Improving the tactical and operational decision making procedures in Chemical Supply Chains

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Improving the tactical and operational decision making procedures in Chemical Supply Chains

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A mis padres.

Success consists of going from failure to failure without loss of enthusiasm.

Winston Churchill (1874-1965)

Summary

Nowadays, market trends have made companies modify the way of doing business. The current context of globalization, economic crisis, political conditions and competence among enterprises involves a continuous challenge for achieving their Key Performance Indicators. This wide range of indexes include profitability, cost reduction, satisfaction of market demand, environmental and impacts or development of new products, among other factors that improve the customer service. The successful achievement of these indicators depends on the supply chain efficiency. Thus, companies work towards the optimization of their overall supply chain in response to the competition from other companies as well as to take advantage of the flexibility in the world market restrictions. This is done by the exploration of any resource flow (including raw materials and intermediates and final products, or energy), as well as any echelon of the supply chain network (such as suppliers, production plants, distribution centres and final markets). In this point, the Supply Chain Management addresses the process of planning, implementing and controlling the supply chain operations in an efficient way, throughout the management of material, information and financial flows across a network of entities within a supply chain. This includes the coordination and collaboration of processes and activities involved in this network. However, the complexity of considering the overall supply chain as well as the presence of uncertainty (i.e., demand, prices, process parameters) introduce more complexity in the coordination of all the activities or processes which take place through the supply chain.

The aim of this thesis is to develop techniques to enhance the decision making process in industrial processes, by the development of new mathematical models to better coordinate all available information and to improve the synchronization production and demand, considering different time scales.

Hence, this thesis presents a general overview of production process requirements within a supply chain and a review of the current state of the art, which has allowed to identify the open issues in the area in the context of Process Systems Engineering. Moreover, the first part of the thesis also presents an analysis of existing approaches, methods and tools used through this thesis.

The second part of this work deals with the integrated management of production and demand constraints. This part first explores how the profitability of the supply chain can be improved by considering simultaneously production side and demand side management under deterministic conditions. Thus, discrete and hybrid time formulations have been presented to study the performance of the time representation. Furthermore, the discrete time formulation has been extended to deal with the external and internal uncertainty, through the implementation of a reactive approach, which allows to update input parameters in case of variation from the initial and/or previous conditions. This part is also addresses the coordinated management of production and demand as well as the use of external and internal resources. Therefore, a new generalized mathematical formulation which integrates all resources involved in the production process within a supply chain is presented.

The third part of this thesis is focused on the integrated supply chain optimization. Particularly, this part concerns the integration of hierarchical decision levels, by the exploitation of mathematical models that assess the consequences of considering simultaneously scheduling and planning decisions when designing a supply chain network. The Synthesis State Task Network concept is introduced to extend its typical representation of a process to incorporate information associated to the synthesis problem by the implementation of synthesis blocks. Finally, an integrated information management system based on an ontological framework is presented. The aim of this information platform is to coordinate all available information for decision making. This integrated platform will allow monitoring the real-time evolution of industrial processes within a supply chain. Moreover, this system may be used as an Operator Training System.

Finally, the last part of this thesis provides the final conclusions and further work to be developed.

Resumen

A día de hoy, las tendencias del mercado han hecho que las empresas modifiquen su manera de hacer negocios. El contexto actual de globalización, crisis económica, condiciones políticas y la competencia entre las empresas implica un continuo desafío para conseguir los indicadores clave de rendimiento. Existe un amplio rango de indicadores, que incluyen rentabilidad, reducción de costes, satisfacción de la demanda del mercado, impacto medioambiental o la rapidez en el desarrollo de nuevos productos, entre otros factores que mejoran el servicio al cliente. El éxito en el logro de estos indicadores depende de la cadena de suministro. Por lo tanto, las empresas trabajan para la optimización de su cadena de suministro en respuesta a la competencia de otras empresas, así como también para tomar ventaja de la flexibilidad en las restricciones del comercio mundial. Esto se hace mediante al análisis del flujo de materiales (incluyendo materias primas y productos intermedios y finales), así como cualquier escalón de la red de la cadena de suministro (por ejemplo, proveedores, plantas de producción, centros de distribución y mercados finales). Llegados a este punto, la gestión de la cadena de suministro aborda el proceso de planificación, ejecución y control de las operaciones de la cadena de suministro de forma eficiente, a través de la gestión de los materiales, la información y los flujos financieros a través de la red que conforma la cadena de suministro. Esto incluye la coordinación de los diferentes procesos y actividades que participan en esta red. Sin embargo, la complejidad de considerar toda la cadena de suministro en su conjunto, así como la presencia de incertidumbre (como por ejemplo, demanda, precios, parámetros de proceso) introducen un grado de complejidad en la coordinación de todas las actividades o procesos que tienen lugar en la cadena de suministro.

El objetivo de esta tesis consiste en desarrollar técnicas que permitan la mejora del proceso de toma de decisiones en procesos industriales, y especialmente el desarrollo de nuevos modelos matemáticos que contemplen la coordinación de toda la información

disponible y la sincronización de la producción y la demanda, teniendo en cuenta diferentes horizontes temporales.

Por lo tanto, inicialmente esta tesis presenta una visión general de los procesos de producción, así como también una revisión del estado del arte, lo que ha permitido identificar las cuestiones abiertas en el área de la Ingeniería de Sistemas de Proceso. Además, en la primera parte de la tesis se presenta un análisis de los diferentes enfoques, metodologías y herramientas que se utilizan a lo largo de esta tesis.

La segunda parte de este trabajo se ocupa de la gestión integrada de la producción y la demanda. Esta parte explora cómo la rentabilidad de la cadena de suministro se puede mejorar teniendo en cuenta de manera simultánea le gestión de la producción y la demanda en condiciones determinísticas. Se ha desarrollado un modelo matemático que utiliza una formulación de tiempo discreto y una formulación híbrida, con el objetivo de evaluar el impacto de la representación temporal. Esta formulación se ha extendido para hacer frente a la incertidumbre tanto externa como interna, a través de la aplicación de un enfoque reactivo, que permite actualizar parámetros de entrada en el caso de variación sobre las condiciones iniciales y/o anteriores. Esta parte también trata la gestión coordinada de la producción y la demanda teniendo en cuenta la gestión de los recursos externos e internos. Para ello, se presenta una nueva formulación matemática generalizada que integra todos los recursos que intervienen en el proceso de producción.

La tercera parte de esta tesis se centra en la optimización integrada de la cadena de suministro. Particularmente, esta parte se refiere a la integración de los diferentes niveles jerárquicos de decisión, mediante la explotación de modelos matemáticos que evalúan las consecuencias de considerar simultáneamente decisiones a nivel operacional y táctico y el diseño de una red de cadena de suministro. Se presenta la representación gráfica consistente en la red de síntesis y tareas-estados para incorporar la información asociada al problema de síntesis. Por último, se presenta un sistema de gestión integrado de información en un entorno ontológico, cuyo objetivo es coordinar toda la información disponible para la toma de decisiones. Esta plataforma integrada permite seguir la evolución en tiempo real de diferentes procesos industriales, así como también puede ser usada como un sistema de entrenamiento de operarios.

Finalmente, la última parte de esta tesis ofrece las conclusiones finales y el trabajo futuro a desarrollar.

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Contents

List of figures

List of tables

Glossary

ABET	Accreditation Board for Engineering and Technology
AIMMS	Advanced Interactive Multidimensional Modeling System
AMPL	A Mathematical Programming Language
CH	Control Horizon
CP	Constraint Programming
CPU	Central Processing Unit
CR	Critical Region
ESE	Energy Systems Engineering
EU	European Union
EWMO	Enterprise-Wide Modelling and Optimization
GA	Genetic Algorithm
GAMS	General Algebraic Modeling System
GloMIQO	Global Mixed Integer Quadratic Optimization
ISA	International Society of Automation
KKT	Karush, Kuhn and Tucker
KPI	Key Performance Indicator
LP	Linear Programming
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non-Linear Programming
MIP	Mixed Integer Programming
MOO	Multi-Objective Optimization
MPC	Model Predictive Control
NLP	Non-Linear Programming
OPC	Object Linking and Embedding for Process Control
OTS	Operator Training Simulators
R&D	Research and Development
RH	Rolling Horizon
PH	Prediction Horizon
PSE	Process Systems Engineering
RTN	Resource Task Network
SC	Supply Chain

SCM	Supply Chain Management
SH	Scheduling Horizon
STN	State Task Network
TSSP	Two stage stochastic programming
UC	Unit Commitment
UNESCO	United Nations Educational, Scientific and Cultural Organization

Part I – Overview

Chapter 1. Introduction

1.1. Introductory perspective

According to the European Chemical Industry Council (2014), the European Union (EU) is the second largest chemicals producing area in the world. Whereas world chemical sales in 2013 were valued at €3,156 billion, the EU accounts for 16.7% of the total, worth €527 billion, and employing directly 1.16 million workers. The vast majority of European Union chemical sales (83.6%) are generated in seven EU members, which are Germany, France, Italy, Netherlands, Spain, Belgium and United Kingdom

Moreover, the EU is the world's top exporter and importer of chemicals, accounting the 42.5% (€430 billion) of total global trade in 2013. Of the thirty largest chemical companies in the world, twelve are headquartered in Europe (e.g., BASF, Bayer, Shell, Ineos, Total) representing around 10% of world chemical sales. Pharmaceuticals and chemicals form the first- and second-leading EU manufacturing sector in terms of value-added per employee in 2006, respectively. It is also noteworthy that food and beverages industry hold the seventh place in this list.

