer satisfaction levels and the maximum financial returns by synchronizing the SC members activities. Recently, Enterprise Wide Modeling and Optimization has emerged as a new promising research field[5;6]. One of its key features is the integration of information and decision-making among the various functions that comprise the SC and across different hierarchical decision levels.

Currently, chemical enterprises are supported not only by production operations but also by product R&D as well as by strategic functions such as financial planning and marketing as shown in Fig. 1. With the aim of maximizing growth and creation of firms value, companies need these functional components to be well coordinated by an integrated model. This fact can enhance the enterprise capabilities of adapting and responding to uncertainties arising from internal processes as well as the external environment. Decisions within organizations ought to be carried out quantitatively understanding the trade-offs among the risks and benefits that imply the different available options. Despite the fact of being necessary and the research efforts devoted so far to this end, there are challenges to overcome so as to provide such a quantitative support for integrated decision-making, which will allow optimizing the overall enterprise resources (e.g., materials, cash, personnel) utilization. In the light of the foregoing, the main objective of this thesis is therefore to contribute to the development of *integrated* mathematical models for *centralized* SCs considering the specific characteristics of chemical related sectors.

The main body of this thesis has been divided in four parts. This extended abstract is organized accordingly. §2 deals with business functionalities integration in order to bring a systemic view of strategic SCM; while §3 focuses on strategic and tactical issues purely related to process operations. Integration of hierarchical decision levels and uncertainty are addressed in §4. Finally, §5 summarizes the thesis contributions.

2 Strategic Functional Integration

Typically, the business strategy is modeled as a *sequential* and hierarchical process in which functional strategies, such as operations, logistics, marketing, and finances are driven by a higher level strategy[7]. A key element of the strategic framework involves coordinating functional level plans to work in concert so as to achieve the overall business strategy rather than to locally optimize outcomes for individual functions, business units, plants, or stores. Undoubtedly, business functional decisions must be integrated and coordinated in order to tackle the critical decision of resources allocation among the different business activities. While this concept is clearly sound on a conceptual level, actual implementation is typically very difficult[8]. This part describes mathematical models to support functional integration.

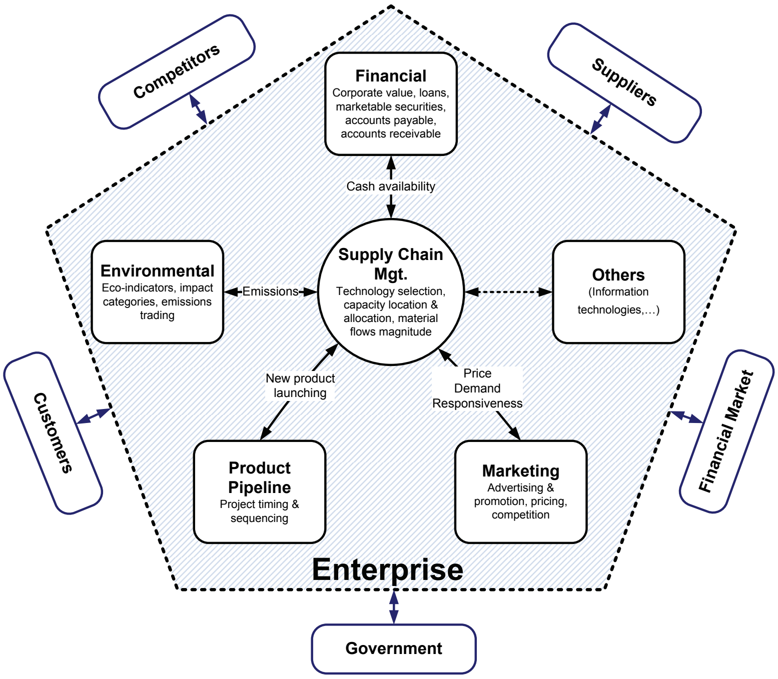


Figure 1: Schematic representation of an integrated SC model

2.1 Enhancing Corporate Value in the Design of Supply Chains

The need to extend the studies and analysis of process operations to incorporate financial considerations has been widely recognized in the literature[3;9–12]. Traditionally, approaches available in the PSE literature to address the design and operation of SCs usually focus on the process operations side and neglect the financial part of the problem. A large proportion of these approaches minimize costs, profit or NPV[13–18]. This is not sufficient to help a business to create and sustain a competitive advantage. To this end, the objective should be sustainable value creation[19]. Metrics which are able to quantify the shareholder's value are worth to explore. Notwithstanding, relatively few integrated corporate financial models have been implemented so far[20–22]. Indeed, the treatment of financial factors is restricted to primary operating and *fixed* capital assets and, typically, some form of NPV with interest rate fixed over the time horizon is used as performance indicator. However, in the planning formulation, they usually ignore the Net Working Capital (NWC), which represents the *variable* capital assets. NWC is constituted by material inventories, accounts receivable (physical distribution), accounts payable (procurement), and cash. All of these components are directly affected by decisions directly associated with tactical SC operations which in turn are subject to the constraints imposed by the SC structure. NWC can be understood as the capital tied up within the cash conversion cycle, which measures how efficiently an enterprise converts its inputs into cash through final product sales. The less capital tied up by SC operations, the better the performance in terms of the business's bottom line. The NWC is not a static figure; it may change from period to period throughout the planning horizon in accordance with SC decisions.

This thesis proposes an MILP formulation that links variables and constraints belonging to two business areas, namely finances and process operations. The Corporate Value (CV) of the firm is adopted as the objective to be maximized as an alternative to the traditional metrics. The CV is computed following a valuation method — the Discounted Free Cash Flows (DFCF) — well entrenched in finance theory[23] which takes into account the NWC in its evaluation. The main advantages of this approach are highlighted through a case study in which the integrated strategy is compared with the traditional approach that computes the maximum-profit or NPV. The comparison is carried out using a multiobjective optimization (ϵ-constraint method). Certainly, an improvement in profit or NPV is only possible if the decision-maker is willing to compromise the firm's CV. In a first case study, the maximum CV solution is almost 300% higher than the one computed by maximizing profit and 267% higher than the one accomplished when maximizing NPV. It is worth to mention that this case study represents a specific situation where there is one market in which the product prices are slightly higher in comparison with the others (1.87%). At such a market, accounts receivable are due within a larger time period. Under this assumption, the design-planning model that accounts for the maximization of a traditional KPI (i.e., either profit or NPV) decides to configure a SC network capable of easily fulfilling the demand of such a market as much as possible. The profit and the NPV are indeed blind KPIs in the sense that they are not capable of properly assessing the financial cost associated with NWC. To further demonstrate the advantages of using the CV and its robustness to assess strategic decisions under different scenarios, the previous case study has been modified and solved. Two modifications have been done: (i) the prices paid by all markets are the same, and (ii) similar due times of account receivables are offered for all markets. Even for this second case, it can be observed that the maximum CV solution is 62% better than the one computed by maximizing profit and 32% superior than the one accomplished when maximizing NPV. Therefore, numerical results show that significant benefits can be obtained if an integrated formulation accounting for the optimization of a suitable financial performance indicator, the CV, is applied. This is a result of the CV capability of properly assessing (i) the expenses associated with the shortages of cash and (ii) the value penalty associated with increments in NWC. Moreover, the integrated solution guarantees the feasibility of the strategic decisions from a financial point of view by ensuring liquidity control. A journal article[24] resulted from the work described in this section.

