

Perspectives in Multilevel Decision-making in the Process Industry

Braulio Brunaud¹ and Ignacio E. Grossmann ^{*1}

¹Carnegie Mellon University
Pittsburgh, PA 15213

June 28, 2017

Abstract

Decisions in supply chains are hierarchically organized. Strategic decisions involve long-term planning of the structure of the supply chain network. Tactical decisions are mid-term plans to allocate production and distribution of materials. Operational decisions correspond to the daily planning of the execution of manufacturing operations. These planning processes are conducted independently with little exchange of information between them. Achieving a better coordination allows to capture benefits that are currently out of reach, and improving communications between different functional areas in a company. We propose a network representation for the multilevel decision structure, and analyze the components involved in finding integrated solutions. An integrated solution is one that maximizes the sum of the benefits of all nodes of the decision network. The task is very challenging. However, significant progress has been made in each of its components. An overview of strategic models, mid-term planning models, and scheduling models, is presented to address the solution of each node in the decision network. Coordination mechanisms to converge to the integrated solutions are also analyzed, including solving large-scale models, multiobjective optimization, bilevel programming, and decomposition. We conclude by summarizing the challenges identified to achieve the full integration of multilevel decision-making in supply chain management.

1 Introduction

Supply chains of the 21st Century are highly globalized. Nowadays, having a product that was manufactured ten thousand kilometers away delivered in two weeks seems very natural. With the information revolution we have become used to receiving orders almost instantaneously. This has put a tremendous

*corresponding author: grossmann@cmu.edu

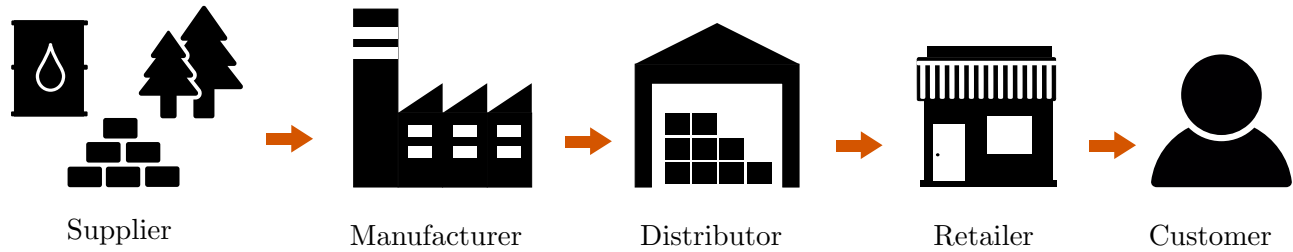


Figure 1. Supply chain example

pressure on supply chains. They are now very complex, and are required to be very responsive. In this scenario, making effective decisions in a timely manner is nearly impossible without a good decision support system (DSS).

The process industry is a good example of this complexity. A typical chemical company has suppliers distributed in different geographical locations, dozens of manufacturing sites, and customers all over the world. Decision-making in the process industry must consider material flows throughout the supply chain together with decisions of the manufacturing process, including batch sizing and timing, defining production rates, parameter setting and control. Process Systems Engineering (PSE) addresses the challenge of optimizing industrial processes with all its complexity (Sargent, 2005). The challenges of integrating the R&D, manufacturing and distribution functions has been recognized in the area of Enterprise-wide Optimization (EWO)(Grossmann, 2005). Several authors have contributed to identify the main challenges and opportunities in EWO. Shah (2005) presents a thorough description of the challenges in the process industry supply chain. He identifies the lack of integration of design and operational decisions as one of the main limitations. More focused on the modeling aspects, Papageorgiou (2009) reviews relevant existing literature until 2008.

A supply chain can be defined as a sequence of steps involved in the manufacturing and distribution of a product. This definition gives an idea of an horizontal process from the raw materials to the finished goods (see Fig. 1). This representation can be helpful to understand the materials flow. However, the information flow is not fully captured by this representation. Information, mainly decisions, flow from the strategic level to the operational level, passing through the tactical level. In order to make optimal decisions, feedback also needs to flow in the opposite direction.

All decision levels are interconnected. For example, decisions on facility location at the strategic level impact the capacity for the tactical plan, and the tactical plan defines inventory targets for the scheduling

of operations. Therefore, a truly optimal solution is one that yields the best possible value for the objective function (whether is maximizing or minimizing) considering the impacts on all the decision levels. Even though information availability inside enterprises has improved by the adoption of enterprise resource planning systems (ERP), planning processes are still executed independently from each other, with little communication between decision levels. Achieving the coordination of all these decision-making processes is very challenging. However, significant progress has been made in the components of the problem. In this paper, we present an overview of the elements involved in solving the problem. The goal is to set the stage to accomplish the integrated optimization of all decision levels across a supply chain.

Decisions in supply chains are hierarchically organized. In general, they can be divided into three levels: strategic, tactical, and operational. The distinction between each level is not absolute, and varies from company to company. The strategic level corresponds to long-term planning decisions that affect the structure of the supply chain network. The tactical level involves mid-term decisions related to the allocation and distribution of materials between manufacturing and storage units (warehouses and distribution centers). Finally, at the operational level, planning of the execution of manufacturing operations is performed. Since the planning horizons for each level are different, the timescales employed when modeling each decision level are also different. Fig. 2 displays general characteristics of the hierarchy of decision levels. Below the operational level there is a control layer. Integration between operational decisions and control is also a matter of research. However, decisions beyond the operational level will not be covered in this paper. For additional details in this area, the reader is referred to the recent reviews by Baldea and Harjunkski (2014) and Dias and Ierapetritou (2016).

As pointed out by Barbosa-Póvoa (2012), the integration of design and planning decisions is fairly well established. However, the integration of planning and scheduling is still an open problem. Maravelias and Sung (2009) recently devoted a review paper specifically to this topic. Garcia and You (2015) identify the challenges when dealing with multilevel systems: modeling, optimization, uncertainty handling, and efficient algorithms design. While, there has been remarkable advance in the different elements required to handle multilevel systems, the integration of all these elements has yet to be addressed. Fig. 3 presents a matrix of the different models identified, classified by decision level and stage of the supply chain.

The current practice is to execute each planning process independently. Achieving the integration allows companies to be more agile in reacting to the dynamic conditions of the process environment, and capturing additional benefits. For example, the timing in which strategic decisions are made is usually

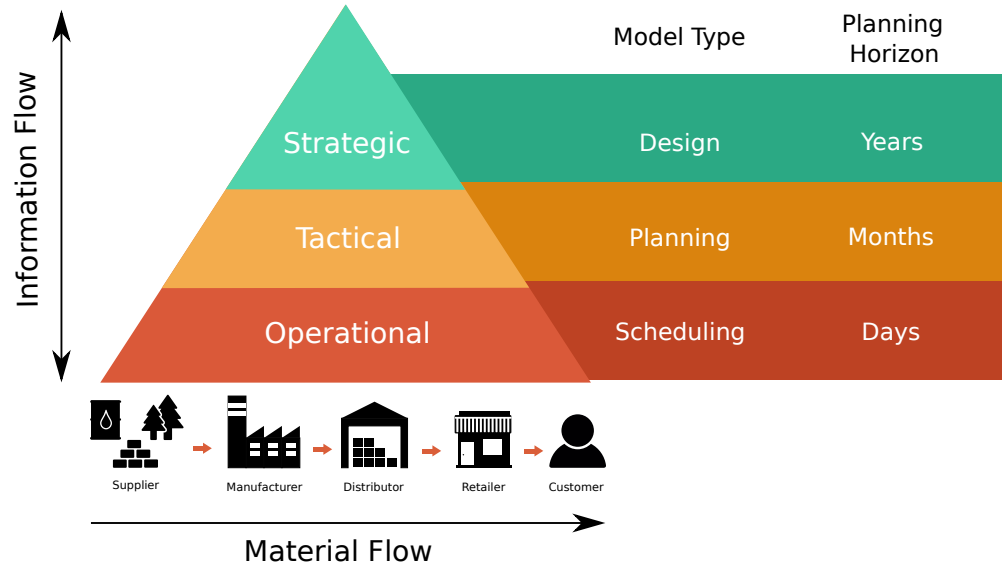


Figure 2. Supply chain decision pyramid

fixed to once a year, and the decisions are treated as static during all that period. Having integrated models enables to identify opportunities in which the strategic planning should be pulled forward to adapt to changing conditions, and thus, advance towards online optimization and supply chain control (Perea-Lopez et al., 2001).

The decision hierarchy also impacts the organizational structure of a company. Managers make decisions that impact the actions their subordinates make. Since the majority of the conflicts in an enterprise are related to communication, achieving a better integration of decision-making processes has the additional benefit of improving the work environment by enhancing the coordination between different functional areas. These benefits are hard to measure, but they are certainly present.

This paper presents an overview of all the elements involved in multilevel optimization through selected examples from the literature, and tries to identify open challenges to achieve the overall integration. Section 2 proposes a network representation for the problem. In sections 3, 4, and 5, models for design, planning and scheduling, respectively, are analyzed in detail. Section 6 explores ways to achieve the coordination between different decision levels. Finally, section 7 summarizes the challenges identified to achieve the multilevel integration goal.