The significant role of the process industry in the EU's economic status is evident. However, in order to maintain its leading position in the world's highly competitive market, EU's process industry must remain active and improve its operational and functional performance through its entire supply chain (SC) network. The faster growth rhythm of Asian countries, especially China and Japan, has created a strong competitor for EU process industries, thus making indispensable the enhancement of the production management through an improved overall SC network management.

Furthermore, nowadays, due to the rapidly changing economic and political conditions, as well as the current context of economic crisis, global companies face a continuous challenge to constantly re-evaluate and optimally configure the operations of their SC for achieving their own Key Performance Indicators, such as profitability, cost reduction, satisfaction of market demand, environmental and impacts, development of new products, product satisfaction, among other factors. Companies seek to optimize their global SCs in response to competitive pressures or to acquire advantage of new flexibility in the restrictions on world trade.

Process industries also follow this trend. Thus, companies need the use and exploitation of mathematical models to predict the behaviour of the overall system, to control the progression of processes, to design any issue involved in the process, to detect any eventual failure, as well as to optimise the system under study. The Process Systems Engineering (PSE) community is aware of this change and today is playing a key role in expanding the system boundaries from chemical process systems to business process systems. PSE is based on processes knowledge and mathematical and experimental techniques to formulate computer models of all units (i.e., equipment, chemical recipe, logistics) that constitute the overall process (i.e., chemical plant, supply chain). The obtained models can be integrated in order to manage the overall system in a coordinated way.

1.2. Supply Chain and Supply Chain Management

The concept of a chemical SC refers to the network of interdependent entities (including retailers, distributors, transporters, production facilities and storage centres and suppliers) that constitutes the processing and distribution channels of products, from the sourcing of its raw materials to its delivery to the end consumer (Beamon,1998). This network of facilities and distribution options performs the following functions (Laínez et al., 2007):

- Procurement of raw materials and services (e.g. water and electricity).
- Transformation of these raw materials into intermediate and specified final products.
- Distribution and delivery of finished products to retailers.
- Treatment of pollutants and residues.

Figure 1.1 represents a typical SC network configuration, based on a production process. The main elements of this particular SC are:

- Suppliers, responsible to provide raw material.
- Production plants, where raw materials are transformed into intermediate and final products.
- Distribution centres, where products are stored and distributed.
- Markets, where products are consumed.

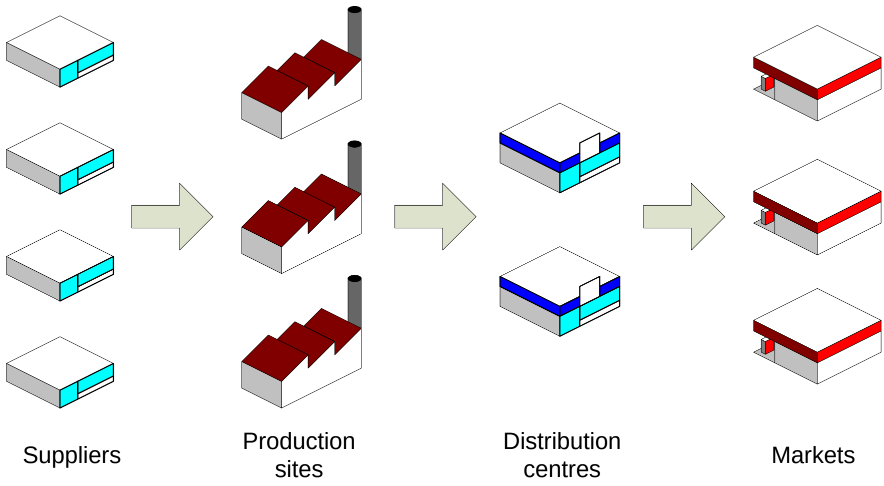

Figure 1.1. Supply chain representation.

Moreover, there are other types of supply chains, which may not be related to the transformation and distribution of materials. In the area of energy, microgrids constitute an example of decentralised supply chain, since involve energy production, storage and consumption (Figure 1.2).

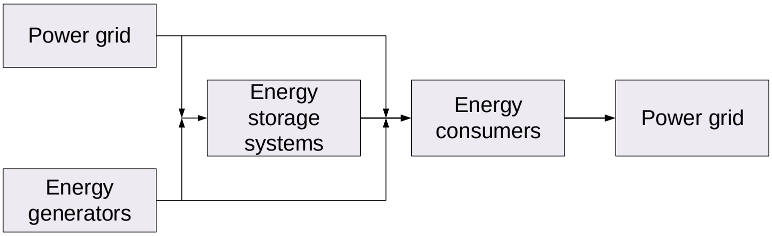

Figure 1.2. Energy supply chain.

On another note, Supply Chain Management (SCM) is the process of planning, implementing and controlling the SC operations in an efficient way. Its concept is related to the management of material, information and financial flows through a network of entities within a SC (including suppliers, manufacturers, logistics, distributors and retailers) that aims at producing and delivering goods or services for the consumers (Tang, 2006). This includes the coordination and collaboration of processes and activities across different functions, including marketing, sales, production, product design, procurement, logistics, finance, and information technology within the network of organizations.

The main objectives of the SCM are (Christopher, 2005):

- To achieve the desired consumer satisfaction levels.

- The maximum financial returns by synchronizing and coordinating the SC members activities.

Figure 1.3 shows the materials, information and cash flows through the SCM:

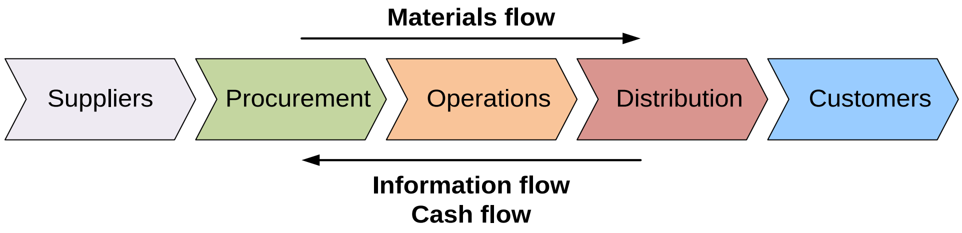

Figure 1.3. Materials, information and cash flows.

The necessity for such coordination grows out of several trends in the marketplace, such as the globalization of market economies. This fact expands the SCM scope in order to consider international issues. In addition, customers' changing expectations regarding value of goods and services, combined with advances in technology and the availability of data, have driven the formation of these international networks (Handfield and Nichols, 1999).

In this context, it is necessary to incorporate a mechanism in order to represent the interconnection and precedence of the several tasks assigned to the overall control system, using data flow graphs. One of these representations was developed by Williams (1989) at the University of Purdue (see Figure 1.4). These representations symbolise the interconnections between influencing external entities on the factory and also identify the interfaces between staff departments which provide services to the factory or express managements' policies in sets of requirements to be fulfilled by the factory.

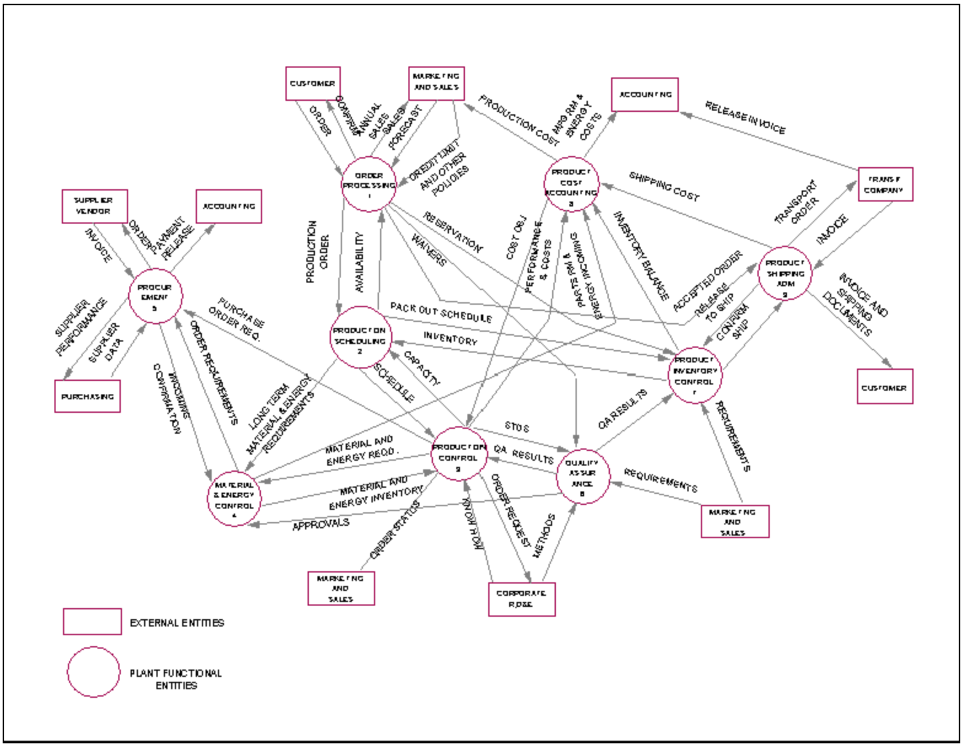

Figure 1.4. Purdue Reference Model.