2.2 Synchronizing Supply Chain and Product Development Decisions

Two enterprise-wide decision problems that have received the most intense attention have been SCM and Product Development Pipeline Management (PDPM). The latter addresses the set of decisions and network of tasks associated with turning a new discovery into a product and introducing it into the corporation's SC[6]. Both of these problems are resource intensive, involve large cash flows and thus their successful solution has a direct bearing on the viability of the enterprise. Both are large scale in terms of the number of decision variables that must be considered, involve activities at multiple time scales, are dynamic in nature, and are subject to a large number of exogenous and endogenous uncertainties. In both, capacity planning decisions are important, that is, whether to produce a new product for launch in an existing facility (and in which one) or whether to plan for new capacity. Moreover, the two of them are interdependent in that typically the cash flow from effective SCM provides all or a significant portion of the investment funding required for PDPM, while SCM relies on a steady flow of new products from PDPM to drive SC growth or at least to sustain the enterprise in the face of competitor's product innovations. They, at root, constitute large-scale, multistage stochastic optimization problems. Given their importance to the viability of the enterprise, the quality of solutions to these decision problems must be measured in terms of enterprise-wide metrics such as corporate value preservation and growth.

One of the industries for which R&D pipeline management is particularly significant is pharmaceuticals. One of the defining aspects of PDPM in this industry is that product candidates are likely to fail during development. When this occurs, not only is the investment in the development of the failed product lost, but the company incurs the opportunity cost of not having developed one of the alternate potential product candidates in its portfolio. Indeed, studies have shown that the US industry average is only one commercial success per seven new product concepts in which development is invested. As a result, as much as 50% of new product development resources are spent on failed products[25]. Planning of new product development activities has been an active research topic in last decades[26–31]. Most of these approaches incorporate as objective function NPV and they do not account for financial issues nor do they incorporate capacity expansion decisions in a SC context. In this thesis, an integrated model is developed which incorporates simultaneous treatment of SC design–planning and PDPM decisions in the pharmaceutical industry. Moreover, this model embeds the financial formulation described in §2.1 enabling the quantitative assessment of the firms' value. The model also considers the endogenous discrete uncertainty associated with clinical trials outcomes during the development process. To tackle this problem, a scenario based multi-stage stochastic MILP formulation is proposed. This model includes financial risk constraints[32] which allow finding optimal solutions within accepted risk levels. The relationship among non-anticipativity constraints is exploited in order to apply a Lagrangean decomposition technique, the Optimal Condition Decomposition[33] (OCD), so as to reduce the computational burden required for solving the integrated model. This allows handling industrial problems of medium scale.

Numerical results of an illustrative example show that the solution calculated by the Integrated Approach (IA) offers improved performance over the Sequential Approach (SA). Under the SA, the SC and product development decisions are firstly made by optimizing the NPV and then the financial decisions are determined by maximizing the CV metric described in §2.1. The IA renders an expected CV of 14.3×10^9 monetary units (m.u.); while a CV of 2.8×10^9 m.u. is obtained by applying the SA. The two approaches also yield different project selection decisions. It is important to point out that the SA selects the projects based on the NPV. For this reason, the SA obtains the highest NPV in the most probable scenario by developing three products, however this requires significant amounts of NWC which leads to a poor CV result for such a scenario. Indeed, the expected CV is low compared to the integrated approach due to this fact. SC capacity allocation decisions are different as well. Furthermore, a significant risk reduction is achieved by using the IA, the probability of obtaining negative CVs is reduced from 59% to 1.5%. Moreover, risk management constraints have been applied to the IA assuming that no negative CVs are desired. For this case, no equipment capacity expansion is proposed. It is worth noticing that the expected CV has decreased to 13.1×10^9 m.u. by using the risk constraints. Nevertheless, there is a reduction in the risk associated to those CVs which are lower than 10.0×10^9 m.u. by up to 10%. With regard to the computational burden, a case study comprising 64 scenarios is solved by using the monolithic model in 24370 CPU seconds, while 1026 CPU seconds are needed by using the OCD scheme (i.e., a 95% reduction in CPU time). Therefore, performance comparison with the traditional sequential decision approach demonstrates the significant economic benefits of the proposed integrated model and that a Lagrangean decomposition can successfully reduce the computational burden for this sort of problems. A journal article[34] and two articles in proceedings of international meetings[35;36] were published as results of the work described in this section.

2.3 Linking Marketing and Supply Chain Models

To be successful, the enterprise model has to contemplate not only the SC, but also the demand chain. Understanding the market and customer behavior is crucial for developing a good business policy. Marketing is a boundary-spanning activity, linking selling entities with buyers and intermediate channels. To operate most effectively, marketing activities must be coordinated with other functional areas of the firm. Business managers should evaluate the existing trade-off between marketing and SC planning decisions in order to enhance the performance of the overall business metric: the shareholders value. Although authors have highlighted the conflicting goals of SC and marketing managers[10;37], it is still typically assumed that under a decentralized decision-making scheme, marketing decisions are made first; determining demand forecasts which are later considered by the SC model to support production-distribution related decisions. By deploying this sequential procedure, the firm may be significantly hampering its overall performance. On the one hand, the primary objective of marketing function is maximizing revenues creation by satisfying customers through the products and services offered. On the other, SCM's objective is typically considered as the minimization of the total SC cost as discussed in §2.1. In general, conflicts arise between marketing and SC because of these contrasting performance indicators which eventually are used to develop incentive structures for managers and their corresponding employees.

The marketing – SC management interface is an issue that deserves further research. A very early work that addresses the coordination of inventory replenishment strategies and pricing policies is presented by Whitin[38] in the 50's. However, very few recent models dealing with this problem can be found in the literature[39–41], most of them are focused on pricing policies. In this thesis, a novel MINLP model considering simultaneously SC design/retrofitting, financial and marketing decisions is presented. For the marketing side, BRANDAID[42], a flexible strategic marketing mix model, is used. This model is basically comprised of three sub-models, namely: advertising sub-model, pricing sub-model and sales force sub-model. The integrated model optimizes the SC and marketing strategic decisions and allows to quantitatively assess the shareholder's value by means of the CV metric (§2.1). A case study is presented to carry out a performance comparison with the traditional SA. Numerical results show that the solution calculated by the IA offers a 47% improvement over the SA solution. The IA obtains such a performance by a 2% decrease in net revenues. The two approaches propose different SC capacity decisions. In order to achieve a greater revenue, the SA induces higher sales for the most expensive product by increasing advertising expenditures. However, it does not consider that the capacity requirements for this product are higher than the rest of the portfolio. These decisions lead to a lower CV. Otherwise, the IA simultaneously assesses the advertising expenditures, the revenue obtained from the products to be sold, and the capacity requirements to carry out their production. The aim is to emphasize the relevance of a correct appraisal of the trade-off existing between the demand which is induced by marketing activities and the SC capacity investments required to meet such a demand. The integrated model evaluates such a trade-off and finds a balanced solution which maximizes the CV. Synchronizing such decisions has an important impact in the firm's value as it is demonstrated in the case study. The model described in this section resulted in an article[43] published in an international journal.