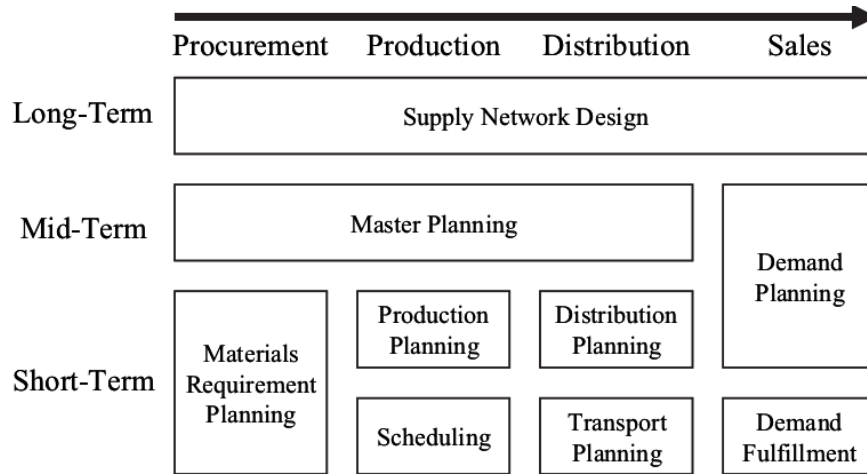


Figure 3. Planning matrix (Meyr et al., 2015)

2 Modeling Structure Network

Supply chains are systems with multiple components that interact exchanging information. Thus, a network representation is ideal to represent the structure and interactions between each of the decision-making components. In this section we propose a standard structure and outline the elements that need to be considered to optimize the whole supply chain. The network representation also motivated [Jalving et al. \(2016\)](#), the developers of PLASMO, a computational package for the Julia programming language ([Bezanzon et al., 2012](#)) to represent networks of models with the JuMP mathematical programming platform ([Dunning et al., 2015](#)).

The structure proposed is presented in Fig. 4. Each node represents the problem that each decision-maker, at a defined level, needs to solve. Each solid-line arc represents the influence of top level decisions in the subnodes. The relationship at an arc can be defined as either passing the value of a variable, or a constraint involving variables of the origin and destination nodes. If the network is solved by simply optimizing each node from the root-node to the leaves, not even feasible solutions are guaranteed. Feedback (dashed-line arcs) is required to converge to the optimal solution. More details on the coordination between nodes are discussed in Section 6.

To further clarify these definitions, consider the following example. In a chemical company, the global planner from a family of specialty chemicals, allocates production for each of the products in his or her portfolio to each production area (Fig. 5). When doing the allocation, the global planner considers transfers between different production areas. Then, the planner for each production area must decide

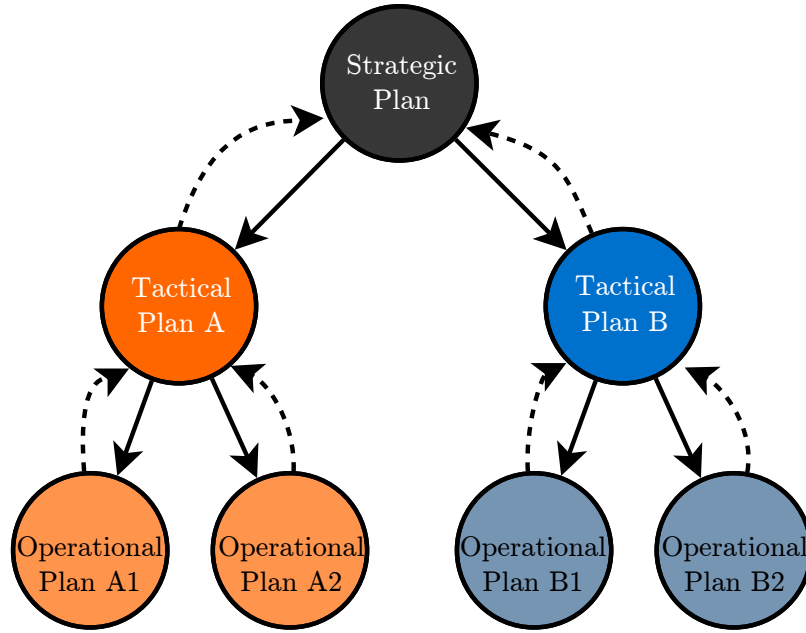


Figure 4. Supply chain decision network structure

how to split the global planner requirement between the different manufacturing plants in the production area. Finally, in each plant a scheduler will perform the short-term planning to execute the manufacturing operations in order to meet the required targets. Without feedback and iteration, it is unlikely that the optimal solution for the network can be obtained. We will refer to the optimal solution of the network (x^*), or integrated solution, to the vector of variables that maximizes the benefit across the whole network.

$$x^* = \arg \max_{x \in X} \sum_{n \in N} z_n \quad (1)$$

where z_n represents the objective function of each node n .

This definition of integrated solution is different to what is found in the literature. Usually only two decision levels are considered, and not even in their full detail. A common approach is to include a relaxation or aggregation of the subproblem as constraints of the top level problem (Maravelias and Sung, 2009). This is done to improve the quality of the solution obtained for the top level. However, the value of the lower decision variables obtained is not meant to be implemented (Fig. 6). Some authors also call

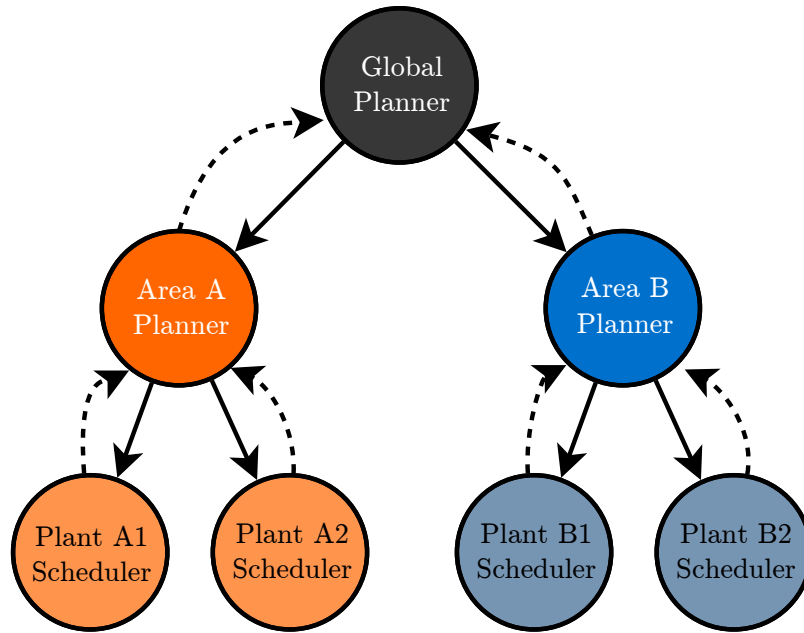


Figure 5. Supply chain decision network structure example

this an integrated solution.

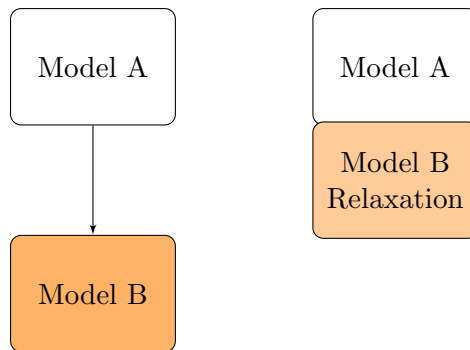


Figure 6. Concept of integrated solution as defined in the literature

Considering the structure proposed in Fig. 4, an optimal solution for the network can be obtained by answering two questions:

1. What is the right model and solution method for each node?
2. How to coordinate the decisions made between nodes?

For the first question, plenty of progress has been made by the development of models for different ap-

plications and decision levels (Bixby et al., 2004). Solution strategies based on mixed-integer programming (Linderoth and Savelsbergh, 1999), constraint programming (Hooker, 2002), metaheuristics (Blum and Roli, 2003), and others, have been proposed. Handling uncertainty is also key in obtaining implementable solutions (Birge and Louveaux, 2011). Sections 3, 4, and 5 are devoted to analyzing details related to this question. The second question has been mainly addressed through decomposition algorithms. This is explored in Section 6.

3 Modeling of Strategic Decisions

Strategic decisions define long-term plans affecting all areas of a company. They represent commitments that span for years, such as the execution of capital projects and contracts. The impact of these decisions is so high that failing to make good decisions can lead to the demise of the company. The associated difficulty is that in order to make these critical decisions, forecasts of several years in the future must be considered. And, as one considers points in time that are more distant to the present, forecasts become more uncertain.

In general, there are three kinds of decisions at the strategic level:

1. Product portfolio selection
2. Contracts
3. Facility installation, expansion, and reduction

In the first kind, a company decides which of its products to maintain in its portfolio based on the projected profitability of serving the forecasted demand. The research in these problems has been focused on improving forecasting methods (de Weck et al., 2003), and also in the handling of new products entering the pipeline (Jain and Grossmann, 1999). The demand depends on the phase of the life cycle in which a product is found (Fig. 7).

From the modeling standpoint, the optimal portfolio can be obtained by allowing the model to not meet the total demand (Eq. 2). However, it is important to consider cases in which demands of products are coupled. For example, a company may be supplying an unprofitable product to a customer to keep serving that same customer with other more valuable products (Rastogi et al., 2011).