These representations also define a system of standardized data and functional models to organize information flows and the decision making process, in order to create a set of standard interfaces which allows information exchange between the overall SC with operation management systems. These models provide a set of data flows and function hierarchies for a generic manufacturing facility, and are addressed to automatable operations including production control, procurement, process support engineering, maintenance management, and other functions directly associated with manufacturing.

1.3. Integrated Supply Chain Management

In order to address the SC management, over the last twenty years most companies, and indeed researchers, tend to use a company-centric view of the SC, where the SC is seen as consisting of the plant in question as a central entity, possibly together with some peripheral partners, typically suppliers and customers. This view involves the integration of production and logistics planning across the enterprise, value-chain management, global network planning and investment appraisal.

Moreover, the trend towards globalization has significantly increased the scale and complexity of current businesses. In this context, corporations have become global networks that are made up of a number of business units and functions.

The SC modelling problem is an extremely complex task. For this reason, it is usually helpful to use the time dimension to establish a hierarchical order so as to facilitate SC coordination (inter and intra enterprise coordination), including:

- Strategic level or long-term planning, which affects decisions related to the structure of the SC and is carried out over a long-term horizon. These decisions include location of production sites and warehouses, the capacity of these facilities, and transportation methods and routes.
- Tactical level or medium-term planning seeks to most efficiently fulfil customer demand over a medium-term horizon. Decisions involve the assignment of production targets to production sites, transportation amounts, and inventory profiles.
- Finally, in an operational level, short-term planning or scheduling is carried out for each individual site within the supply chain upon receiving targets from master planning obtained in the tactical level. The scheduling horizon is in days or weeks, and scheduling decisions include batch-sizing, assignment of tasks to equipment units, and sequencing of tasks.

There are interconnections between these different hierarchical levels of the SC which affects the decision making process. For this reason, SC decisions should be coordinated via integration. Figure 1.5 represents these 3 hierarchical levels and its decisions through a SC network.

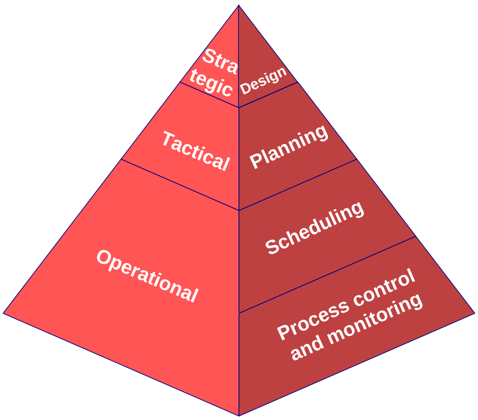

Figure 1.5. Supply chain hierarchical levels.

Operational functions include research and development (R&D), production plants (continuous, discontinuous and discrete) and supply networks. The business departments control their operations through the decisions that enterprises must take about their capital expenditure, the financing of the company, growth strategies and operations. Strategic decisions about capital expenditure and planning include the technology used, the choice of R&D projects and decisions about infrastructure and SCM. Financial decisions are made by identifying the assets and liabilities required from the working capital for larger projects and operations, and by assessing and protecting the company from the risk of change.

Current studies and solutions on these problems, proposed in the fields of PSE and Operations Research, tend only to consider subsets of such decisions, even though a business must act as a cohesive body in which its various functions are coordinated to a certain extent.

Therefore, from a company's viewpoint, overall performance will be below optimum if strategic and tactical decisions are taken separately, as has been the practice to date. However, it is significantly more complex for a company to make decisions that involve its overall interests than to make decisions about specific functions. This explains why integral modelling that reflects the overall running of companies has been virtually unprecedented.

The PSE community faces an increasing number of challenges, while enterprise and SCM remain subjects of major interest that offer multiple opportunities. Further progress in this area is thought to bring with it a unique opportunity to demonstrate the potential of the PSE approach to enhance a company's value. One of the key components of SCM and enterprise-wide modelling and optimization (EWMO) is decision making coordination and integration at all levels (Grossmann, 2004). Most of the recent contributions offer models that separately address problems arising in the three hierarchical decision levels within a standard SC (i.e., strategic, tactical aggregate planning and short-term scheduling).

The nature of the SC planning problem is quite similar to the plant production scheduling problem. Both problems usually search answers to the questions of in what amount, when and where to produce each product comprising the business portfolio so as to obtain financial returns. However, planning brings into play a broader, aggregated view of the problem.

The time scale in planning problems is usually longer than the time scale in product processing. In this way, the sequencing/timing decisions in a scheduling problem are transformed into decisions in a rough capacity problem. In fact, equipment capacity modelling is a highly sensitive aspect that must be taken into account in order to assure consistency and feasibility when problems are being integrated across SC hierarchical decision levels.

Furthermore, at the strategic level, designing a SC network does not only involve selecting the type and size of the equipment, but also allocating this equipment to the different potential SC echelons. Therefore, it is required a SC modelling approach that:

- Considers equipment capacity similarly at strategic and operational levels, so that this capacity can be aggregated and disaggregated in a straightforward and transparent manner;
- Is able to handle strategic decisions associated with technology allocation to sites and not merely site locations;
- Easily represents the transport material and financial flows among SC sites at the scheduling level.

One very significant element to be also considered during the decision making process within a SC is the information availability and reliability. Businesses are subject to internal and external uncertainties. 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, among other factors. 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.

However, the external and internal dynamics of real businesses have not been represented by current models in a way that achieves desired consumer satisfaction levels and acceptable financial returns. Fluctuating demand patterns, increasing customer expectations and competitive markets, coupled with internal disturbances, mean that today's supply networks are not reliable in such an environment unless their external and internal dynamics are appropriately incorporated into the SC model, but nowadays this is not always possible or practical.

For these reasons, the integration of decision making in businesses at various levels will lead significant added value. This requires the coordination of a problem's multiple planning facets in non-conventional manufacturing networks and in multi-site systems. Furthermore, the challenge of solving large multi-scale optimization problems becomes evident when the integration of different decision levels is considered.

Finally, the scheduling details about production equipment will enable the dynamics of SC to be tracked. By considering information from the equipment supervisory module, which can be incorporated into the scheduling formulation, it will be possible to handle the incidents that may arise in the SC in low-level decisions.

1.4. External resources

Different resources are used in the operation of a SC. The need to improve the management of the overall SC has led to the consideration of external resources in the decision making process. In the area of production processes, the most common used resources are water and energy. Thus, a simultaneous management of production and the use of resources is required to take into account environmental and social issues in the industrial processes, in order to reduce their impacts.

One of the main common resources is water. Its use is essential for humanity. However, the availability of this source is limited and decreasing in many areas of the world (Figure 1.6, UNESCO, 2012). Water is used for human necessities as well as in industrial processes. Factories use large amounts of water in industrial processes, which can be used, for example as mass separating agent, reactant, utility or cleaning agent. The scarcity and the strict discharge policies related to the use of water, motivated by the concern associated to the limitation of this natural source, are significant forces to investigate ways to reduce the use of water. This reduction in the use of freshwater and the reduction of wastewater generation is possible by reusing and recycling water.

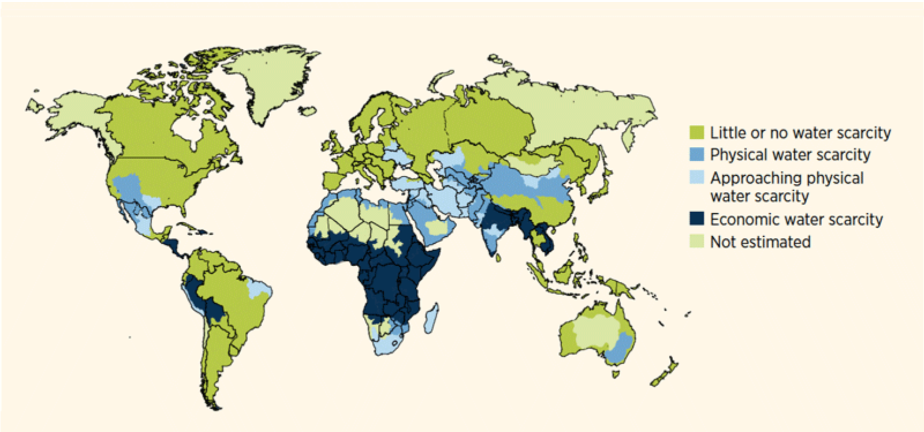

Figure 1.6. Global physical and economic water scarcity.