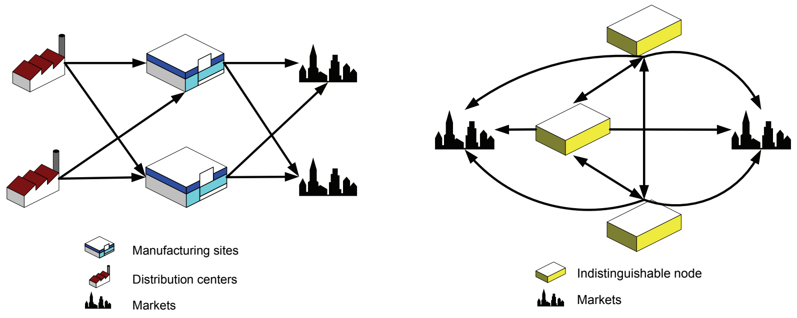
3 Strategic and Tactical Issues in Process Operations

This part focuses on strategic and tactical issues purely related to operations. A novel flexible formulation approach is proposed to solve the challenging design–planning problem of SC networks. By extending the previous model, the SC design is also addressed considering economical and environmental issues.

3.1 Flexible Design–Planning of Supply Chain Networks

Clearly, a SC network is comprised by lateral links, reverse loops, two way exchanges and so forth, encompassing the upstream and downstream activity[44]. Notwithstanding, common characteristics of most existing SC design–planning approaches[13;15;28;45–55] are that among SC components exclusively vertical flows that have only one direction are considered and/or a predefined superstructure which restricts how potential SC members may interchange materials is utilized as departing point as shown in Fig. 2(a). Vertical flows are understood as those material flows between SC components that belong to consecutive echelons type (e.g., flows that go from wholesalers to retailers, from production plants to wholesalers). Models that do not contemplate a superstructure a priori are needed so that the whole set of possible connections is explored (see Fig. 2(b)). Accordingly, new alternatives to enhance value creation may appear. In addition, it still remains the issue of what an appropriate description of production processes at the SC level is. SC design used to be confined to final products and their relation to the production or supply of intermediates is usually disregarded[56]. The inclusion of this aspect may have a strong impact in the design of SCs.

This thesis proposes mathematical model for the flexible design–planning of SC's. Its distinctive features are that (i) considers all feasible links and material (raw material, intermediate and final products) flows among the potential SC components inherently, (ii) does not need any pre-established process network superstructure so that the sub-trains (if any) in which production process is decoupled and their location are determined by the optimization. In order to do so, the problem is formulated as an MILP which translates the State-Task-Network[57]



(a) Traditional framework (b) Flexible framework

Figure 2: Approaches for SC Design

(STN) representation to the SC context. The tasks (i.e., production or distribution activities) are used as the core of the formulation rather than products as occurs in traditional models. This allows treating indistinctively (i) locations related to a processing plant, a distribution center or both of them, as well as (ii) raw materials, intermediates or final products. Here, one of the three case studies used to emphasize the potential of the proposed model is discussed. This is an adapted version of the polystyrene case study introduced by You and Grossmann[53] which concerns a polystyrene SC design. The flexible approach solution leads to an NPV improvement of 74.6% over the traditional approach which considers the published superstructure[53]. The flexible solution establishes a distribution center that transfers final products to customers but it also receives raw materials from suppliers to be sent to other production site. Raw materials are usually not considered to be handled by distribution centers, however improvements can be achieved by doing so. Moreover, production plants are directly shipping final products to some markets and technologies are allocated to sites which have not been considered in the given superstructure. The flexible approach proposes to install some equipment technologies in spite of being more costly than other available options, since the trade-off between the required higher investment and the transportation cost in non-traditional connections results in an overall NPV increase. The case study demonstrates that the features of the proposed model provide opportunities to select value-efficient allocations of production-distribution activities which may lead to more advantageous SC designs. Furthermore, a more appropriate description of manufacturing processes at the SC level has been achieved by translating a recipe representation to the SC environment which may eventually facilitate the consideration of scheduling decisions while designing a SC as will be shown in §4. The work previously described was published as a journal article[58].

3.2 Mapping Environmental Impacts

Corporate approaches to improve environmental performance cannot be undertaken in isolation, so a concerted effort along the SC entities is needed which poses another important challenge to managers. Actually, managerial practice related to environmental issues has expanded from a narrow focus on pollution control within a single firm to include a larger set of inter-organizational management decisions, tools, and technologies that prevent pollution before its generation[59]. The PSE community has developed several methodologies for the characterization of the environmental impacts of chemicals, products, and processes[60–62]. All these methodologies are based on the incorporation of an optimization step to a Life Cycle Assessment (LCA) study which focuses on process conditions of a single SC echelon. Because an LCA ideally covers a cradle-to-grave approach, it can be clearly seen that an LCA fits as a suitable tool for assessing the environmental burdens associated with designing and operating a SC. Mele et al.[63;64] and Hugo and Pistikopoulos[18] show LCA based quantitative tools for supporting the SC design.

From another standpoint, as the planet warms up, so does legislation to reduce greenhouse gas (GHG) emissions worldwide. With estimated economic damage of about US$85 for each ton of CO_2, capping GHG emissions and establishing a price tag on them became inevitable[65]. Indeed, such a setup is already in effect in some countries and for certain industries under the EU Emissions Trading Scheme. Certainly, this scheme will force a change in the way organizations run their SCs[66]. One of the key aspects to have a successful policy is the definition of the free emissions allowance cap for each industry type. It is noteworthy that these policies are applied based on the temporal distribution of emissions. This is disregarded in the models developed since they just evaluate the environmental impacts at the end of the planning horizon. Consequently, the incorporation of constraints associated with the temporal distribution of emissions is needed when studying climate change policies in a SC.