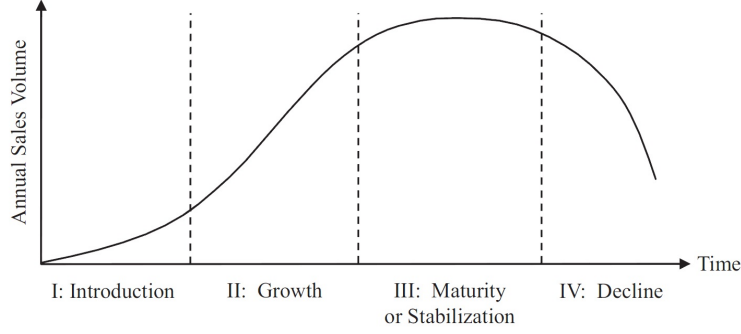


Figure 7. Product life cycle curve

$$\sum_{j \in J_k} x_{jkpt} \leq Demand_{kpt} \quad \forall k \in K, p \in P, t \in T \quad (2)$$

In Eq. (2), K is the set of customers, P is the set of products, T is the set of time periods, and J_k is the set of facilities serving customer k . x_{jkpt} is the flow of material of product p , between facility j delivered to customer k . Uncertainty is present in the demand forecast for both new and mature products.

Contracts are also important strategic decisions. They dictate prices and restrictions on amounts related to supply, sales, and transportation. Modeling of supply and sales contracts has been addressed by Park et al. (2006). They consider the following types of contracts:

Fixed price contracts The purchase price is fixed, independent on the amount purchased

Discount after a certain amount The first σ_1 units are sold to a price ϕ_1 . The units in excess of σ_1 are sold to a price ϕ_2

Bulk discount When the amount ordered surpasses σ_1 , the price for the entire order decreases to ϕ_2

Fixed duration contracts In fixed duration contracts, a minimum purchase and a contract duration is defined. The longer the contract, the larger the minimum purchase, and the lower the price

All the contract options can be modeled using Generalized Disjunctive Programming (Grossmann and Trespalacios, 2013), and formulated as mixed-integer linear programming (MILP) models using the convex hull reformulation (Balas, 1998). For sales contracts, the same four types and conditions are used. An example of the application of these formulations was presented by Drouven and Grossmann (2016). The authors optimized a strategic plan for shale gas extraction considering different kinds of contracts.

Transportation contracts optimization has been addressed by Yano (1992). In addition to the amounts and prices, these contracts consider multiple transportation modes and the provision of urgent services.

The third kind of strategic decision, capacity installation, expansion, and contraction, has been widely studied. Martínez-Costa et al. (2014) present a review of strategic models related to capacity expansion. They describe the main decisions and factors involved in strategic planning. Among the list of decisions considered in the models they reviewed, they include tactical decisions such as production and demand allocation. These articles use the same approach described in Fig. 6 from Section 2. Another observation they make is the consideration of location of facilities. With the exception of temporary facilities, all problems related to facility location yield strategic models. A comprehensive review of these models is presented by Melo et al. (2009). Capacity increases can be simple equipment purchases or more complex construction projects to install new plants or even building a new site. Martínez-Costa et al. (2014) do not make a particular difference between both cases.

To better understand the modeling approach for strategic decisions, we now analyze two examples from the literature related to the process industry. The first example selected is the model proposed by Levis and Papageorgiou (2004) to optimize a pharmaceutical supply chain. The model is set to plan clinical trials and manufacturing capacity. The planning horizon is ten years divided in one year periods. The manufacturing capacity is controlled deciding the number and timing of installation of production lines. The installation of the first production line at a site, called header suite by the authors, must include the installation of general services. The capacity decisions are translated into available production time, which restricts the production and sales. The objective is to maximize the expected Net Present Value (NPV), considering uncertainty in the success of clinical trials.

The model considers three constraints to handle the expansion decisions:

1. A production line exists if it was present in the previous period, or if it was decided to install it before considering the construction lead time.

$$y_{it} \Rightarrow y_{it-1} \vee b_{it-\lambda_i} \quad (3)$$

where i is the production suite, t is the time period, λ_i is the construction time of suite i , y_{it} indicates the existence of suite i in period t , and b_{it} indicates that the construction of suite i starts at period t .

2. A non-header suite can only be installed if a header suite was installed before.
3. A symmetry breaking constraint. Suite $i - 1$ must be installed before suite i .

The second group of constraints corresponds to production, inventory, and sales constraints. An interesting observation is that the sales are bounded by the demand, which allows the model to perform portfolio planning.

$$sales_{kpt} \leq Demand_{kpt} \quad \forall k, p, t \quad (4)$$

The rest of the constraints are specific to the pharmaceutical industry. A scale-up operation is required when a product is manufactured at a plant for the first time, and then qualification runs are required to demonstrate the plant is producing in compliance to the regulations. To solve the resulting model the authors propose a hierarchical algorithm in which the strategic decisions are taken first with aggregated production, and then the tactical plan is solved in reduced space.

A second relevant example of strategic planning models is the problem studied by You et al. (2010). The objective of the model is to determine the expansion strategy of multiple chemical sites, together with the supply chain planning. The planning horizon considered is ten years divided in yearly periods. Each site has a defined number of slots in which a production train can be installed. Each train corresponds to a reactor and the associated downstream facilities. The sizes of the production trains, both installed and available for installation is predefined. Additionally to the timing and size of expansions, the model decides which production family should the production train be dedicated to. Besides expansion, options for shutting down a production train, or convert it to another product family are considered.

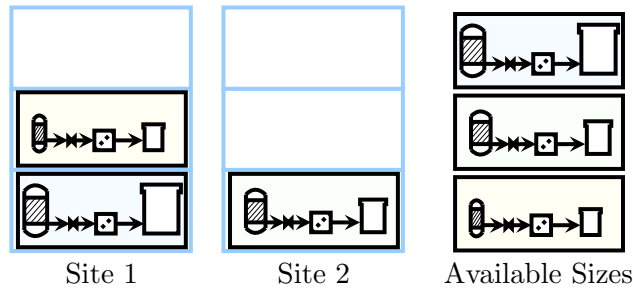


Figure 8. Site expansion modeling approach from You et al. (2010)

The model considers three processes related to capacity: installation, shutdown, and transformation of production trains to another product family. Blocks of logical constraints are defined for each process. The model also considers tactical planning decisions at the product level. Since the strategic decisions are made

at the strategic level, appropriate conversions are included in the production constraints. Due to the model complexity, the authors develop two solution strategies: bilevel decomposition (Iyer and Grossmann, 1998) and Lagrange decomposition (Guignard and Kim, 1987). Just like the previous example, the sales variables are bounded by the demand. However, in this model the sales must be within a certain demand range (Eq. 5).

$$MinDemand_{kpt} \leq Sales_{kpt} \leq MaxDemand_{kpt} \quad \forall k, p, t \quad (5)$$

Comparing both examples it is possible to identify some similar characteristics and some differences in modeling.

1. In both examples the capacity is discrete. It can be increased or reduced by changing the number of capacity units, manufacturing suites in the case of the first example, and production trains in the second. Therefore, the constraints related to capacity involve binary or integer variables, and logical relations.
2. Both examples consider yearly periods and ten years of planning horizon. This is the right timing for strategic decisions. However, for the tactical decisions considered, the time discretization yields aggregated plans. Further refinement of the time grid is required to correctly optimize the tactical decisions in detail.
3. The first example only considers expansion, whereas the second considers expansion, shutdown, and transformation.
4. The effect of installing the first capacity unit is included in the first example.
5. The demand satisfaction constraints are inequalities in both cases. This would make them suitable for portfolio optimization. For the second example *MinDemand* would need to be set to zero.

Because of the discrete nature of strategic decisions, these problems usually yield MILP models. They are solved either with standard branch-and-cut solvers or heuristics. The models found in the literature have similar characteristics to the examples selected. However, no general modeling approach has been defined yet.

The preferred method for handling uncertainty at the strategic level is stochastic programming, because it is assumed that longer planning horizons give more opportunities to reevaluate decisions and take

recourse actions (Snyder, 2006). In process engineering design, the flexibility analysis has been proposed (Swaney and Grossmann, 1985), which has strong connections to robust optimization (Zhang et al., 2016). This approach has not been applied yet to supply chains. The use of the flexibility analysis for supply chain design has been limited (Mansoornejad et al., 2011; Sahay and Ierapetritou, 2015; Wang et al., 2016).

4 Supply Chain Planning

Optimization of tactical decisions has been addressed in the area of supply chain planning. With the strategic decisions already fixed, the goal is to optimize the material flows and inventories in the supply chain network. The base model used to represent this decision level is the lot-sizing problem (Karimi et al., 2003). The planning horizon ranges from six months to a couple of years, divided in monthly periods. The flow between the different echelons (suppliers, manufacturing sites, distribution centers, and customers) in the network must be determined (Fig. 9). Because the models are multiperiod, inventory levels are simultaneously determined.