Regarding the energy, its use of energy at domestic and industrial levels is essential. However, as global population and standard of life increases, the energy demand also increases. It is expected that global demand will be increasing at an average of 1.5% every year to 2035 (Figure 1.7, Orr, 2013), which can involve a failure to meet this growing energy demand if the energy supply is not sufficient and sustainable. In this area, Energy Systems Engineering involves all the decision making procedures associated to an energy supply chain from the primary energy source to the final energy delivery to the customer. The main objectives of managing energy systems are to reduce costs, to reduce the environmental impact and to satisfy energy demand.

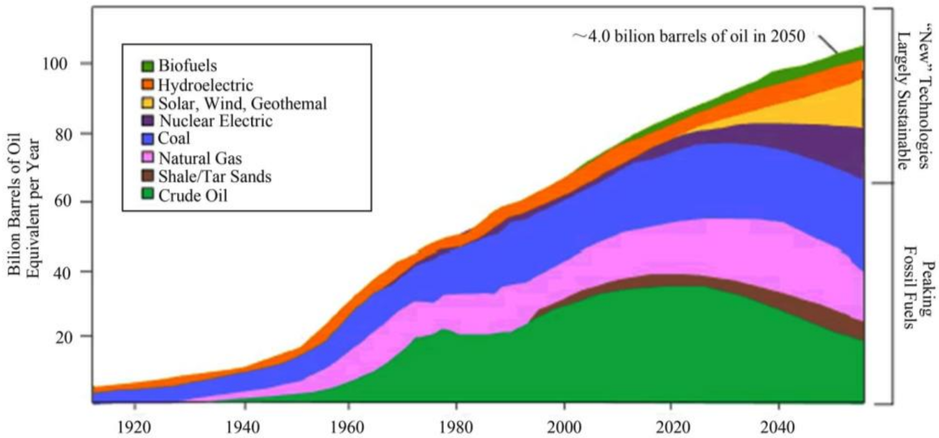

Figure 1.7. World energy demand forecast.

1.5. Main objectives

In the current context of economic crisis, improving the efficiency of the industrial processes is essential to ensure the viability of the companies, such as the coordination of the management of the entire SC, new market trends, uncertain conditions and market diversification.

This thesis aims to enhance the decision making of industrial processes, facing nowadays open issues. In order to achieve this main goal, the key objectives of this thesis are next detailed:

- The modelling and optimization of Supply Chain Management problems using rigorous mathematical optimization approaches and also to propose alternative robust and efficient methods. Thus, the development of robust dynamic mathematical models will be applied for:
  - ✓ The simultaneous management of production and demand under different time representations (Chapter 4).
  - ✓ The integration of external and internal uncertain sources (Chapter 5).
  - ✓ The management of resources within the production process (Chapter 6).
  - ✓ The coordination of production and environmental aspects (Chapter 6).
  - ✓ Real-time scheduling (Chapter 8).
- The development of decision making models in order to improve the Supply Chain Management, by integrating the SC hierarchical levels and reflecting external and internal dynamics of real processes or enterprises (Chapter 7).

- The integration and characterization of all information related to a supply chain (at strategic, tactical and operational level) in a unique information management structure, in order to coordinate the decision making process between the different hierarchical levels and also between the different echelons involved in the SC (Chapter 8).
- The development an open software prototype for the implementation of these methodologies and algorithms (Chapter 8).

1.6. Thesis outline

This thesis has been structured in order to introduce progressively the contributions to the coordinated management of production and demand. Figure 1.8 illustrates the outline of the thesis, which has been divided in four main parts.

Part I, in addition to this introductory chapter, describes, in Chapter 2, a state of the art of the applications and the techniques used to address specific problems in SC decision making, and finally allows identifying some trends and challenges. Also, Chapter 3 provides the different methods and tools and techniques to optimize complex optimization problems.

Part II analyses the integrated management of production and demand constraints. Chapter 4 aims to analyse different time representation alternatives within a mathematical formulation, considering simultaneously not only production, but also demand management, in deterministic conditions. Chapter 5 considers this coordinated decision making process taking into account uncertain conditions, through the use of reactive procedures (i.e., rolling horizon approach) and proactive procedures (i.e., stochastic programming). To complete this part, Chapter 6 extends the approach to include the use of resources, such as water and energy, in the decision making.

Part III studies the integration of different hierarchical levels and all available data within the decision making process associated to the SC. Particularly, Chapter 7 aims to improve process productivity by the coordination of different decision making levels and developing mathematical models able to integrate the features of more than one decision level in the SCM. Moreover, Chapter 8 presents an open communication system in order to integrate all available information associated to a chemical/industrial process, as well as to automate the decision making process.

Finally, Chapter 9 in Part IV summarizes the main contribution of this thesis and draws up concluding remarks for future work.

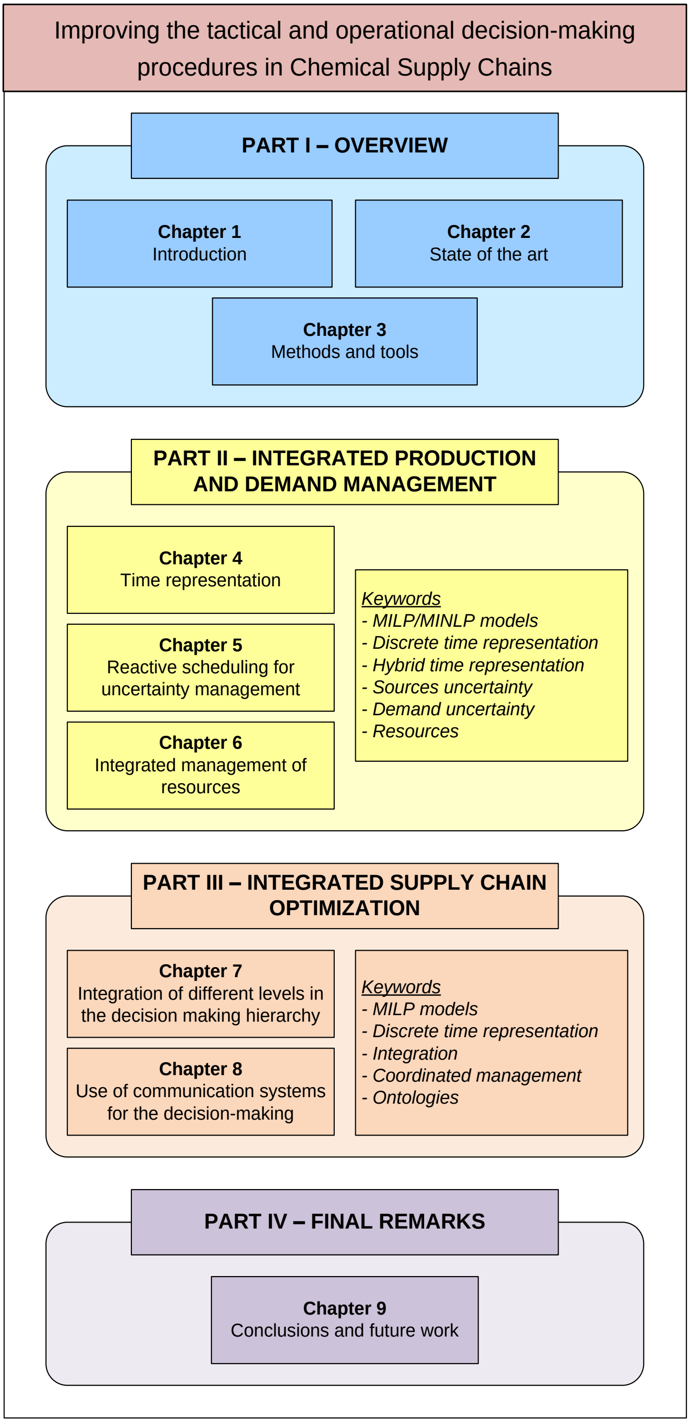

Figure 1.8. Thesis outline.

Chapter 2. State of the art

The intrinsic complexity of the decision making processes within a SC has brought forth the development of a wide variety of problem models and solution algorithms. The selection and adoption of a given approach depends on the characteristics of each problem and in many situations, case specific adaptations seem to be applicable.

In this area, PSE is a branch of chemical engineering which covers a set of methods and tools to support decision making for the creation and operation of a SC, including modelling, simulation, optimization, planning and control tasks. PSE manages knowledge and mathematical tools in order to develop complex mathematical models to represent a unit process, a production facility or an overall SC.