This thesis proposes an approach which represents a comprehensive step over previous works[18;63;64] by modeling CO_2 trading schemes and the temporal distribution of emissions. The design–planning approach presented in §3.1 is utilized. This model is suitable to collect all SC nodes information through a single variable set, which eases the environmental formulation. The environmental metric IMPACT 2002+[67] is used, which presents an implementation which categorizes the environmental interventions in four damage levels (human health, ecosystem quality, climate change-global warming potential, resources). The resulting model is solved by using a multiobjective optimization which allows observing possible environmental trade-offs between damage categories and the economic indicator. A case study concerning different technologies for the production of Maleic Anhydride (MA) SC is used to illustrate the advantages of the proposed approach. Numerical results show that the maximum NPV SC configuration is based on benzene feedstock, whereas the minimization of the environmental impact indicator results in a butane based SC. Raw material production is the most important factor contributing to the overall environmental impact in both cases. It is important to point out that the benzene based SC would have been selected if a SC approach is not followed and the supplier impacts are disregarded. This extended SC scope is expected to better aid effective environmental strategies since firms have an important influence over the environmental footprint through their "purchase" decisions. In addition, it is noteworthy that the optimal SC configuration considering the emissions trading scheme corresponds to the benzene based SC independently of the value for the free emissions cap and the emission right price. Under the trading scheme, the minimum *overall* impact configuration (butane based) will be a favorable alternative by no means since it is the one which most emits CO_2. The benzene based SC shows a greater overall impact, being human health its most impacting damage category due to benzene's carcinogenicity. However, a CO_2 trading emission scheme would favor benzene based production, thus leading to a change from butane based — the most environmental friendly option — to benzene based MA production. The results obtained for this specific case study question the suitability of applying a CO_2 trading scheme to every industry sector: different regulatory schemes may be required in different industrial scenarios. Current regulations merely consider climate change damage which certainly is a very important factor; however, other aspects such as human health, ecosystem quality and abiotic resources usage should be also considered so that effective industry changes with regard to the environment are induced. As a direct result of this work, an article was published[68].

4 Decision Levels Integration and Treatment of Uncertainty

For competitive customer service to be maintained, SC managers need to consider the dynamics of a rapidly changing market environment as well as the dynamics of internal SC operations. External uncertainties include those related to the cost of raw materials and products (unless they are subject to monopoly conditions), fluctuations in the exchange rate, and uncertainties in market size and demand due to competition and macroeconomic factors. Examples of internal uncertainties include the success rate of R&D projects, given the technological risks involved, and disruptions to production, such as production failures and unforeseen stoppages. These operational SC risks and disruptions can have severe long-term effects on the firm's financial performance. An empirical analysis of the effect of SC disruptions on stock prices shows that companies experience 33% to 40% lower stock returns and 13.5% higher share price volatility as a result of this sort of problems[69].

Evidently, market uncertainty and internal business operations make it difficult to synchronize the activities of all SC echelons; this causes significant deviations from previous objectives and plans. Therefore, for a SC to be managed efficiently it is important to systematically review variability and to take it explicitly into account in decision making processes. These actions ensure a robust response to changes in the business environment, increase the accuracy of decisions and improve business performance. For these reasons, research is called for into the characterization of dynamics in SCs and the application of control methodologies to improve the SCs responsiveness[3]. In the literature, a Model Predictive Control (MPC) framework has been used for the review process[70–74]. MPC incorporates the most recent information on the market and internal business into the planning process. Such a framework is commonly based on deterministic predictive models. However, predictions based on these models may be sub-optimal or even infeasible when the real scenario unfolds. Other well-known approach that is presented as a robust manner of making decisions under uncertainty is using stochastic optimization[75–78]. Particularly, some studies have developed approaches that focus on limiting a phenomenon known as the "bullwhip effect", which is the increase in fluctuation of demand upstream in the SC[71;74]. However, incorporating low-level decisions (local scheduling, supervisory control and diagnosis, incident handling) and the implications of incorporating these decisions for the dynamics of the entire SC (production switching between plants, dynamic product portfolios) have not yet been fully studied.

In addition, one of the key components of enterprise wide modeling and optimization is decision-making coordination and integration at all levels as was stated in §1. Most of the recent contributions offer models that separately address problems arising in the three, standard SC hierarchical decision levels[13;28;55;79–81] (i.e., strategic, tactical aggregate planning and short-term scheduling). As indicated by Grossmann[3], this is a major pending research problem that requires more attention. The SC planning problem is similar to the production scheduling problem in that both usually seek answers to the questions of in what amount, when and where to produce each of the products comprising the business portfolio so as to obtain financial returns. Nevertheless, planning brings into play a broader, aggregated view of the problem. The time periods used in planning problems are usually longer than task processing times; thus, the sequencing/timing decisions in scheduling are transformed into rough capacity decisions in the tactical planning. Indeed, equipment capacity modeling is the core aspect that must be taken into account in order to assure consistency and feasibility when problems are being integrated across different SC hierarchical decision levels. Moreover, the strategic decisions of determining the optimal SC network structure play a vital role in the alternatives available for the later optimization of SC operations.

In this section, uncertainty and process dynamics are incorporated into enterprise-wide models and hierarchical

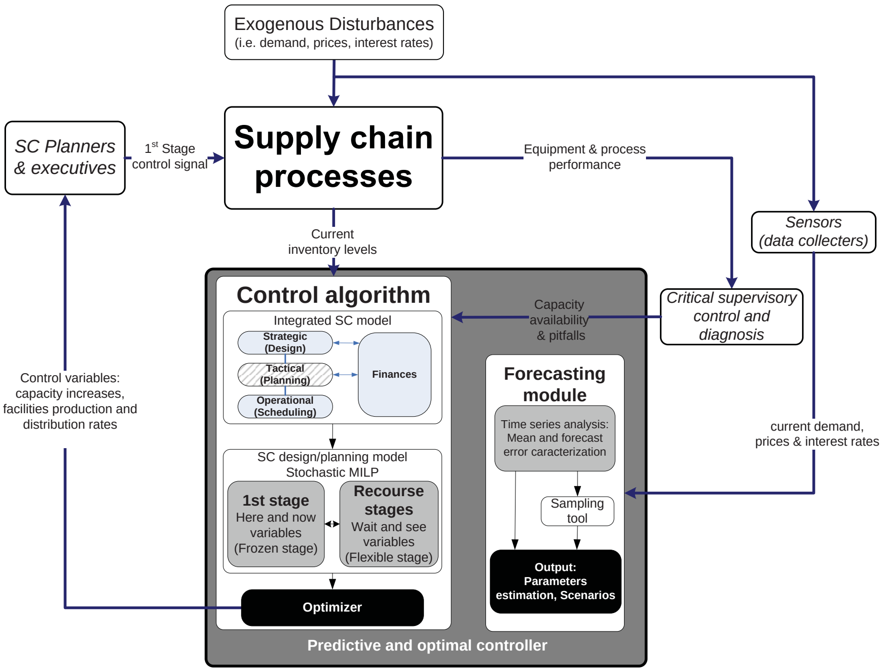


Figure 3: Proposed MPC strategy

decision levels are also integrated. An MPC methodology is proposed which employs a scenario based multistage stochastic MILP as predictive model as shown in Figure 3. Demand uncertainties are taken into account. A operations and a financial formulation is included in the mathematical model. The average CV is adopted again as the objective function and calculated by means of a DFCF method. Here, it is important to point out that a disadvantage attributed to DFCF methods is that they do not account for the managerial flexibility needed to alter the course of an investment over time as uncertain factors unfold. Certainly, deterministic DFCF methods assume a single decision pathway with average outcomes. Real options analysis has been proposed as an alternative to overcome this drawback. This analysis considers multiple decision pathways by adjusting mid-course strategies to deal with the uncertainty[82]. Likewise, stochastic optimization assumes that some actions are taken in a *first stage* after which a random event occurs and then *recourse decisions* can be made in response to the unveiled scenario. However, a stochastic DFCF model, as the one proposed in this section, offers more realistic solutions because it considers the so-called *non-anticipativity* constraints; whereas, real options typically lead to "wait-and-see" solutions by assuming complete knowledge of information during the decision-making process.