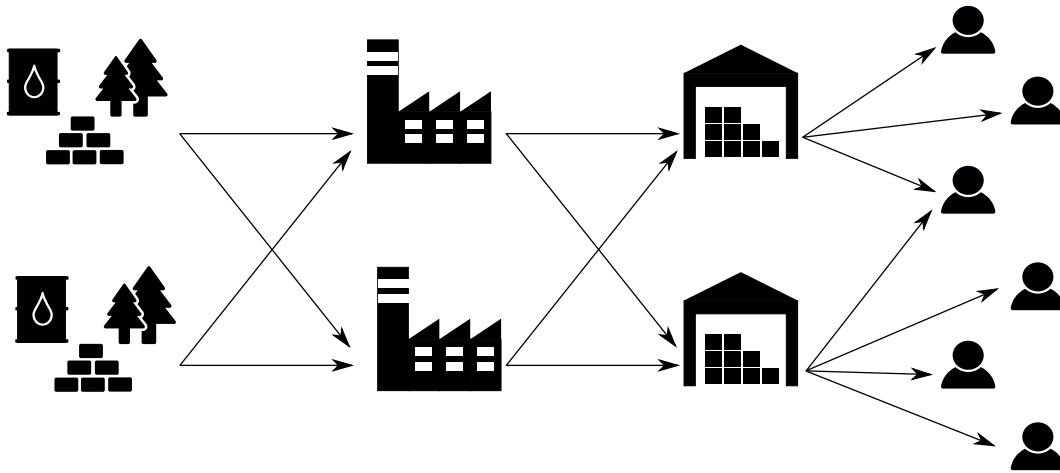


Figure 9. Supply chain planning network

The basic constraints of the problem are the inventory balance (Eq. 6), and constraint satisfaction (Eq. 7),

$$inv_{jpt} = inv_{jpt-1} + \sum_i x_{ijpt} - \sum_k x_{jkpt} \quad \forall j, p, t \quad (6)$$

$$\sum_j x_{jkpt} = Demand_{kpt} \quad \forall k, p, t \quad (7)$$

where i is a manufacturing site, j is a distribution center, k is a customer, p is a product, and t is a time period. The variables inv and x represent inventory and flow, respectively.

A large variety of application-specific constraints complement these models. In the simplest case, the problem yields LP models. However, it is frequent to find MILP models in the literature when start-up or fixed transportation costs are considered. NLP models are also defined when material blending is present, for example, oil blending problems (Loterio et al., 2016). To handle uncertainty, inventory optimization considering safety stocks has been studied (You and Grossmann, 2011).

5 Process Scheduling

Once the mid-term planning is completed, the short-term scheduling to plan the execution of the manufacturing operations is required. The planning horizon spans from two days to four weeks, and the horizon is divided in days or even hours. General modeling frameworks have been defined to address the problem. The resulting models are difficult to solve, motivating intensive research in the area. Harjunkski et al. (2014) and Méndez et al. (2006) present comprehensive reviews of models and applications of process scheduling. We focus on analyzing general characteristics between the modeling frameworks to identify key elements for multilevel optimization.

A major issue in scheduling models is time representation (Floudas and Lin, 2004). Discrete time is the most used as it is easier for tracking resource constraints. However, continuous time is more accurate, although computationally more difficult.

The State-Task-Network (STN) formulation, proposed by Kondili et al. (1993), involves the transformation of materials (called states) by employing tasks. Fig. 10 displays an example of a STN. In the diagram, each circle represents a state and each rectangle represents a task. The process stoichiometry is represented by the coefficients at each arc. Process equipment is not represented in the diagram. However, they are considered in the model.

The main decision variables are:

1. y_{ijt} : a binary variable indicating if task i is performed in equipment j at the beginning period t
2. b_{ijt} : the size of the batch processed at equipment j in period t , executing task i
3. s_{kt} inventory of state k in period t

There are two groups of constraints:

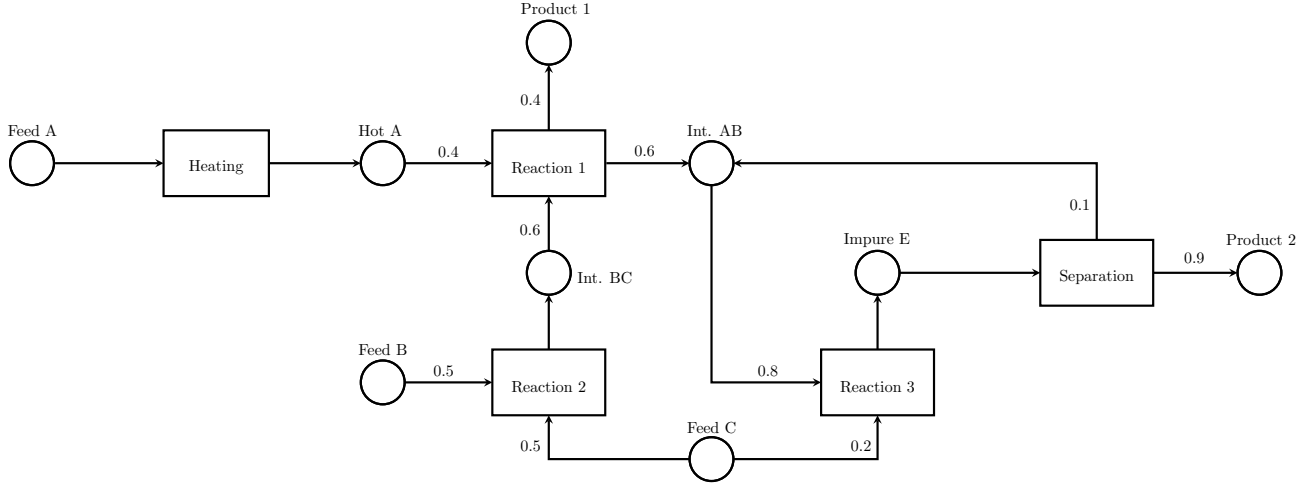


Figure 10. State-task-network. Example 1 from Kondili et al. (1993)

Logical constraints They ensure no more than one task is assigned to an equipment at a given period, and also that no task is assigned while the equipment is executing a task.

Material balances For each state a material balance is required. Each circle from Fig. 10 acts as a storage tank.

The minimal STN model with discrete time representation is given by Eqs. 8–13.

$$\text{Max} \quad \sum_k \eta_k s_{kT} \quad (8)$$

$$\text{s.t.} \quad \sum_{i \in I_j} \sum_{\tau=t-PT_{ij}+1}^t y_{ij\tau} \leq 1 \quad \forall j, t \quad (9)$$

$$s_{kt} = s_{kt-1} + \sum_{i \in I_k^P} \rho_{ik}^p \sum_{j \in J_i} b_{ij(t-PT_{ij})} - \sum_{i \in I_k^C} \rho_{ik}^c b_{ijt} + \Pi_{kt} - D_{kt} \quad \forall k, t \quad (10)$$

$$V_{ij}^{\min} y_{ijt} \leq b_{ijt} \leq V_{ij}^{\max} y_{ijt} \quad \forall i, j \in J_i, t \quad (11)$$

$$C_k^{\min} \leq s_{kt} \leq C_k^{\max} \quad \forall k, t \quad (12)$$

$$b_{ijt}, s_{kt} \geq 0, y_{ijt} \in \{1, 0\} \quad (13)$$

The objective value is to maximize the profit involving the final inventory s_{kT} in period T . The parameters η_k is the inventory value. Π_{kt} and D_{kt} are parameters indicating planned material or product deliveries. PT_{ij} is the processing time of task i in unit j . The parameters ρ_{ik}^p and ρ_{ik}^c define the proportion of state k produced or consumed by task i . $V_{ij}^{\min/\max}$ is the minimum/maximum batch size, and $C_k^{\min/\max}$

is the minimum/maximum inventory of state k .

Pantelides (1994) proposed the Resource-Task-Network (RTN) formulation in which processing equipment is explicitly considered. The RTN framework is less intuitive, but more general than STN. There is no difference made between equipment units and materials, since all are treated as resources. For example, the stoichiometric relation for the separation task would be represented as follows:

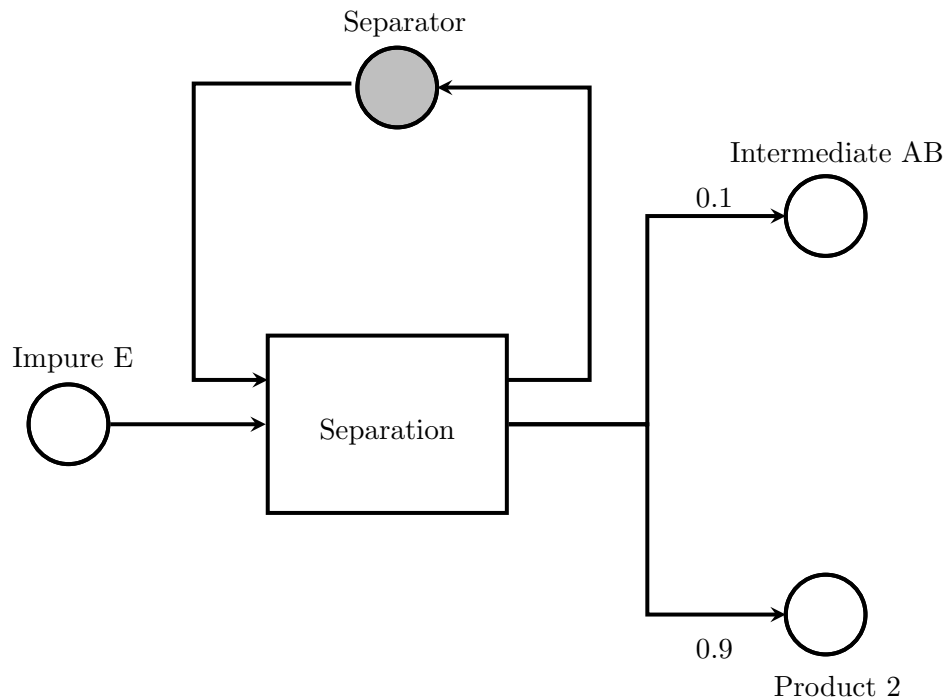
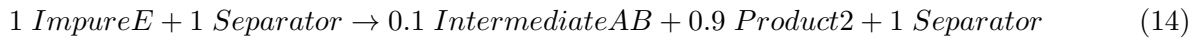


Figure 11. RTN representation of the separation task from Fig. 10

In this way, any resource including materials, equipment, utilities, and human resources, can be seamlessly incorporated into the model, requiring a single balance constraint.