This chapter includes a summary of the major contributions made so far of the topics covered throughout this thesis. The problems that are still open or have special interest will be illustrated for the development of this Thesis. Particularly, this chapter is focused on reviewing the most important works related to the optimization of SCs. In addition, previous works addressed to optimize decision making at different hierarchical levels will be reviewed, as well as decision making based on the integration of these hierarchical levels, the consideration of utilities in the decision making and the consideration of uncertainty in the process.

2.1. Hierarchical decision making

The decision making process within a SC usually can be decomposed in 3 hierarchical levels, according to the time horizon: strategic, tactical and operational (Chapter 1.3). The main decision associated to each decision levels as well as its time horizon are shown in Figure 2.1.

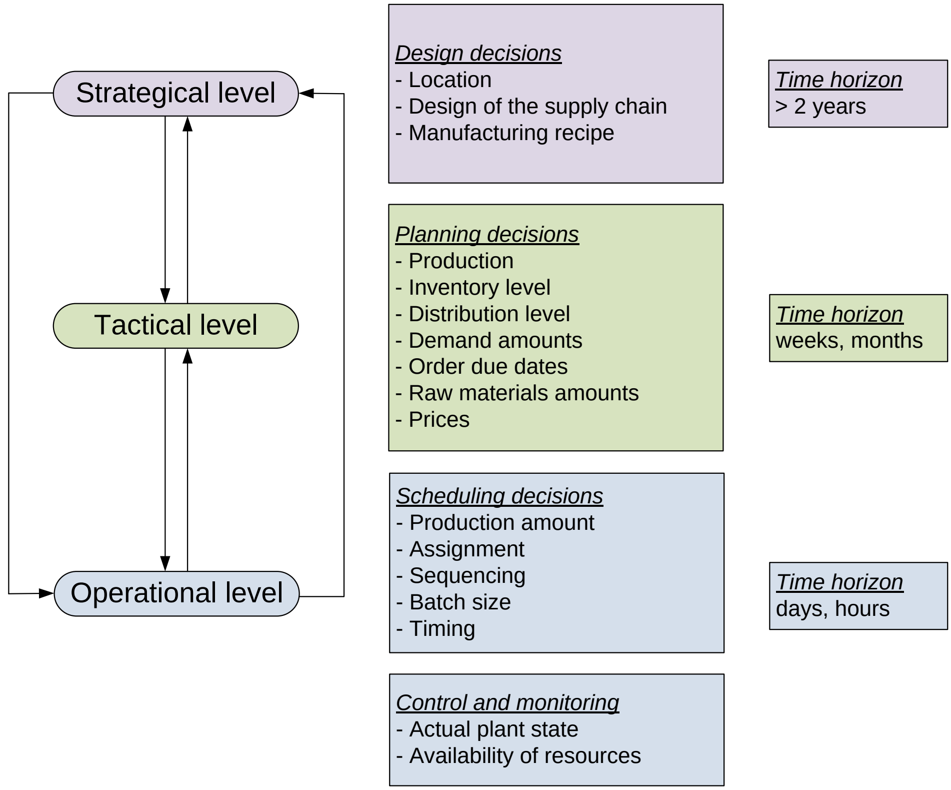

Figure 2.1. Decision making levels.

2.1.1. Strategical level

The SC strategical level (long-term planning) is used in order to synthesize and design the network related to the production and distribution of a set of products. The associated decision making which are involved in this hierarchical level includes the optimal sourcing, manufacturing and distribution network for the new and existing products of a SC, which includes the location of the production plants, warehouses, the production capacities of each plant, technology installed, and the selection of vendors and suppliers all considering several available locations for each plant, market, supplier and warehouse. All these variables can be optimized under an established criteria (i.e., annual profit, total capital cost, net present value, network flexibility, environmental damage, customer service, etc.).

The most common approaches are to formulate a Mixed Integer Linear Programming (MILP), considering fixed costs (investments) and variable costs (manufacturing, procurement, distribution and taxes, among other costs). This kind of problems is usually solved for a time horizon of two to five years. Moreover, these problems have been mainly tackled with operations research approaches at a global level of detail.

The SC synthesis and design problem has its origins in the location and planning problem, which has been a subject of study in Operations Research since the mid-1950s. However, it was first mathematically structured in a MILP form by Balinski (1965). Posteriorly, Brown et al. (1987) developed a mathematical model related to a distribution and distribution industrial network optimization for the biscuit company of Nabisco™, involving opening and closing of plants and its assignment of production.

Several approaches are addressed to exploit the flexibility of the SC network. Ferrio and Wassick (2008), proposed a MILP problem formulation destined to the redesign of existing networks. In this new approach, direct shipping is taken into account, although potential linkages must be predefined. Also, Naraharisetti et al. (2008) developed a MILP redesign formulation, which considers the alternative of investments and disinvestments, as well as decisions including technology upgrade, production, allocation and distribution. More recently, Laínez et al. (2009), proposed an approach based on a flexible SC that allows material flows of any raw material, intermediate material and final product between each facility in order to maximize the net present value. Longinidis and Georgiadis (2014) incorporates the leasing within a new MILP formulation, which combines the SC design and sales and leaseback techniques.

More recently, Kalaitzidou et al. (2014) presented a general MILP formulation for the design of SC networks, considering flexibility on facilities' location and operation. This work addresses the design of a multiproduct and multiechelon network consisting of generalized production/warehousing nodes that can receive any material from any potential supplier or any other generalized production or warehousing node and deliver any material to any market or any other generalized production or warehousing node.

Additionally, the management of the use of utilities (such as water and energy) plays and important role in the SC design. Some works related to this issue can be found in Yang et al. (2014) and Gao et al. (2015). Chapter 2.6 explains the current state of the art related to the management of production process and use of utilities at operational level.

Furthermore, there are several approaches focused on the simultaneous consideration of multiple key performance indicators. As examples, Laínez et al. (2010) have developed a Mixed Integer Non-Linear Programming (MINLP) formulation that optimizes the SC and marketing strategic decisions, evaluating the trade-off between marketing and SC decisions. Pérez-Fortes et al. (2012) introduced the environmental and social criteria within a multi-objective MILP, in order to design a regional and sustainable SC. A complete review of the design of sustainable SC can be found in Eskandarpour et al. (2015) and García et al. (2015), where research opportunities and challenges in the field of SC design, including energy and sustainability issues, are analysed.

Although the traditional approaches consider demand uncertainty, there is a challenge to study the incorporation of uncertainty associated to environmental impacts or the acquisition of raw materials in flexible SC design (see Chapter 2.2). Also, one future extension related to the strategic level is the integration of other indicators, such as the capacity risk in the design of SC in order to optimize the safety stock level (see Chapter 2.3).

2.1.2. Tactical level

The tactical level comprises the mid-term planning, for a time horizon of several months. The mid-term production planning in the industry (SC planning) is typically used in order to determine production levels, inventory levels, distribution of final and intermediate products in a network of product sites, distribution centres and final consumers, including a set of constraints associated with the availability of raw materials acquisition and capacity constraints in production facilities and warehouses. In other words, this kind of problems is addressed to optimize the production, storage and distribution sources to satisfy market requirements, considering a fixed infrastructure within a SC. The constraints associated with the tactical decision making level mainly consider the availability of raw materials, and maximum/minimum production, distribution and storage capacities. The problem can be formulated as a linear programming model (since the production, storage and distribution can be continuous variables), but, in order to be more realistic in most of the cases the formulation corresponds to a MILP model, due to the constraints associated to discrete decision making (i.e., produce or not).

The tactical level formulations address the problem of chemical SC production planning for multi-product, multi-site production networks including production-distribution options, which can be applied to different kind of processes. For example, Wilkinson et al. (1996) presented an optimal production and distribution planning of a wide case study, which takes into account different products, production plants and distribution centres. t is found that the ability of the model to capture effects such as multipurpose operation, intermediate storage and changeovers give rise to counter-intuitive results, such as producing materials further away from demand than expected.

McDonald and Karimi (1997) have developed deterministic models formulated as mixed-integer linear programs. This work deals with multi-period midterm planning models for multiproduct processes. The main goal is to determine the optimal allocation of resources.

More recently, Tsiakis and Papageorgiou (2008) also considered production and distribution networks with special emphasis on product site allocation among sites and outsourcing possibility.

SC planning techniques have also been applied also for pharmaceutical (Papageorgiou et al., 2001, Sousa et al., 2011; Susarla et al., 2012), agrochemical (Sousa et al., 2008), clinical applications (Chen et al., 2012) and to refineries. As examples, Neiro and Pinto (2004) proposed a multi-period large scale MINLP for modelling petroleum SCs, by considering refineries, terminals and pipeline networks. The non-linearities are included in the model in order to characterize the properties of each product. More recently, Santibañez-Aguilar et al. (2015) presented a dynamic optimization model for the optimal planning of a distributed biorefinery, which incorporates a Model Predictive Control (see Chapter 3.5.2) in order to predict the behaviour of the storage levels and orders of the SC.