In order to integrate different decision levels, the SC design-planning model presented in §3.1, which translates a recipe representation to the SC context, is coupled with a STN scheduling formulation. This approach enables to assess the impact of considering scheduling aspects of process operations in the capacity decisions included in the design of a SC network. Additionally, the scheduling details enable the dynamics of the SC to be better tracked. The challenge of solving large multi-scale optimization problems becomes evident when decision level integration is considered. Therefore, an OCD decomposition technique is applied to reduce the computational burden associated with the model solution. The validation of the proposed approach and the resulting potential benefits are highlighted by using the polystyrene SC case study presented in §3.1. An horizon of 48 monthly periods is considered. The results are compared with the traditional SA which does not considers the scheduling when dealing with the design of the SC network. The scheduling model is taken into consideration in the first month for the IA. To approximate the multistage stochastic problem solution, the two stage shrinking horizon method presented in the work of Balasubramanian and Grossmann[83] is used. In addition the performance of the SC designs proposed by the SA and IA are evaluated by simulating demand scenarios for the 48 planning periods and using the MPC framework which is equivalent to following a rolling horizon scheme.

Numerical results show that the SC configuration proposed by the IA outperforms by 15.5% in terms of average CV the one proposed by the SA when they are tested using the production scheduling simulation. For the SA, the capacity aggregation considered at the design level results in higher nominal plant productivity since idle times introduced by task sequencing and changeovers are disregarded. However, significant deviations, around -22.9%, in predicted production levels are found when the SA proposed network design is deployed into simulated scenarios. The IA avoids this situation by incorporating the scheduling formulation into the design problem. Indeed, deviations from predicted production levels for the IA are around 1.5% when the IA network design is deployed into simulated scenarios. The case study also emphasizes how to deal with equipment failure using the proposed MPC framework and a supervisory control module. It should be highlighted that the planning model utilized in this control strategy is able to consider movement of raw materials, intermediates and final products among the different facilities comprising the SC network. Such flexibility increases the number of alternatives available to resolve the incidences since production and its corresponding input materials can be transfered accordingly from one site to another. Such flexibility is not usually considered in traditional SC planning models. Furthermore, the capacity of other sites have been contemplated in order to resolve the incidences considered in the case study. It is demonstrated that by using the proposed MPC framework SC transparency is gained, the decision making process to resolve the incidents is performed at the SC level and not merely at the plant level, thus allowing to select the best "re-planning" option in terms of value creation. It is important to point out that the proposed control strategy allows to handle uncertainty and incidences by combining reactive and preventive approaches. A pro-active treatment of uncertainty is included by means of stochastic programming. The review and update process that is required to tackle incidences and changes in random factors is performed by introducing the SC stochastic holistic model into an MPC framework. The novel control framework constitutes a step-forward in closing the loop for the dynamic SC management and a supporting platform for the supervisory module handling the incidences that may arise in the SC. The previous work resulted in the publication of two journal articles[84;85].

Finally, due to the discrete decisions involved (e.g., equipment assignment, task allocation over time) scheduling problems are inherently combinatorial in nature, and hence very challenging from the computational complexity point of view[86]. Therefore, a modest growth in problem size can lead to a significant increase in the computational requirements[87]. Furthermore, stochastic programs become deterministic equivalent programs with the utilization of a scenario tree. The size of the deterministic scheduling formulation can easily grow out of hand for a large number of scenarios, which renders the direct solution approaches numerically intractable and thus necessitates special methods, such as decomposition and aggregation[88]. Hence, it turns out that one of the major challenges in the area of scheduling under uncertainty is to reduce the computational cost required to solve this kind of problems (NP complete problems which are complicated by the consideration of uncertainty). It is noteworthy that solution procedures based on knowledge of the specific problem have been recognized to exhibit a good potential in providing advances in this direction[89]. Here, a new approach for solving scheduling problems under exogenous uncertainty has been developed. The approach is based on the S-graph[90] framework which has proven to be a rigorous and efficient tool for solving deterministic scheduling problems. The proposed framework does not only inherit the advantages of S-graph, but it also has an advantage against stochastic programming techniques; namely, the computational effort needed to solve the problem does not increase by increasing the number of scenarios. Such convenience relies on the fact that the search space size is independent on the number of considered scenarios. As the number of scenarios increases a larger LP that is used as a performance evaluator is to be solved but still due to its nature the computational times for its solution are significant small. Therefore, the presented framework has a great potential to solve industrial scale problems of scheduling under uncertainty. Note that this approach for scheduling under uncertainty can be integrated with the control strategy previously proposed. This work has been published as a journal article[91].

5 Concluding Remarks

The advantages and contributions of the integrated solution approaches proposed in this thesis have been highlighted along this document. This thesis is a further step in an attempt to tackle research challenges related to the integrated SCM such as a novel and better representation of production-distribution processes at the SC level, functionally integrated approaches, considerations of uncertainty, and decomposition strategies. In §2 mathematical models to approach the enterprise business functionalities integration problem are presented. Firstly, the design and retrofit of SCs taking into account financial concerns is addressed. The proposed MILP model pursues the maximization of a suitable financial key performance indicator, the CV of the firm. The CV is computed by a DFCF method which incorporates the NWC into the evaluation. The NWC constitutes a dynamic capital that is usually neglected in traditional approaches. This model is extended to incorporate for the first time new product pipeline management and also to deal with the endogenous nature of specific (clinical trials) uncertainties during the development process. To tackle this problem, a scenario based multi-stage stochastic MILP formulation is proposed. Moreover, the model is able to account for financial risk restrictions that may be imposed by stockholders. A specific type of Lagrangian decomposition technique (OCD) has been adapted to successfully achieve substantial reduction in the computational burden associated with the solution of this kind of problems. Another novel extension of the model developed in §2.1 is presented to interface SC operations and marketing functions. An MINLP model that integrates a marketing engineering contribution, the BRANDAID model, is presented. The relevance of a correct appraisal of the trade-off existing between the demand, which can be induced by marketing expenditure and pricing decisions, and the SC capacity investments required to meet such a demand is pointed out.