Resource balance For every resource a balance constraint is required. The start of a task is controlled by the availability of resources to perform it, including the processing equipment.

The main decision variables are:

1. y_{it} : a binary variable indicating if task i starts at the beginning of period t
2. b_{it} : the size of the batch processed in period t , executing task i

3. r_{kt} : inventory of resource k in period t

The simplest discrete time RTN model is given by Eqs. 15–18

$$Max \quad \sum_k \eta_k r_{kT} \quad (15)$$

$$s.t. \quad r_{kt} = r_{kt-1} + \sum_{i \in I_r} \sum_{\tau=0}^{PT_i} (\mu_{ir\tau} y_{i(t-\tau)} + \nu_{ir\tau} b_{i(t-\tau)}) + \Pi_{rt} \quad \forall k, t \quad (16)$$

$$V_{ik}^{min} y_{it} \leq b_{it} \leq V_{ik}^{max} y_{it} \quad \forall i, r \in R_i, t \quad (17)$$

$$b_{it}, r_{kt} \geq 0, y_{it} \in \{1, 0\} \quad (18)$$

Parameters μ_{ikt} and ν_{ikt} indicate fixed and variable proportion of production (positive value) or consumption (negative value) of resource k for task i at interval τ relative to start of processing of the task i (Méndez et al., 2006).

Recently, Zyngier and Kelly (2012) proposed a new representation for scheduling problems, called Unit-Operation-Port-State-Superstructure (UOPSS). It starts from the process flow diagram, a physical equipment perspective, and extends it to include logical units (operations). It includes five types of units:

1. Process
2. Pool
3. Pipeline
4. Pileline (stacks)
5. Parcel

For each unit there is a defined set of constraints (Zyngier and Kelly, 2009). The UOPSS models include three groups of constraints:

Logical Balances Logical constraints involving binary variables to handle start-up, shutdown, and other logical relationships required by the model

Quantity Balances Material balances of the different states and resources present in the model

Logistic Balances Constraints that relate quantity variables to logical variables

For example, consider that the separator from Fig. 11 could perform another operation to separate an input F into Product 2 and another species G . The UOPSS representation for this case is displayed in Fig. 12.

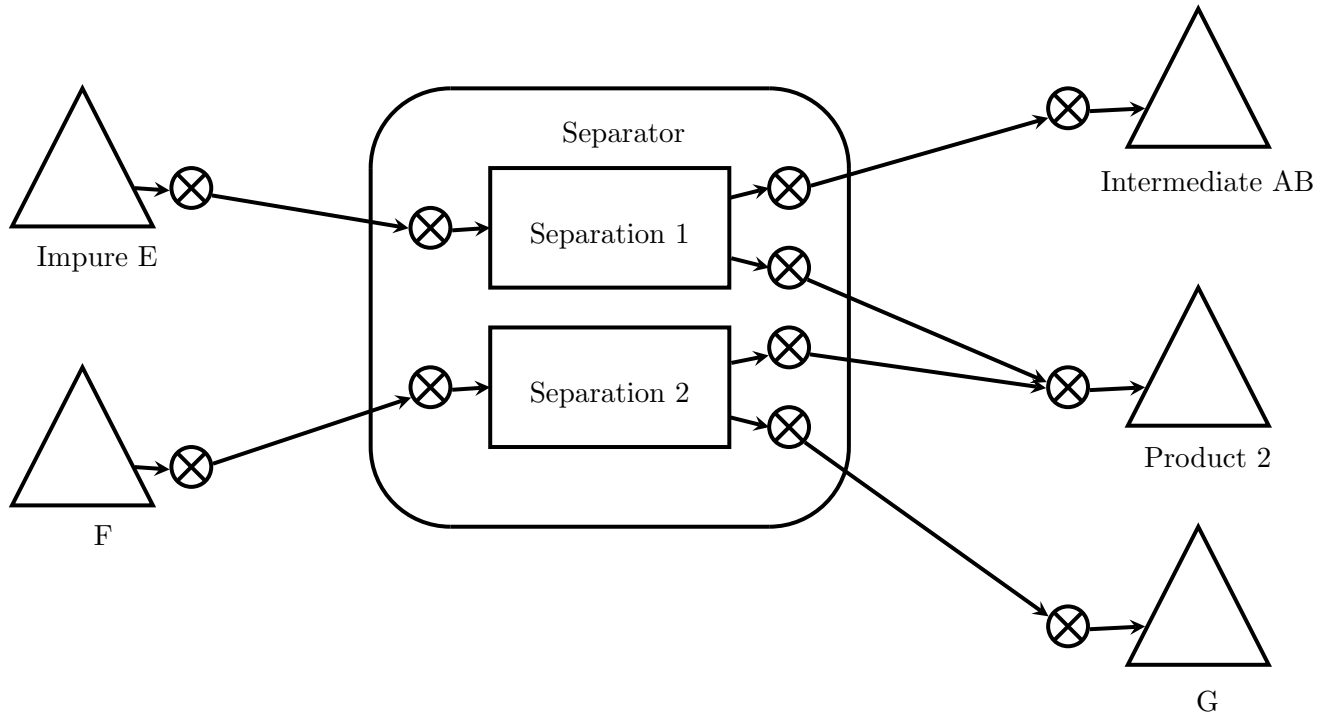


Figure 12. UOPSS representation example

Storage tanks are represented by triangles, the operations by rectangles, and the ports by circles. The diagram displays the explicit physical connectivity, in this case between the storage tanks and the separator, and also includes the process perspective with the inclusion of logical units, separation modes in the example. Storage tanks are an example of pool units, whereas the separator is a process unit. Both STN and RTN have been extensively used in many applications. Since, UOPSS is more recent, its application has not been as extensive as the other two representations. How the three approaches compare is still an open question.

Industrial size scheduling problems are very difficult to solve. Due to the combinatorial nature of scheduling models, several solution methods have been proposed. Besides using MILP solvers, heuristics, and constraint programming methods have also been used. [Jain and Grossmann \(2001\)](#) proposed an hybrid method for combining MILP and constraint programming, [Maravelias and Grossmann \(2004\)](#) applied this algorithm to batch scheduling.

Since the duration and yield of operations are inherently uncertain, scheduling under uncertainty

is a research area of high interest. Aytug et al. (2005) and Li and Ierapetritou (2008) have published comprehensive reviews on the topic. Lappas and Gounaris (2016) recently proposed an Adaptive Robust Optimization framework for short-term scheduling.

6 Model Network Coordination

As discussed in the previous sections, models for each of the decision levels have been proposed. The integration of multiple decision levels has not been completely solved. In this section we present an overview of different approaches to coordinate the solutions obtained for each node of the decision network.

Optimization models are formulated to resolve trade-offs between opposing decision objectives. For example, in a facility location problem there is a trade-off between fixed costs arising from opening facilities and distribution costs. Lowering distribution costs by opening many facilities, in order to be as close as possible to the customers, increases the fixed costs for keeping more facilities opened. Thus, there is a conflict between the objectives of different decision levels. To resolve the conflict, i.e. find an optimal solution that maximizes the benefit of the sum of all objective functions, can be approached in several ways. They include: large-scale models, multiobjective optimization, agent-based optimization, and decomposition.

6.1 Large-scale models

The first approach is to combine the models from each node into a single large-scale model. If the model can be solved it will yield the optimal solution for the system in a single step. The evident challenge is tractability. The larger the model the harder it is to solve. Especially considering that the solution time scales exponentially with the model size. Another downside of this approach is that the effective exploitation of parallel computing depends on the solver capabilities.

This approach is the same as if a manager requiring to develop a production plan for the next year, would ask his three direct reports to have a large meeting with all the stakeholders involved in the decision. Finding a solution that satisfies all the meeting attendees within the duration of the meeting can be tremendously challenging. In many cases, no agreement will be reached within the available time. The more participants in the meeting, the harder it is to reach an agreement.

6.2 Multiobjective optimization

Multiobjective optimization (MO) is another approach for finding the optimal solution for the decision network. The idea behind MO is to acknowledge the existence of two or more objectives and try to determine the trade-off between them. This is specially useful for situations in which the objectives cannot be added because they have different units, for example, when sustainability objectives are considered (Pinto-Varela et al., 2011; Guillén-Gosálbez and Grossmann, 2009). Recently, Širovnika et al. (2016) proposed a rigorous way of combining such objectives with the concept of Sustainability Net Present Value.

The output from a MO is a representation of the variation of one objective with respect to the other. This defines a family of Pareto-optimal solutions (Fig. 13). This gives more flexibility to the decision maker to select the operation point in the Pareto front using any criterion desired depending the valuation given the objectives considered.