Some works proposes decomposition techniques, such as two-level optimization or Lagrangean decomposition. Jackson and Grossman (2003) developed a multi-period MINLP for the production planning and product distribution optimization of several continuous multiproduct plants which are located in different sites and supply different markets. The model related to each production facility is represented using nonlinear process models, solving the problem by using Lagrangean decomposition. This decomposition technique was used in order to solve large-scale instances of the problem. Moreover, Ryu and Pistikopoulos (2007) proposed a MILP model for multi-period SC planning problems, transforming the problem into two-level optimization problems. In order to solve this problem, firstly, demands in disjunctive geographical locations are aggregated, as proposed in a previous work (Ryu and Pistikopoulos, 2005). Secondly, individual single-site multi-period planning problems are constructed based on their allocated demands. Also, Verderame and Floudas (2008) developed a model which relates the operation planning and the mid-term of a multipurpose and multiproduct batch chemical, taking into account transportation tasks and multiple sites. Furthermore, Camacho-Vallejo et al. (2015) presented a two-level mathematical formulation addressed to the problem of planning the production and distribution in a SC. In this proposed formulation, the problem is solved in order to determine the production levels to be sent from the distribution centres to the retailers trying to minimize the transportation costs. Posteriorly, the second level consists in minimizing the operational costs.

The consideration of multiple criteria in the decision making process has been addressed in recent works. Fahimnia et al. (2015) presented a MINLP model to evaluate the trade-off between economic aspects and environmental impact, by introducing carbon emissions, energy consumption and waste generation in the proposed model. Also, Boukherroub et al. (2015) proposed a multi-objective model, which takes into account economic, environmental and social impacts.

Finally, Papageorgiou (2009), Mula et al. (2010) and Díaz-Madroñero et al. (2014) presented reviews of mathematical models in planning. According the mentioned reviews, the main challenges in planning are related to water and energy SC, in order to establish a water network which includes water supply and waste water treatment, and energy network, including new decentralized grids. In addition, it is significant to remark the future study of optimizing transport and production planning in a coordinated way, including forms of transport, routes, environmental restrictions, and integration of the suppliers' nodes into the supply chain's optimization models. Also, typical and new sources of uncertainty must be studied taking into account that multiple SCs cooperation and competition for the market demand has not been yet analysed.

2.1.3. Operational level

The scheduling or operational level is a critical issue in both batch and continuous processes. Mathematical models developed to support this activity include decisions of what, where, how and when to operate. In summary, the decision making problem aims to obtain the best possible scheduling: lot-sizing (assignment of equipment and resources to tasks), production allocation (resources utilization profiles), sequencing and timing (start and end times). But scheduling decisions also affect other factors, including process feasibility, sustainability or safety, and so other objectives can be considered, related to production, environmental impact, etc. In the last decades, there have been significant advances in the application of short-term scheduling methodologies, especially to solve industrial problems. One of the main issue in scheduling formulation is the time representation (see Chapter 2.5).

Traditional approaches are based on detailed scheduling related to a production plant, without taking into account its incorporation into a SC. Recent works are related to the integration of the operational level within the SC (see Chapter 2.3).

Scheduling reviews have been presented during the last decades. Shah (1998) reviewed the single and multisite detailed scheduling. In a recent review of scheduling problems, the modelling of representative optimization approaches for the different problem types can be found in Méndez et al. (2006) and Harjunkoski et al. (2014). According to the last review, although there are very significant progresses in the field of short-term scheduling, systematic solution of large-scale problems, concerning to complex enterprise, using mathematical programming remains a challenge to solve.

Several works have been published in order to improve the operational decision making at the plant level. For example, Pinto and Grossmann (1995) developed a MILP formulation of short-term scheduling of batch plants with multiple stages which may contain equipment in parallel. The operational level is also used in order to predict the starting point and end times for each operation, as presented by Pekny and Reklaitis (1998). Some works are focused on multi-tasks and multi-product plants (Méndez and Cerdá, 2007; Marques de Souza Filho et al., 2013; MirHassani and BeheshtiAsl, 2013), multiperiod optimization models (Kabra et al., 2013), discrete scheduling models under multi-objective optimization (Capón-García et al., 2014), and focused on the sequence-dependent issues (Cóccola et al., 2014).

Moreover, operational applications for multi-product, multi-task and batch processes have been studied for single-stage production plants (Castro et al., 2008, Castro and Grossmann, 2012) and multi-stage (Prasad and Maravelias, 2008).

Furthermore, several works include material storage policies. For example, Aguirre et al. (2011 and 2014) solve a short-term scheduling of a semiconductor industry problem, developing an MILP-based tool to synchronize detailed schedule of production activities and transfer operations following strict intermediate storage policies, including zero wait restriction. This model is quite remarkable because proofs the adaptability of the scheduling model across all kind of industries.

In order to represent the production sequences of the chemical processes, two general graph frameworks are available, namely the State-Task Network (STN) and the Resource-Task Network (RTN). The STN was initially proposed by Kondili et al. (1993), and consists of a direct graph which includes two nodes: the state node and the task node. Posteriorly, Pantelides (1994) extended such framework to the RTN representation in order to describe processing equipment, storage, material transfer and utilities as resources in a unified way.

With regard to the STN representation, which allows handling many complexities in this kind of processes. In addition, they formulated a MILP based on a discrete time representation in order to solve short-term scheduling, taking into account equipment allocation, storage levels, the availability of raw materials, and the batch size and production deliveries in order to maximize the profit of the process. In addition, this work proposed a detailed scheduling model in order to optimize multiple products and multiple tasks plants. In this work, it was defined the STN to represent the process information, separating the process in nodes linked to the task nodes, where each connection represents the precedence of the task. Recipe networks are then adequate for serial processing structures, and better represent the information of the process, and the complexity associated to different information becomes a challenge to manage.

Furthermore, several authors use the STN representation for discrete time formulations, such as Maravelias and Grossmann (2003b and 2006), who developed an algorithm to minimize the makespan of multipurpose batch plants and where the relationship between discrete and continuous time MILP formulation was studied, respectively. In addition, the STN representation is also used for continuous time formulations in several works. For example, Maravelias and Grossmann (2003a) proposed a continuous time MILP model for short-term scheduling of multipurpose batch plants, including resource constraints, variable batch sizes and processing times, storage policies, batch mixing/splitting and sequence-dependent changeover times. Posteriorly, Bose and Bhattacharya (2009) developed a MILP formulation in order to generate an optimal schedule for a sequence of several continuous processing units for processing products using the STN representation.

The main challenges related to operational level are focused on the integration under uncertainty of this hierarchical level within a SC (see Chapters 2.2 and 2.3), and the development of strategies to reduce the computational effort required to find optimal solutions still remain as open issues to be studied.

2.2. Uncertainty

In general, process are dynamic and therefore, different kinds of unexpected events may occur quite frequently. These disturbances may affect the nominal operating conditions (i.e., schedule of the production facility). Different uncertainty management techniques are briefly described in Chapter 3.5. Also, more details regarding optimization under uncertainty in process industries can be found in Sahinidis (2004). This section focuses the state-of-the-art related to the presence of uncertainty in the different hierarchical levels of a SC.

The consideration of uncertainty can be crucial to ensure the generation of feasible solutions of good quality and practical interest. Different sources of uncertainty affect each hierarchical level of the SC (Figure 2.2). Because of the interactions between the different levels of decision making, uncertainties from one level will affect decisions made in other levels. For instance, variable demands do not only alter tactical planning decisions, but also the process scheduling in the operational level (Bonfill et al., 2008). The most frequently adopted approach in the literature is the stochastic programming, which is a proactive approach where a solution with the maximum expected performance is obtained by including estimated scenarios in the model.

In the literature, it is possible to find several works related to two-stage or multi-stage stochastic formulations. In a strategic framework, Tsiakis et al. (2001) proposed a MILP model for the SC design problem under uncertainty, in order to minimize the total annualized cost of a multiproduct, multi-echelon SC network, considering different demand scenarios. The decision making included the number, location of distribution centres to be introduced and its capacity, transportation routes and production rates. Guillén-Gonsálbez et al. (2005b) proposed the multi-objective stochastic MILP model in order to optimize the SC design problem taking into account economic profit, customer satisfaction and financial risk. The decisions to be determined are number, locations and capacities of production plants and distributions centres, production rates and flows of materials. The resulting strategy combines genetic algorithms and mathematical programming tools by Guillén-Gonsálbez et al. (2006b). Also, a stochastic model was introduced by Lin and Wang (2011) in order to design a SC under supply and demand uncertainty with embedded supply chain disruption mitigation strategies.

Furthermore, there are several approaches focused on the consideration of multiple objectives. As example, You and Grossmann (2008) have extended the SC design problem in order to consider responsiveness and economic Key Performance Indicators (KPIs) as the objectives to be maximized under demand uncertainty.