The strategic problem of designing a SC network is addressed in §3 by translating the recipe concept to the whole SC environment. Instead of a rigid predefined network structure, the proposed approach utilizes a new SC design and planning model that permits material flows of any kind between any kind of facilities. It is noteworthy that a main feature of the proposed model is that it does not require any pre-established process network superstructure thus allowing to optimally define the sub-trains in which production process is decoupled and their respective locations. As a result, processing facilities outputs may be intermediate materials. This is one key feature in modeling the complex global SCs behavior. It is demonstrated that great potential to improve firm's economic performance can be gained by exploring the whole range of available alternatives when designing a SC. This model enables to do this exploration in a straightforward manner. This model is extended to consider the optimization of SC planning and design accounting economical and environmental issues. An LCA approach has been selected in order to incorporate the environmental aspects to the model. The implications of emissions trading schemes are evaluated.

§4 deals with managing uncertainty and integrating hierarchical decision levels. A stochastic version of the model developed in §3.1 is integrated with an STN scheduling formulation and included in an MPC strategy. Capacity has been utilized as the linking aspect when integrating SC design, planning and scheduling. The control strategy presented allows handling uncertainty and incidences by combining reactive and preventive approaches. It is illustrated that better transparency and broader visibility of SC is obtained when resolving incidences with the proposed MPC framework. Lastly, a new approach based on the S-graph is presented to handle batch scheduling under exogenous uncertainty. This approach has the advantage of reducing the computational cost as the formulation size does not increase with the number of considered scenarios.

The work carried out in this thesis resulted in eight articles which have been published in international journals[24;34;43;58;68;84;85;91].

Literature Cited

[1] CEFIC, "Facts and figures: The European chemical industry in a worldwide perspective," Conseil Européen des Fédérations de l'Industrie Chimique, Tech. Rep., 2010.

[2] A. McKinnon, "Supply chain excellence in the European chemical industry," CEFIC and The European Petrochemical Association, Tech. Rep., 2004.

[3] I. Grossmann, "Challenges in the new millennium: product discovery and design, enterprise and supply chain optimization, global life cycle assessment," *Computers & Chemical Engineering*, vol. 29, pp. 29–39, 2004.

[4] C. S. Tang, "Perspectives in supply chain risk management," *International Journal of Production Economics*, vol. 103, pp. 451–488, 2006.

[5] I. Grossmann, "Enterprise-wide optimization: A new frontier in process systems engineering," *AIChE Journal*, vol. 51, pp. 1846–1857, 2005.

[6] V. Varma, G. Reklaitis, G. Blau, and J. Pekny, "Enterprise-wide modeling & optimization - an overview of emerging research challenges and opportunities," *Computers & Chemical Engineering*, vol. 31, pp. 692–711, 2007.

[7] C. Fine and A. Hax, "Manufacturing strategy: A methodology and an illustration," *Interfaces*, vol. 15, pp. 28–46, 1985.

[8] C. Bozarth and W. Berry, "Measuring the congruence between market requirements and manufacturing: A methodology and illustration," *Decision Sciences*, vol. 28, pp. 121–150, 1997.

[9] G. Applequist, J. Pekny, and G. Reklaitis, "Risk and uncertainty in managing chemical manufacturing supply chains." *Computers & Chemical Engineering*, vol. 24, pp. 2211–2222, 2000.

[10] J. Shapiro, *Modeling the Supply Chain.* Duxbury, 2006.

[11] ——, "Challenges of strategic supply chain planning and modeling," *Computers & Chemical Engineering*, vol. 28, pp. 855–861, 2004.

[12] N. Shah, "Process industry supply chains: Advances and challenges," *Computers & Chemical Engineering*, vol. 29, pp. 1225–1235, 2005.

[13] J. Bok, I. Grossmann, and S. Park, "Supply chain optimization in continuous flexible process networks," *Industrial & Engineering Chemistry Research*, vol. 39, pp. 1279–1290, 2000.

[14] J. Gjerdrum, N. Shah, and L. Papageorgiou, "Transfer prices for multienterprise supply chain optimization," *Industrial & Engineering Chemistry Research*, vol. 40, pp. 1650–1660, 2001.

[15] J. Kallrath, "Combined strategic and operational planning: An MILP success story in chemical industry," *OR Spectrum*, vol. 24, pp. 315–341, 2002.

[16] G. Berning, M. Brandenburg, K. Gürsoy, J. Kussi, V. Mehta, and F.-J. Tölle, "Integrating collaborative planning and supply chain optimization for the chemical process industry," *OR Spectrum*, vol. 24, pp. 371–401, 2002.

[17] C. Chen and W. Lee, "Multi-objective optimization of multi-echelon supply chain networks with uncertain demands and prices," *Computers & Chemical Engineering*, vol. 28, pp. 1131–1144, 2004.

[18] A. Hugo and E. Pistikopoulos, "Environmentally conscious long-range planning and design of supply chain networks," *Journal of Cleaner Production*, vol. 13, pp. 1471–1491, 2005.

[19] W. Klibi, A. Martel, and A. Guitouni, "The design of robust value-creating supply chain networks: A critical review," *European Journal of Operational Research*, 2009, doi:10.1016/j.ejor.2009.06.011.

[20] G. Yi and G. Reklaitis, "Optimal design of batch-storage network with recycle streams," *AIChE Journal*, vol. 49, pp. 3084–3094, 2003.

[21] ——, "Optimal design of batch-storage network with financial transactions and cash flows," *AIChE Journal*, vol. 50, pp. 2849–2865, 2004.

[22] G. Guillén-Gosálbez, M. Badell, A. Espuña, and L. Puigjaner, "Simultaneous optimization of process operations and financial decisions to enhane the integrated planning/scheduling of chemical supply chains," *Computers & Chemical Engineering*, vol. 30, pp. 421–436, 2006.

[23] J. Grant, *Foundations of Economic Value Added.* John Wiley and Sons, 2003.

[24] J. M. Laínez, G. Guillén-Gosálbez, M. Badell, A. Espuña, and L. Puigjaner, "Enhancing corporate value in the optimal design of chemical supply chains," *Industrial & Engineering Chemistry Research*, vol. 46, pp. 7739–7757, 2007.

[25] M. Hynes-III, "Addressing escalating drug development cost through improved resource management: a pharmaceutical product resear and development case study," in *Proceedings Foundations of Computer-Aided Process Operations (FOCAPO 2008)*, M. Ierapetritou, M. Bassett, and S. Pistikopoulos, Eds., CACHE-AIChE-Informs. CACHE Corp, 2008, pp. 103–107.

[26] C. Schmidt and I. Grossmann, "Optimization models for the scheduling of testing tasks in new product development," *Industrial & Engineering Chemistry Research*, vol. 35, pp. 3498–3510, 1996.

[27] C. Maravelias and I. Grossmann, "Simultaneous planning for new product development and batch manufacturing facilities," *Industrial & Engineering Chemistry Research*, vol. 40, pp. 6147–6164, 2001.

[28] L. Papageorgiou, G. Rotstein, and N. Shah, "Strategic supply chain optimization for the pharmaceutical industries," *Industrial Chemistry Engineering Research*, vol. 40, pp. 275–286, 2001.