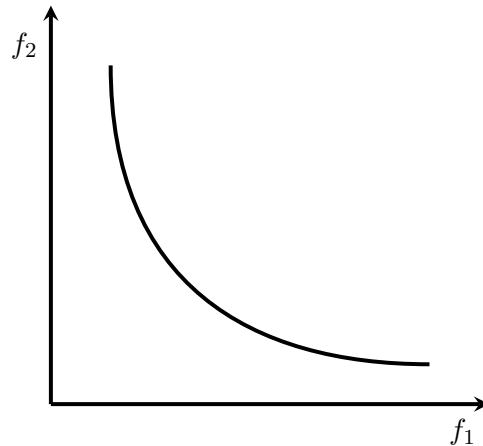


Figure 13. Pareto front output from solving a bi-objective problem

6.3 Decomposition

Large-scale problems have been effectively solved employing decomposition. The problem is partitioned into two or more parts that are solved iteratively, exchanging information between them. Since the solution time of a problem increases exponentially with its size, the time it takes to conduct one iteration is far less than the solution time it takes to solve the full-space problem. The success of these algorithms is based on the fact that many problems can be solved in less than a couple hundred iterations in a fraction of the time required to solve the full-space problem.

In Benders decomposition (Benders, 1962) the problem is solved iteratively exchanging information

between the decision makers. The problem is partitioned between a master problem and one or more subproblems. The master problem proposes a value for its variables, and the subproblems inform back their best solution given the proposed values received. Thus, the subproblem is a function of the variables of the master problem. Since the master problem only considers part of the full problem, it yields a lower bound of the optimum (in case of minimization). The subproblems yield a full feasible solution, as every feasible solution is an upper bound of the optimum. The iterations can continue until both bounds match to a desired tolerance.

Coming back to the analogy of the manager needing to elaborate a production plan for the next year, Benders decomposition corresponds to the process in which the manager and his or her reports work separately in making the decisions within their scope. They only exchange the results of their decision-making process, iterating until they reach an agreement. This process represents how decisions are made in practice. The difference is that only a few iterations are performed. Therefore, there are large improvement opportunities in the current decision-making processes. A second interesting observation is that Benders decomposition could also represent any bargaining process, opening strong connections with game theoretical approaches.

Mathematically, the objective value of the subproblems is a function of a decision made by the master problem. Usually, problems with the block angular structure displayed in Fig. 14 are amenable to Benders decomposition, because selecting the linking variables as part of the master problem, decomposes the problem into several subproblems that can be solved in parallel. This is exactly the case in two-stage stochastic programming.

To clarify these concepts consider the example defined by Eq. 19

$$\begin{aligned}
 P : \text{Min} \quad & c^T x + d^T y \\
 \text{s.t.} \quad & Ax \leq b \\
 & Ey \leq f \\
 & Gx + Hy \leq q \\
 & x \in X, y \in Y
 \end{aligned} \tag{19}$$

The problem P can be partitioned into a master problem and a subproblem. For example, x may represent the vector of strategic variables, whereas y represents the vector of tactical variables. Then the

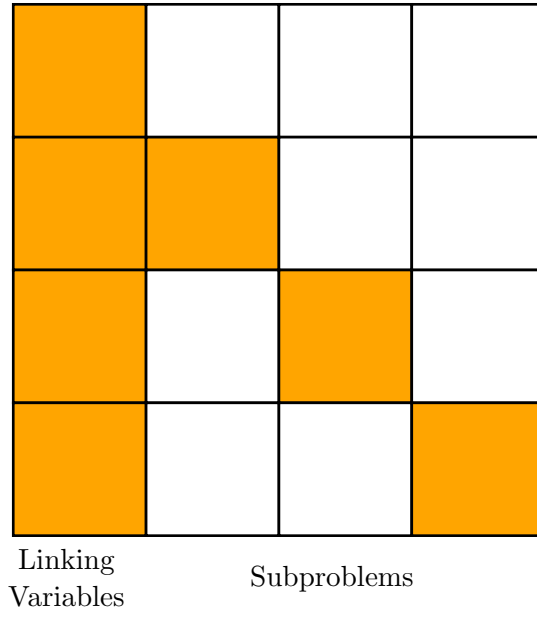


Figure 14. Block angular structure with linking variables

strategic problem (or master problem) is defined by Eq. 20, and the subproblem by Eq. 21.

$$BM : Min \quad c^T x + \theta \tag{20a}$$

$$s.t. \quad Ax \leq b \tag{20b}$$

$$\theta \geq \theta^k - \lambda^k(x^k - x) \quad k = 1 \dots K \tag{20c}$$

$$g(x, x^l) \leq 0 \quad l = 1 \dots L \tag{20d}$$

$$\theta \geq \theta^{LB} \tag{20e}$$

$$x \in X, \theta \in \mathbb{R} \tag{20f}$$

$$SP(x) : Min \quad d^T y \quad (21a)$$

$$s.t. \quad Ey \leq f \quad (21b)$$

$$G\hat{x} + Hy \leq q \quad (21c)$$

$$x - \hat{x} = 0 \quad (21d)$$

$$y \in Y \quad (21e)$$

The problem BM (Benders master) optimizes the strategic decisions. It acknowledges that there is a part of the problem that is unknown to itself (the tactical problem) by including the variable θ in the objective function. The feasible space for this variable is iteratively approximated by a family of cuts (Eq. 20c). The variable θ is bounded by θ^{LB} , otherwise the problem P would be unbounded. The objective value of subproblem SP is a function of the vector x . In other words, the tactical decision depends on the strategic decision. At iteration k , a value for x is given and the optimal solution for SP is determined. From the subproblem, the objective function and λ^k , the dual variables of Eq. 21d, to construct the cut from Eq. 20c. This corresponds to the coordination-feedback process described by Mesarovic et al. (1970).

When the subproblem is a linear programming problem (LP), the duals λ^k are well defined, and the cut from Eq. 20c can be easily generated. However, when the subproblem is a mixed-integer linear problem (MILP) the duals are not defined, and additional efforts are required to obtain tight cuts. Mathematically, finding the optimum for the decision network is equivalent to solving a multistage stochastic programming problem with mixed-integer recourse (MSMIP). When Fig. 4 is rotated in 90 degrees the usual representation for a multistage scenario tree is obtained. Therefore, all the methods developed for solving MSMIPs are applicable to multilevel systems.

The simplest feedback that a subproblem can provide is feasibility. The decision proposed by the master problem can be either feasible or not. When the subproblem is infeasible, a cut to exclude such solutions must be incorporated in the master problem (Eq. 20d). When the subproblem is an LP, the cut is given by Eq. 22, where ν^l is the Farkas proof of infeasibility, an unbounded extreme ray of the dual problem.

$$0 \leq \nu^l(x^l - x) \quad (22)$$

When the subproblem is a mixed-integer problem, the duals are not defined, and other cuts need to be defined. Balas and Jeroslow (1972) proposed “no-good” cuts for the case of binary master variables (Eq. 23)

$$\sum_{i:x_i^l=0} x_i + \sum_{i:x_i^l=1} (1 - x_i) \geq 1 \quad (23)$$

When the subproblem is feasible, the feedback is given in terms of the objective value and the dual information. When the subproblem is an LP a standard Benders cut is generated (Eq. 24).

$$\theta \geq \theta^k - \lambda^k(x^k - x) \quad (24)$$

Again, when the subproblem is a mixed-integer problem the dual information is not available, and additional considerations to generate cuts are required. The first option is to only use the objective value. Laporte and Louveaux (1993) proposed the cut from Eq. 25 for the case of binary master variables. θ^{LB} is a lower bound of the objective value of the subproblem.

$$\theta \geq \theta^k - (\theta^k - \theta^{LB}) \left(\sum_{i:x_i^k=0} x_i + \sum_{i:x_i^k=1} (1 - x_i) \right) \quad (25)$$

The cut is tight at the optimal solution, but in general very weak. The cut pushes the master problem to agree with the subproblem in the value of θ^k unless it changes components of the master variables vector x . The number of components that need to be changed to “override” the effect of the cut, depends on the quality of the bound θ^{LB} . In the worst case, when $\theta^{LB} = 0$, by changing only one component the cut becomes useless.

The second option is to solve a convex relaxation of the subproblem to approximate the objective

value and obtain dual information. Zou et al. (2017) propose three additional cut options for the case of binary master variables.

Benders Cut. Solving the LP relaxation of the subproblem it is possible to generate the cut from Eq.

24. The cuts are valid and finite. However, their use does not guarantee convergence to the optimal solution.

$$\theta \geq \theta^{LP} - \lambda^{LP}(x^k - x) \quad (26)$$

Lagrange Cut. The subproblem can be relaxed defining a Lagrange relaxation by dualizing Eq. 21d.

Since the Lagrange relaxation is at least as tight as the LP relaxation, the cut obtained dominates the Benders cut. However, they are more expensive to obtain.

$$\theta \geq \theta^{LR} - \lambda^{LR}(x^k - x) \quad (27)$$

Strengthened Benders Cut. An intermediate option between the previous two, is using the dual values from the LP relaxation to initialize the Lagrange relaxation. The objective value of the first iteration can be used to define a cut. This family of cuts is also valid and finite, but does not necessarily dominate Benders cuts.

$$\theta \geq \theta^{LR_1} - \lambda^{LP}(x^k - x) \quad (28)$$

In the equations a superindex LP indicates the LP relaxation, LR indicates the Lagrange relaxation, and LR_1 is the first iteration of the Lagrange relaxation.