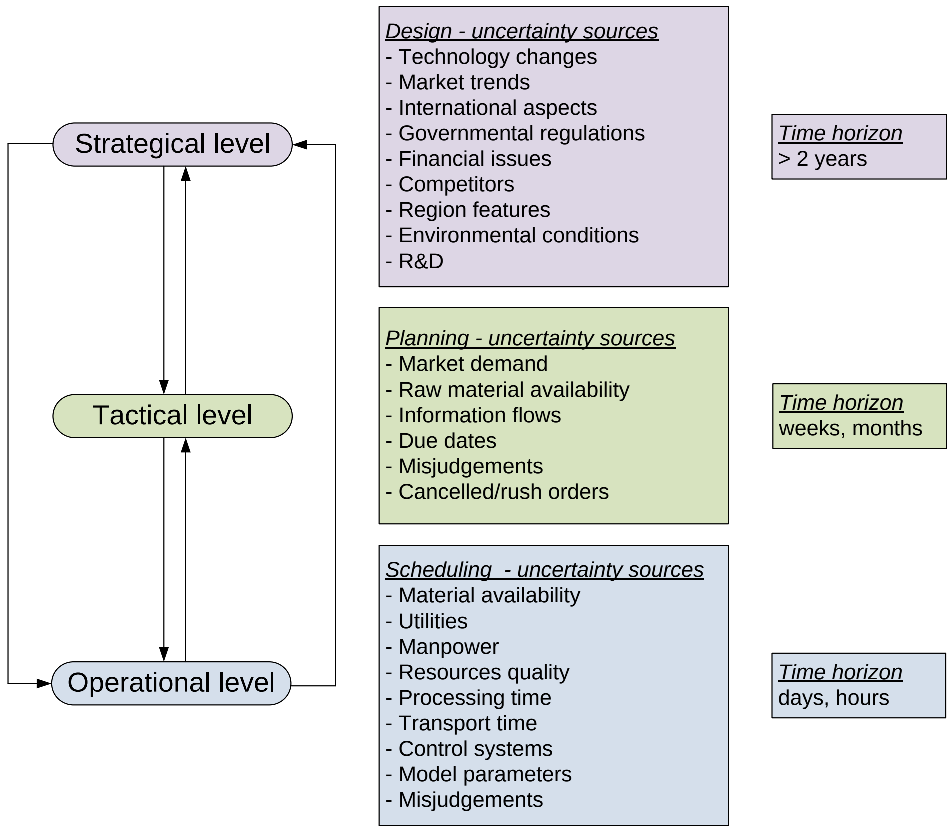

Figure 2.2. Sources of uncertainty.

In a SC planning framework, Ierapetritou and Pistikopoulos (1996) developed a two-stage stochastic formulation that includes uncertainty in model/process parameters and product demands at the design stage of multiproduct/multipurpose batch plants. Petkov and Maranas (1997) proposed a MINLP stochastic model, including uncertain product demand, for multi-period planning and scheduling of multiproduct plants. In addition, Gupta and Maranas (2000 and 2003) developed a two-stage stochastic programming approach, using the framework of multisite mid-term SC planning under demand uncertainty. In this work, the production decisions are solved using linear programming, while SC decisions are postponed to be solved posteriorly using a MINLP formulation. The main characteristic of the proposed model is the identification of optimal supply policies under low, intermediate and high demand. More recently, Rodríguez and Vecchetti (2012) developed a stochastic model to deal with the uncertain demand including the selection of price levels. Moreover, Lakkhanawat and Bagajewicz (2008) developed a stochastic programming for refinery planning which integrates pricing decisions. The two-stage stochastic program with fixed recourse considers the demand and client budget uncertainties. More recently, Felfel et al. (2015) proposed a multi-stage stochastic MILP formulation focused on a multi-product, multi-period and multi-site SC under demand uncertainty. The aim of this work was to maximize the profit. Another proactive approach is the use of game theory formulation, which is a technique for analysing situations in which there are different elements affected by the decision making process. Zamarripa et al. (2011a) developed a multi-objective MILP formulation in order to optimize the SC planning by introducing the use of game theory for decision making in cooperative and competitive scenarios. Moreover, Ryu et al. (2004) proposed a multi-parametric framework to capture conflicting interests of multiple elements in the context of SC planning problems, where operation strategies under varying demand are obtained by using parametric optimization techniques. Furthermore, Chu et al. (2015) developed a new simulation-base optimization framework for optimizing distribution inventory systems, where the objective is to minimize the storage cost.

In the SC scheduling level, Guillén-Gosálbez et al. (2006a) developed a multistage stochastic MILP optimization model to address the scheduling of SCs with embedded multipurpose batch chemical plants under demand uncertainty. Moreover, Adhitya et al. (2007a) report a heuristic based re-scheduling for refinery operations. They broke a schedule into operation blocks. Re-scheduling is performed by modifying these blocks in the original schedule using simple heuristics to generate a new schedule that is feasible for the new problem data. In a posterior work, Adhitya et al. (2007b) developed a model-based approach for rescheduling SC operations in response to disruptions. More recently, Kopanos et al. (2008) developed a MILP formulation for the rescheduling of programmed tasks, by applying a penalty cost in case of deviations from the established target, to preserve schedule stability. Also, the rolling-horizon approach has been used for scheduling problems (Kopanos and Pistikopoulos, 2014), in order to optimize the problem according to the current available information.

The majority of presented works are focused on an element of uncertainty, typically the demand uncertainty. A challenge is the study of a unified view of all the elements that create uncertainty in a SC, and its consequences in all the elements within a SC.

Previous works are related to a partial view of the SC, usually associated with the production function, which allows the incorporation of low-level decisions. However, the coordination or integration of a set of interlinked SCs has become a challenge. 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, studied by Perea-López et al. (2003) and Mestan et al. (2006). More recently, Hwarng and Xie (2008) investigated the effect of variability in a multi-level SC under the influence of several factors. 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, due to the high computational effort of the incorporation of low-level decisions data.

2.3. Integration of decision levels

Chapters 2.1 and 2.2 were focused on the study of each hierarchical level under deterministic and uncertain conditions. However, a current important challenge is the integration of the decision making process and the optimization of different decision levels within a SC (strategic, tactical and operational level), in order to ensure coherence among different decisions, usually associated to different time and economic scales. The necessity of coordinating these decision levels has led to the development of several hierarchical modelling approaches, in order to improve the decision making process.

2.3.1. Integration in deterministic conditions

Several authors enhance the importance of integrating planning and scheduling levels, due to the fact that operational plans must be in accordance with planning plans, including production, distribution and other related activities related to each enterprise or SC. The interest in integrating scheduling and planning is increasing, due to the fact that it is essential to guarantee a quick and rational respond to demand fluctuations, to optimize the existing resources, and due to economic benefits for this integration are substantial. In this context, Kallrath (2002a) provided an overview of planning and scheduling in industrial processes of batch and continuous processes. Guillén-Gonsálbez et al. (2005a) developed an integrated planning and scheduling model including financial risks. Sung and Maravelias (2007) and posteriorly Maravelias and Sung (2009) have developed a hybrid planning-scheduling optimization technique, where the optimal schedule is obtained in off-line optimization and then integrated to the planning model as a convex approximation of the production levels. More recently, Muñoz et al. (2015) presented a Lagrangian decomposition approach in an ontological framework (see Chapter 3.8.1), in order to improve information sharing and communication between all elements/partners of the overall SC.

According to the review presented by Verderame et al. (2010), future challenges could be addressed in the formulation, within the field of integrating planning and scheduling, of accurate mathematical models and, at the same time, resolvable in a manageable time, or with an appropriate computational effort, using commercial solvers.

In addition, this kind of models are usually formulated by aggregating scheduling models where the production capacity of the plant is approximated, although this method guides to the planning model overestimating the production capacity of the plant. Next steps could be addressed to formulate planning models, providing very tight upper bounds on the production capacity for different plants.

In addition, there are numerous works describing methodologies for solving simultaneously strategic and planning operations. It should be noted that, in most of developed mathematical approaches, these models are based on information of previous decision making models, typically associated to design and planning tasks, as can be found in the literature. Kallrath (2002b) described a methodology for strategic and operational planning in a multi-site production network. The objective was to optimize the total net profit of a global network, including operating modes of equipment in each time period, production and supply of products, minor changes in the infrastructure and raw material purchases. More recently, Mota el al. (2015) developed a multi-objective formulation for supply chain design and planning, introducing economic issues as well as environmental and social impacts.

Furthermore, the integration of strategic and operational levels has received recent attention. The objective of this integration is to determine the requirements to install or to invest with the detailed consideration of plant processes. In this field, Corsano et al. (2014) developed a MILP formulation to deal with the integration of these two hierarchical levels, using three solution strategies, which are a bi-level algorithm, a Lagrangian decomposition and a hybrid approach that combines the previous two methods.