[29] A. Levis and L. Papageorgiou, "A hierarchical solution approach for multi-site capacity planning under uncertainty in the pharmaceutical industry," *Computers & Chemical Engineering*, vol. 28, pp. 707–725, 2004.

[30] D. Subramanian, J. Pekny, and G. Reklaitis, "A simulation-optimization framework for research and development pipeline management," *AIChE Journal*, vol. 47, pp. 2226–2242, 2001.

[31] M. Colvin and C. Maravelias, "A stochastic programming approach for clinical trial planning in new drug development," *Computers & Chemical Engineering*, vol. 32, pp. 2626–2642, 2008.

[32] A. Barbaro and M. Bagajewicz, "Managing financial risk in planning under uncertainty," *AIChE Journal*, vol. 50, pp. 963–989, 2004.

[33] A. Conejo, F. Nogales, and F. Prieto, "A decomposition procedure based on approximate newton directions mathematical programming," *Mathematical Programming, Series A*, vol. 93, pp. 495–515, 2002.

[34] J. M. Laínez, L. Puigjaner, and G. Reklaitis, "Financial and financial engineering considerations in supply chain and product development pipeline management," *Computers & Chemical Engineering*, vol. 33, no. 12, pp. 1999 – 2011, 2009.

[35] J. M. Laínez, G. V. Reklaitis, and L. Puigjaner, "Enhancing value in supply chains by integrating capacity allocation decisions and r&d pipeline management," in *Foundations of Computer-Aided Process Operations (FOCAPO)*, M. Ierapetritou, M. Bassett, and S. Pistikopoulos, Eds. Austin, TX: CACHE, 2008, pp. 489 – 492.

[36] ——, "Managing financial risk in the coordination of supply chain and product development decisions," in *European Symposium on Computer Aided Process Engineering*, J. Jeżowski and J. Thullie, Eds. Amsterdam: Elsevier, 2009, pp. 1027 – 1032.

[37] J. Eliashberg and R. Steinberg, *Marketing-Production Joint Decision Making*, ser. Handbooks in Operations Research and Management Science. Amsterdam: Elsevier Science Publishers, 1997, vol. 5, ch. 18.

[38] T. Whitin, "Inventory control and price theory," *Management Science*, vol. 2, pp. 61–80, 1955.

[39] X. Chen and D. Simchi-Levi, "Coordinating inventory control and pricing strategies with random demand and fixed ordering cost: The finite horizon case," Massachusetts Institute of Technology, Tech. Rep., 2002.

[40] G. Guillén-Gosálbez, M. Bagajewicz, S. E. Sequeira, A. Espuña, and L. Puigjaner, "Management of pricing policies and financial risk as a key element for short term scheduling optimization," *Industrial & Engineering Chemistry Research*, vol. 44, pp. 557–575, 2005.

[41] G. Guillén-Gosálbez, C. Pina, A. Espuña, and L. Puigjaner, "Optimal offer proposal policy in an integrated supply chain management environment," *Industrial & Engineering Chemistry Research*, vol. 44, pp. 7405–7419, 2005.

[42] J. Little, "BRANDAID: A marketing-mix model, Part 1: Structure," *Operations Research*, vol. 23, pp. 628–655, 1975.

[43] J. M. Laínez, G. V. Reklaitis, and L. Puigjaner, "Linking marketing and supply chain models for improved business strategic decision support," *Computers & Chemical Engineering*, vol. 34, no. 12, pp. 2107 – 2117, 2010.

[44] R. Lamming, "Japanese supply chain relationships in recession," *Long Range Planning*, vol. 33, pp. 757–778, 2000.

[45] M. Balinski, "Integer programming: methods, uses, computation," *Management Science*, vol. 12, pp. 254–313, 1965.

[46] G. Brown, G. Graves, and M. Honczarenko, "Design and operation of a multicommodity production/distribution system using primal goal decomposition," *Management Science*, vol. 33, pp. 1469–1480, 1987.

[47] A. Cakravastia, I. Toha, and N. Nakamura, "A two-stage model for the design of supply chain networks," *International Journal of Production Economics*, vol. 80, pp. 231–248, 2002.

[48] J. Ryu and E. Pistikopoulos, "Design and operation of an enterprise-wide process network using operation policies. 1. Design," *Industrial & Engineering Chemistry Research*, vol. 44, pp. 2174–2182, 2005.

[49] F. Mele, G. Guillén-Gosálbez, A. Espuña, and L. Puigjaner, "An agent-based approach for supply chain retrofitting under uncertainty," *Computers & Chemical Engineering*, vol. 31, pp. 722–735, 2007.

[50] J. Ferrio and J. Wassick, "Chemical supply chain network optimization," *Computers & Chemical Engineering*, vol. 32, pp. 2481–2504, 2008.

[51] M. Bansal, I. Karimi, and R. Srinivasan, "Selection of third-party service contracts for chemical logistics," *Industrial & Engineering Chemistry Research*, vol. 47, pp. 8301–8316, 2008.

[52] R. Sousa, N. Shah, and L. Papageorgiou, "Supply chain design and multilevel planning - an industrial case," *Computers & Chemical Engineering*, vol. 32, pp. 2643–2663, 2008.

[53] F. You and I. Grossmann, "Design of responsive supply chains under demand uncertainty," *Computers & Chemical Engineering*, vol. 32, pp. 3090–3111, 2008.

[54] K. Al-Qahtani and A. Elkamel, "Multisite refinery and petrochemical network design: Optimal integration and coordination," *Industrial & Engineering Chemistry Research*, vol. 48, pp. 814–826, 2009.

[55] L. Fan, Y. Kim, C. Yun, B. Park, S. Park, B. Bertok, and F. Friedler, "Design of optimal and near-optimal enterprise-wide networks for multiple products in the process industry," *Industrial & Engineering Chemistry Research*, vol. 48, pp. 2003–2008, 2009.

[56] M. Melo, S. Nickel, and F. Saldanha, "Facility location and supply chain management – a review," *European Journal of Operational Research*, vol. 196, pp. 401–412, 2009.

[57] E. Kondili, C. Pantelides, and R. Sargent, "A general algorithm for short term scheduling of batch operations," *Computers & Chemical Engineering*, vol. 17, pp. 211–227, 1993.

[58] J. M. Laínez, G. Kopanos, A. Espuña, and L. Puigjaner, "Flexible design–planning of supply chain networks," *AIChE Journal*, vol. 55, pp. 1736–1753, 2009.

[59] R. Klassen and P. Johnson, *Understanding Supply Chains: Concepts, Critiques & Futures*. Oxford: Oxford University Press, 2004, ch. The Green Supply Chain, pp. 229–251.

[60] S. Stefanis, A. Livingston, and E. Pistikopoulos, "Minimizing the environmental impact of process plants: A process systems methodology," *Computers and Chemical Engineering*, vol. 19, pp. S39–S44, 1995.