Gade et al. (2014) also propose to start from the LP relaxation adding Gomory cuts when variables of the subproblem that are known to be integer take a fractional value in the relaxation. By successively adding cuts, the objective value of the relaxation is strengthened, and dual information is available. Sherali and Fraticelli (2002) proposed generating cuts by applying their Relaxation-Linearization Technique. It involves lifting the space by considering one binary variable at a time, which limits its application to small problems.

All the previous cut options proposed for mixed-integer subproblems are either not tight enough or expensive to obtain. They are also limited to binary master variables. This is one of the biggest challenges

in multilevel optimization.

The situation can be compensated by exploiting parallel computing. Every problem that can be solved with Benders decomposition can also be solved by Lagrange decomposition (Guignard and Kim, 1987) by disaggregating the master variables and adding non-anticipativity constraints. If the problem P (Eq. 19) decomposes into $|I|$ subproblems, then the y variable can be written as $y_i : i \in I$, where y_i is the local variable corresponding to the subproblem i . In principle, the vector x does not have a component for each subproblem, but the variables can be duplicated adding non-anticipativity constraints.

$$x_i : i \in I \tag{29}$$

$$x_i - x_{i+1} = 0 \quad \forall i \in I \tag{30}$$

The constraints from Eq. 30 can be dualized to apply Lagrange decomposition. Since a multilevel optimization problem can be solved with both Benders and Lagrange decomposition, both algorithms can be run in parallel exchanging information between them. This is the idea behind cross decomposition (Van Roy, 1983; Mitra et al., 2014).

6.4 Game theory approaches

As briefly discussed in the previous section, finding the optimal solution of a decision network is equivalent to finding the solution of a bargaining process. So far these approaches have only been used to identify optimal decisions in the presence of external decision makers, such as coordination between multiple echelons (Zamarripa et al., 2013), and coordination between enterprises and customers (Garcia-Herreros et al., 2016). Florensa et al. (2017) showed that these approaches can also be applied to multilevel systems. The modeling of these problems leads to bilevel programming models (Vicente and Calamai, 1994), in which the subproblems are embedded as constraints in the master problem. Eq. 31 is an example of a bilevel programming problem.

$$\begin{aligned}
 BPP : \text{Min} \quad & c^T x \\
 \text{s.t.} \quad & Ax \leq b \\
 & \text{Min} \quad d^T y \\
 & Ey \leq f \\
 & Gx + Hy \leq q \\
 & x \in X, y \in Y
 \end{aligned} \tag{31}$$

The problem can be solved by replacing the inner problem by its Karush-Kuhn-Tucker conditions and reformulating the resulting problem (Colson et al., 2005). The application of bilevel programming to the integration of supply chains is still to be addressed.

7 Challenges

Multilevel supply chain optimization is required to design enterprise-wide decision systems. The decision network representation is much more than a useful representation to model and solve the problem, but a natural representation of the way companies are organized the make decisions. This is reflected in the similarity between organizational structures and the decision structures discussed in Section 2. Efficiently modeling and solving multilevel systems will result in more responsive supply chains that make better decisions and are more competitive. There are several challenges that need to be addressed to succeed in this area.

The first challenge in multilevel optimization is the availability of a modeling platform that allows for model seamlessly representing the nodes of the decision structure as building blocks and their connections. PLASMO (Jalving et al., 2016) is a step in the right direction but it has not even been released.

The second challenge is the lack of standardized models for strategic and tactical decisions. For process scheduling, there are multipurpose general frameworks available. It is not clear that the same thing can be achieved in higher levels of the decision-making pyramid. These generalizations should also include the right aggregation of lower levels to ensure that feasibility is maintained, and to accelerate the solution process. Generalization can be especially challenging at the tactical level due to the variety of conditions found in each application. However, the availability of commercial software for this purpose (Funaki, 2009) is an indication that such generalization is indeed possible.

The third challenge is coordination. The algorithms available are applied to specific mathematical structures of each node. The feedback process (cut generation) is the most difficult part. Decomposition algorithms that can deal with any type of node, in the most general case nonconvex mixed-integer nonlinear problems (MINLP), are required. Recently, this area has made significant process driven by the research in stochastic programming with mixed-integer recourse.

Finally, uncertainty is a reality present in every decision-making problem. There are several options to address uncertainty, such as stochastic programming, robust optimization, and the flexibility analysis. The modular modeling in multilevel optimization allows to combine them, using the most appropriate approach for each level. This has not been attempted yet. Stochastic programming integrates particularly well with the decision structure, maintaining the same mathematical structure, adding extra nodes to the decision network.

In summary, supply chain multilevel optimization is an important frontier in decision-making. It will bring new benefits to make manufacturing processes smarter. Significant progress has been made in several components of the problem, but the integration of those components, and the solution of additional challenges is still needed.

References

- Aytug, H., Lawley, M. A., McKay, K., Mohan, S., and Uzsoy, R. (2005). Executing production schedules in the face of uncertainties: A review and some future directions. *European Journal of Operational Research*, 161(1):86–110.
- Balas, E. (1998). Disjunctive programming: Properties of the convex hull of feasible points. *Discrete Applied Mathematics*, 89(1):3–44.
- Balas, E. and Jeroslow, R. (1972). Canonical cuts on the unit hypercube. *SIAM Journal on Applied Mathematics*, 23(1):61–69.
- Baldea, M. and Harjunkski, I. (2014). Integrated production scheduling and process control: A systematic review. *Computers & Chemical Engineering*, 71:377–390.
- Barbosa-Póvoa, A. P. (2012). Progresses and challenges in process industry supply chains optimization. *Current Opinion in Chemical Engineering*, 1(4):446–452.

- Benders, J. F. (1962). Partitioning procedures for solving mixed-variables programming problems. *Numerische Mathematik*, 4(1):238–252.
- Bezanzon, J., Karpinski, S., Shah, V., and Edelman, A. (2012). Julia: A fast dynamic language for technical computing. In *Lang.NEXT*.
- Birge, J. R. and Louveaux, F. (2011). *Introduction to stochastic programming*. Springer Science & Business Media.
- Bixby, R. E., Fenelon, M., Gu, Z., Rothberg, E., and Wunderling, R. (2004). Mixed integer programming: a progress report. *The Sharpest Cut*, pages 309–325.
- Blum, C. and Roli, A. (2003). Metaheuristics in combinatorial optimization: Overview and conceptual comparison. *ACM Computing Surveys (CSUR)*, 35(3):268–308.
- Colson, B., Marcotte, P., and Savard, G. (2005). Bilevel programming: A survey. *4OR: A Quarterly Journal of Operations Research*, 3(2):87–107.
- de Weck, O. L., Suh, E. S., and Chang, D. (2003). Product family and platform portfolio optimization. In *ASME 2003 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference*, pages 175–185. American Society of Mechanical Engineers.
- Dias, L. S. and Ierapetritou, M. G. (2016). Integration of scheduling and control under uncertainties: Review and challenges. *Chemical Engineering Research and Design*, 116:98–113.
- Drouven, M. G. and Grossmann, I. E. (2016). Multi-period planning, design and strategic models for long-term, quality-sensitive shale gas development. *AIChE Journal*.
- Dunning, I., Huchette, J., and Lubin, M. (2015). JuMP: A modeling language for mathematical optimization. *arXiv:1508.01982 [math.OC]*.
- Florensa, C., Garcia-Herreros, P., Misra, P., Arslan, E., Mehta, S., and Grossmann, I. E. (2017). Capacity planning with competitive decision-makers: Trilevel milp formulation, degeneracy, and solution approaches. *European Journal of Operational Research*.
- Floudas, C. A. and Lin, X. (2004). Continuous-time versus discrete-time approaches for scheduling of chemical processes: a review. *Computers & Chemical Engineering*, 28(11):2109–2129.

- Funaki, K. (2009). State of the art survey of commercial software for supply chain design. *Georgia Institute of Technology Report*.
- Gade, D., Küçükyavuz, S., and Sen, S. (2014). Decomposition algorithms with parametric gomory cuts for two-stage stochastic integer programs. *Mathematical Programming*, 144(1-2):39–64.
- Garcia, D. J. and You, F. (2015). Supply chain design and optimization: Challenges and opportunities. *Computers & Chemical Engineering*, 81:153–170.
- Garcia-Herreros, P., Zhang, L., Misra, P., Arslan, E., Mehta, S., and Grossmann, I. E. (2016). Mixed-integer bilevel optimization for capacity planning with rational markets. *Computers & Chemical Engineering*, 86:33–47.
- Grossmann, I. E. (2005). Enterprise-wide optimization: A new frontier in process systems engineering. *AIChE Journal*, 51(7):1846–1857.
- Grossmann, I. E. and Trespalacios, F. (2013). Systematic modeling of discrete-continuous optimization models through generalized disjunctive programming. *AIChE Journal*, 59(9):3276–3295.
- Guignard, M. and Kim, S. (1987). Lagrangean decomposition: A model yielding stronger lagrangean bounds. *Mathematical Programming*, 39(2):215–228.
- Guillén-Gosálbez, G. and Grossmann, I. E. (2009). Optimal design and planning of sustainable chemical supply chains under uncertainty. *AIChE Journal*, 55(1):99–121.
- Harjunkoski, I., Maravelias, C. T., Bongers, P., Castro, P. M., Engell, S., Grossmann, I. E., Hooker, J., Méndez, C., Sand, G., and Wassick, J. (2014). Scope for industrial applications of production scheduling models and solution methods. *Computers & Chemical Engineering*, 62:161–193.
- Hooker, J. N. (2002). Logic, optimization, and constraint programming. *INFORMS Journal on Computing*, 14(4):295–321.
- Iyer, R. R. and Grossmann, I. E. (1998). A bilevel decomposition algorithm for long-range planning of process networks. *Industrial & Engineering Chemistry Research*, 37(2):474–481.
- Jain, V. and Grossmann, I. E. (1999). Resource-constrained scheduling of tests in new product development. *Industrial & Engineering Chemistry Research*, 38(8):3013–3026.

- Jain, V. and Grossmann, I. E. (2001). Algorithms for hybrid MILP/CP models for a class of optimization problems. *INFORMS Journal on Computing*, 13(4):258–276.
- Jalving, J., Abhyankar, S., Kim, K., Hereld, M., and Zavala, V. M. (2016). A graph-based computational framework for simulation and optimization of coupled infrastructure networks. *IET Generation, Transmission & Distribution*, To Appear.
- Karimi, B., Ghomi, S. F., and Wilson, J. (2003). The capacitated lot sizing problem: a review of models and algorithms. *Omega*, 31(5):365–378.
- Kondili, E., Pantelides, C., and Sargent, R. (1993). A general algorithm for short-term scheduling of batch operations. milp formulation. *Computers & Chemical Engineering*, 17(2):211–227.
- Laporte, G. and Louveaux, F. V. (1993). The integer l-shaped method for stochastic integer programs with complete recourse. *Operations Research Letters*, 13(3):133–142.
- Lappas, N. H. and Gounaris, C. E. (2016). Multi-stage adjustable robust optimization for process scheduling under uncertainty. *AIChE Journal*, 62(5):1646–1667.
- Levis, A. A. and Papageorgiou, L. G. (2004). A hierarchical solution approach for multi-site capacity planning under uncertainty in the pharmaceutical industry. *Computers & Chemical Engineering*, 28(5):707–725.
- Li, Z. and Ierapetritou, M. (2008). Process scheduling under uncertainty: Review and challenges. *Computers & Chemical Engineering*, 32(4):715–727.
- Linderoth, J. T. and Savelsbergh, M. W. (1999). A computational study of search strategies for mixed integer programming. *INFORMS Journal on Computing*, 11(2):173–187.
- Lotero, I., Trespalacios, F., Grossmann, I. E., Papageorgiou, D. J., and Cheon, M.-S. (2016). An MILP-MINLP decomposition method for the global optimization of a source based model of the multiperiod blending problem. *Computers & Chemical Engineering*, 87:13–35.
- Mansoornejad, B., Pistikopoulos, E. N., and Stuart, P. (2011). Incorporating flexibility design into supply chain design for forest biorefinery. *J-FOR Journal of Science & Technology for Forest Products and Processes*, 1(2):54–66.

- Maravelias, C. T. and Grossmann, I. E. (2004). A hybrid MILP/CP decomposition approach for the continuous time scheduling of multipurpose batch plants. *Computers & Chemical Engineering*, 28(10):1921–1949.
- Maravelias, C. T. and Sung, C. (2009). Integration of production planning and scheduling: Overview, challenges and opportunities. *Computers & Chemical Engineering*, 33(12):1919–1930.
- Martínez-Costa, C., Mas-Machuca, M., Benedito, E., and Corominas, A. (2014). A review of mathematical programming models for strategic capacity planning in manufacturing. *International Journal of Production Economics*, 153:66–85.
- Melo, M. T., Nickel, S., and Saldanha-Da-Gama, F. (2009). Facility location and supply chain management—a review. *European Journal of Operational Research*, 196(2):401–412.
- Méndez, C. A., Cerdá, J., Grossmann, I. E., Harjunkski, I., and Fahl, M. (2006). State-of-the-art review of optimization methods for short-term scheduling of batch processes. *Computers & Chemical Engineering*, 30(6):913–946.
- Mesarovic, M. D., Macko, D., and Takahara, Y. (1970). Theory of multilevel hierarchical systems. *New York, Academic*.
- Meyr, H., Wagner, M., and Rohde, J. (2015). Structure of advanced planning systems. In *Supply Chain Management and Advanced Planning*, pages 99–106. Springer.
- Mitra, S., Garcia-Herreros, P., and Grossmann, I. E. (2014). A novel cross-decomposition multi-cut scheme for two-stage stochastic programming. *Computer Aided Chemical Engineering*, 33:241–246.
- Pantelides, C. C. (1994). Unified frameworks for optimal process planning and scheduling. In *Proceedings on the Second Conference on Foundations of Computer Aided Process Operations*, pages 253–274. CACHE Publications New York.
- Papageorgiou, L. G. (2009). Supply chain optimisation for the process industries: Advances and opportunities. *Computers & Chemical Engineering*, 33(12):1931–1938.
- Park, M., Park, S., Mele, F. D., and Grossmann, I. E. (2006). Modeling of purchase and sales contracts in supply chain optimization. In *SICE-ICASE, 2006. International Joint Conference*, pages 5727–5732. IEEE.

- Perea-Lopez, E., Grossmann, I. E., Ydstie, B. E., and Tahmassebi, T. (2001). Dynamic modeling and decentralized control of supply chains. *Industrial & Engineering Chemistry Research*, 40(15):3369–3383.
- Pinto-Varela, T., Barbosa-Póvoa, A. P. F., and Novais, A. Q. (2011). Bi-objective optimization approach to the design and planning of supply chains: economic versus environmental performances. *Computers & Chemical Engineering*, 35(8):1454–1468.
- Rastogi, A. P., Fowler, J. W., Carlyle, W. M., Araz, O. M., Maltz, A., and Büke, B. (2011). Supply network capacity planning for semiconductor manufacturing with uncertain demand and correlation in demand considerations. *International Journal of Production Economics*, 134(2):322–332.
- Sahay, N. and Ierapetritou, M. (2015). Flexibility assessment and risk management in supply chains. *AIChE Journal*, 61(12):4166–4178.
- Sargent, R. (2005). Process systems engineering: A retrospective view with questions for the future. *Computers & Chemical Engineering*, 29(6):1237–1241.
- Shah, N. (2005). Process industry supply chains: Advances and challenges. *Computers & Chemical Engineering*, 29(6):1225–1235.
- Sherali, H. D. and Fraticelli, B. M. (2002). A modification of benders’ decomposition algorithm for discrete subproblems: An approach for stochastic programs with integer recourse. *Journal of Global Optimization*, 22(1-4):319–342.
- Širovnika, D., Zoreb, Ž., Čučekb, L., Pintaričb, Z. N., and Kravanja, Z. (2016). System synthesis by maximizing sustainability net present value. *Chemical Engineering Transactions*, 52:1075–1080.
- Snyder, L. V. (2006). Facility location under uncertainty: a review. *IIE Transactions*, 38(7):547–564.
- Swaney, R. E. and Grossmann, I. E. (1985). An index for operational flexibility in chemical process design. part i: Formulation and theory. *AIChE Journal*, 31(4):621–630.
- Van Roy, T. J. (1983). Cross decomposition for mixed integer programming. *Mathematical programming*, 25(1):46–63.
- Vicente, L. N. and Calamai, P. H. (1994). Bilevel and multilevel programming: A bibliography review. *Journal of Global Optimization*, 5(3):291–306.

- Wang, H., Mastragostino, R., and Swartz, C. L. (2016). Flexibility analysis of process supply chain networks. *Computers & Chemical Engineering*, 84:409–421.
- Yano, C. A. (1992). Optimizing transportation contracts to support just-in-time deliveries: the case of one contracted truck per shipment. *IIE Transactions*, 24(2):177–183.
- You, F. and Grossmann, I. E. (2011). Stochastic inventory management for tactical process planning under uncertainties: Minlp models and algorithms. *AIChE Journal*, 57(5):1250–1277.
- You, F., Grossmann, I. E., and Wassick, J. M. (2010). Multisite capacity, production, and distribution planning with reactor modifications: Milp model, bilevel decomposition algorithm versus lagrangean decomposition scheme. *Industrial & Engineering Chemistry Research*, 50(9):4831–4849.
- Zamarripa, M. A., Aguirre, A. M., Méndez, C. A., and Espuña, A. (2013). Mathematical programming and game theory optimization-based tool for supply chain planning in cooperative/competitive environments. *Chemical Engineering Research and Design*, 91(8):1588–1600.
- Zhang, Q., Lima, R. M., and Grossmann, I. E. (2016). On the relation between flexibility analysis and robust optimization for linear systems. *AIChE Journal*.
- Zou, J., Ahmed, S., and Sun, X. A. (2017). Stochastic dual dynamic integer programming. *Optimization Online*, 2017.
- Zyngier, D. and Kelly, J. D. (2009). Multi-product inventory logistics modeling in the process industries. In *Optimization and Logistics Challenges in the Enterprise*, pages 61–95. Springer.
- Zyngier, D. and Kelly, J. D. (2012). UOPSS: a new paradigm for modeling production planning & scheduling systems. In *Symposium on Computer Aided Process Engineering*, volume 17, page 20.