[61] A. Azapagic, "Life cycle assessment and its application to process selection, design and optimisation," *Chemical Engineering Journal*, vol. 73, pp. 1–21, 1999.

[62] A. Azapagic and R. Clift, "The application of life cycle assessment to process optimisation," *Computers and Chemical Engineering*, vol. 23, pp. 1509–1526, 1999.

[63] F. Mele, A. Espuña, and L. Puigjaner, "Environmental impact considerations into supply chain management based on life-cycle assessment," in *Innovation by Life Cycle Management LCM 2005 International Conference*, 2005.

[64] F. Mele, M. Hernández, and J. Bandoni, "Optimal strategic planning of the bioethanol industry supply chain with environmental considerations," in *Proceedings Foundations of Computer-Aided Process Operations (FOCAPO 2008)*, M. Ierapetritou, M. Bassett, and S. Pistikopoulos, Eds., CACHE-AIChE-Informs. CACHE Corp, 2008, pp. 517–520.

[65] N. Stern, "Stern review on the economics of climate change," *HM Treasury, London, UK*, p. http://www.sternreview.org.uk/, 2006.

[66] K. Butner, D. Geuder, and J. Hittner, "Mastering carbon management: Balancing trade-offs to optimize supply chain efficiencies," *IBM Institute for Business Value*, vol. GBE03011-USEN-00, 2008.

[67] S. Humbert, M. Margni, and O. Jolliet, "Impact 2002+: User guide draft for version 2.1," Industrial Ecology & Life Cycle Systems Group, GECOS, Swiss Federal Institute of Technology Lausanne (EPFL), Lausanne, Switzerland, Tech. Rep., October 2005.

[68] A. D. Bojarski, J. M. Laínez, A. Espuña, and L. Puigjaner, "Incorporating environmental impacts and regulations in a holistic supply chains modeling: An LCA approach," *Computers & Chemical Engineering*, vol. 33, no. 10, pp. 1747 – 1759, 2009.

[69] K. Hendricks and V. Singhal, "An empirical analysis of the effect of the effect of supply chain disruptions on long-run stock price performance and equity risk of the firm," *Production and Operations Management*, vol. 14, pp. 35–52, 2005.

[70] S. Bose and J. Pekny, "A model predictive framework for planning and scheduling problems: a case study of consumer goods supply chain," *Computers & Chemical Engineering*, vol. 24, pp. 329–335, 2000.

[71] E. Perea-López, B. Ydstie, and I. Grossmann, "A model predictive control strategy for supply chain optimisation," *Computers & Chemical Engineering*, vol. 27, pp. 1201–1218, 2003.

[72] E. Perea-López, I. Grossmann, B. Ydstie, and T. Tahmassebi, "Dynamic modeling and decentralized control of supply chains," *Industrial & Engineering Chemistry Research*, vol. 40, pp. 3369–3383, 2001.

[73] P. Seferlis and N. Giannelos, "A two-layered optimisation-based control strategy for multi-echelon supply chain networks," *Computers & Chemical Engineering*, vol. 28, pp. 799–809, 2004.

[74] E. Mestan, M. Türkay, and Y. Arkun, "Optimization of operations in supply chain systems using hybrid systems approach and model predictive control," *Industrial & Engineering Chemistry Research*, vol. 45, pp. 6493–6503, 2006.

[75] M. Ierapetritou and E. Pistikopoulos, "Batch plant design and operations under uncertainty," *Industrial & Engineering Chemistry Research*, vol. 35, pp. 772–787, 1996.

[76] A. Gupta and C. Maranas, "A two-stage modelling and solution framework for multisite midterm planning under demand uncertainty," *Industrial & Engineering Chemistry Research*, vol. 39, pp. 3799–3813, 2000.

[77] P. Tsiakis, N. Shah, and C. Pantelides, "Design of multi-echelon supply chain networks under demand uncertainty," *Industrial & Engineering Chemistry Research*, vol. 40, pp. 3585–3604, 2001.

[78] A. Bonfill, A. Espuña, and L. Puigjaner, "Addressing robustness in scheduling batch processes with uncertain operation times," *Industrial & Engineering Chemistry Research*, vol. 44, pp. 1524–1534, 2005.

[79] J. Jackson and I. Grossmann, "Temporal decomposition scheme for nonlinear multisite production planning and distribution models," *Industrial and Engineering Chemistry Research,*, vol. 42, pp. 3045–3055, 2003.

[80] S. Jetlund and I. Karimi, "Improving the logistics of multi-compartment chemical tankers," *Computers & Chemical Engineering*, vol. 28, pp. 1267–1283, 2004.

[81] A. Bonfill, A. Espuña, and L. Puigjaner, "Decision support framework for coordinated production and transport scheduling in SCM," *Computers & Chemical Engineering*, vol. 32, pp. 1206–1224, 2008.

[82] J. Mun, *Real options analysis: tools and techniques for valuing strategic investments and decisions*, 2nd ed., ser. Wiley finance series. New York: John Wiley & Sons, 2005.

[83] J. Balasubramanian and I. Grossmann, "Approximation to multistage stochastic optimization in multiperiod batch plant scheduling under demand uncertainty," *Industrial & Engineering Chemistry Research*, vol. 43, pp. 3695–3713, 2004.

[84] L. Puigjaner and J. M. Laínez, "Capturing dynamics in integrated supply chain management," *Computers & Chemical Engineering*, vol. 32, no. 11, pp. 2582 – 2605, 2008.

[85] L. Puigjaner, J. M. Laínez, and C. R. Alvarez, "Tracking the dynamics of the supply chain for enhanced production sustainability," *Industrial & Engineering Chemistry Research*, vol. 48, no. 21, pp. 9556–9570, 2009.

[86] J. Pekny and G. Reklaitis, "Towards the convergence of theory and practice: A technology guide for scheduling/planning methodology," in *Third International Conference on Foundations of Computer-Aided Process Operations*, J. Pekny and G. Blau, Eds., 1998, pp. 91–111.

[87] X. Lin and C. Floudas, "Continuous-time versus discrete-time approaches for scheduling of chemical processes: a review," *Computers and Chemical Engineering*, vol. 28, pp. 2109–2129, 2004.

[88] L. Cheng, E. Subrahmanian, and A. Westerberg, "Design and planning under uncertainty: Issues on problem formulations and solutions," *Computers & Chemical Engineering*, vol. 27, pp. 781–801, 2003.

[89] Z. Li and M. Ierapetritou, "Process scheduling under uncertainty using multiparametric programming," *AIChE Journal*, vol. 53, pp. 3183–3203, 2007.

[90] E. Sanmartí, L. Puigjaner, T. Holczinger, and F. Friedler, "Combinatorial framework for effective scheduling of multipurpose batch plants," *AIChE Journal*, vol. 48, pp. 2557–2570, 2002.

[91] J. M. Laínez, M. Hegyháti, F. Friedler, and L. Puigjaner, "Using S-graph to address uncertainty in batch plants," *Clean Technologies and Environmental Policy*, vol. 12, pp. 105–115, 2010.