It is important to mention that complex enterprises require not only the use of computer simulation, optimization and control techniques but also to automate the decision making process. Muñoz et al. (2011) presented an ontological framework for integration of all available information in a coordinated information platform to coordinate all decision making within the overall SC. Ontologies provide structures for the integration of information sources (Muñoz et al., 2010). Thus, they can be used in order to integrate different decision levels, including communication and knowledge, and helping to knowledge reuse and sharing, with the aim of increasing the efficiency of cost, time and resources (Fensel, 2010). It is worthy to mention that ontologies are considered as a tool to reduce or eliminate conceptual and terminological confusion and come to a shared understanding. The use of ontologies to integrate and organise all information will be discussed in Chapter 3.8.1.

Finally, it is remarkable the significant interest to integrate different objectives, for example financial aspects, environmental impacts, or time changeovers, among other parameters. In this point, it is worthy to mention that SCM is focused in solving the problem as a whole, providing solutions to the problem of integration and coordination of the different decisions in the different hierarchical levels. As example, Laínez et al. (2009) integrated process operations and financial issues to improve the decision making in chemical processes, developing a SC design-planning model.

According to the literature review, one important challenge is to coordinate the integration of financial, environmental, uncertainty, risks and production aspects to explore their synergistic benefits. Moreover, another open issue consist of ensuring consistency, feasibility and optimality across models that are applied over large changes in time scales.

2.3.2. Integration under uncertain conditions

The integration of different hierarchical levels within the decision making process under uncertain conditions has received attention in the last years. Regarding the integration of tactical and operational levels, Yue and You (2013) presented a stochastic MINLP formulation to tackle the presence of uncertainty in the suppliers. The main decisions to be taken include the optimal selection of production schemes, purchase amounts of raw materials, sales of final products as well as production levels.

The integration of strategic and tactical levels has been also studied. In this area, Cardoso et al. (2013) developed a stochastic MILP formulation for the design and planning of SC with reverse flows under demand uncertainty, in order to maximize the net present value. The main decisions are focused on sizing and location of production plants, distribution centres and retailers, definition of equipment units to install and inventory levels. Posteriorly, Zeballos et al. (2014) presented a stochastic MILP formulation for the integration of design and planning of a multi-period and multi-product SC under demand and supply uncertainty, considering multiple scenarios.

In the field of integration of strategic and operational levels under uncertain conditions, Lee (2014) developed a two-stage stochastic program formulation that addresses optimization of an energy supply chain in the presence of uncertainties, such as market, politics and technology changes. The case under study considers the energy production through renewable sources as well as the use of energy storage systems.

Although the integration of hierarchical levels under uncertain conditions has been studied, it is foreseen the need to dedicate further research efforts in order to extend the developed formulations to the introduction of more uncertainty sources as well as the integration of production and demand within the overall production process.

2.4. Management of production and demand

This section concerns the simultaneous management of production and demand within a supply chain. In particular, this section is focused on the energy supply chains, since the proposed formulations will be applied to a case study based on an energy network in Chapters 4 and 5. After an explanation to contextualize the necessity to manage energy supply chains, a review of the production side and the demand side management is presented.

Traditional power grids are based on centralized supply chains where large power plants generate electricity to be used posteriorly at industrial or domestic level (Wang and Singh, 2009). The optimization of the associated large-scale centralized production management problem is complicated by the need to include in the model the elements required to solve the transmission problems arising from the physical distance between the energy generation plant and the consumer, although usually, the flexibility in this classical energy supply chain is very limited, due to the need to match energy production and demand in the framework of an uncertain scenario. Furthermore, the generation of energy in centralized networks usually exploits non-renewable sources (i.e., fossil fuels), which has a negative environmental impact (i.e., climate change, pollution).

On the other hand, most of renewable energy producers (i.e., photovoltaic panels, wind turbines) have relatively less capacity but are installed in a more distributed manner at different locations, potentially near the energy consumers, which reduces energy transmission losses in comparison with traditional power grids. These infrastructures may be locally interconnected in order to achieve the higher degree of flexibility required to match generation and demand. In this sense, the resulting supply chains, known as microgrids, usually include an extensive number of measuring devices as energy meters, to obtain prompt and reliable information on energy consumptions, since the access to real-time information becomes essential to exploit the above mentioned flexibility, to improve the efficiency and reliability of the grid (reducing the incidence of adverse events, as blackouts), the proactive maintenance schedule, and finally the customer savings.

A major drawback of renewable energy systems is the apparent mismatch of the volatility of energy production from renewable sources and energy demand. This fact means that although the of renewable energy sources use represents a big opportunity (e.g., reduce the dependence from non-renewable sources), these generators have the disadvantage that the natural source can be intermittent and unpredictable, and forecast techniques are not completely reliable. Thus, the simultaneous consideration of energy production and demand is essential to manage appropriately a microgrid, in order to match energy production and demand.

The growing interest in energy microgrids has led to the development of several mathematical management models and representation schemes related to their management, as well as to their design, including the energy production management, the energy demand side management and the simultaneous management of energy production and demand.

Regarding the energy production management, different mathematical models were developed in order to minimize the operational cost of a given network. In this field, Zamarripa et al. (2011b) have developed a mathematical model to determine the production and storage levels to satisfy a deterministic energy demand, by minimizing the operational cost. More recently, a MILP model for the energy production planning related to an energy supply chain network based on a residential microgrid, which consists of a number of interconnected combined heat and power systems, under the objective of minimizing the total operational cost, has been presented by Kopanos et al. (2013). These mathematical formulations take into account energy generation constraints, such as production limits, ramping limits and minimum up and down times, which involve the presence of non-linear constraints. The aim of these approaches is to find how a given set of energy generators should satisfy a given demand in order to minimize the total operational costs. This is a very challenging optimization problem in the area of Energy Systems Engineering because of the huge number of possible combinations of the status of the generating units in the network (Bhardwaj et al., 2012). Several works were focused on the management of energy production of fixed and given demand. Carrión and Arroyo (2006) presented a discrete time MILP formulation which minimizes the energy cost of a given network. More recently, Zondervan et al. (2010) developed a Mixed Integer Non-Linear Programming (MINLP) formulation for process industries, in which the objective was to minimize the operational cost according to the availability and price of energy, by determining the optimal schedule of process tasks.

The energy demand side management of industrial process represents an emerging challenge. In this area, Della Vedova and Facchinetti (2012) developed a real-time scheduling approach to model and control the electrical availability. The aim was to reduce the presence of peaks of power consumption, which are negative for energy providers, for the grid and for the users, due to the fact that the presence of peaks reduces the grid efficiency and also because energy prices are based in peaks.

Furthermore, the management of both energy production and demand has been studied in a sequential way, by adapting the process schedule to the energy availability from an external power grid. Regarding industrial processes, Nolde and Morari (2010) have developed a continuous time MILP in order to minimize the total energy cost, by managing the energy consumption. The aim of the proposed formulation was to adapt the schedule of a steel plant, introducing a penalization for any variation from the contracted energy consumption from the plant to the energy supplier. Other works related to the simultaneous management of production and demand were focused on adapting the scheduling of the industrial process to the price of the energy in each period of time. Mitra et al. (2012) developed a discrete time MILP in order to adjust production planning according to time-dependent electricity pricing schemes for a continuous process. Also, the demand response has been studied by Hadera et al. (2014) for a steel plant, in order to reduce energy costs. Moreover, Mohsenian-Rad and León-García (2010) developed an offline residential energy consumption scheduling approach based in electricity pricing models.

But, although energy production management has been studied in the last years, the overall scheduling of a microgrid taking into account the simultaneous management of energy production and energy demand (including the possibility to shift energy consumptions) under uncertainty has not been reported and still represents an open challenge to the research community. The development of a new mathematical model to manage a microgrid can be applied to obtain the optimal schedule of energy consumptions, producing several benefits such as the reduction of energy peaks and the reduction of non-renewable energy requirements. Along this line, a discrete time MILP formulation for the integrated management of energy production and demand was developed by Silvente et al. (2012a). More recently, Silvente et al. (2015a) presented a comparison between discrete time and hybrid time MILP formulations related to a microgrid in order to maximize its profit. Also, a first MILP hybrid approach was presented by Silvente et al. (2013) with the aim of minimizing the operational cost of the overall system, and very recently Marietta et al. (2014) and Silvente et al. (2014 and 2015b) have presented a discrete time MILP formulation with flexible time windows for the allocation of energy loads into a rolling horizon framework.

2.5. Time representation

Different alternatives can be used for the time representation in a mathematical formulation, including discrete, continuous and hybrid time representations. Discrete and continuous time representations have been reviewed and discussed in several works (Floudas and Lin, 2004; Maravelias and Grossmann, 2006 and Stefansson et al., 2011).

2.5.1. Discrete time representation

The discrete time representation is based on dividing the scheduling horizon into a finite number of time intervals, forcing all activities to start/finish at the boundaries of these time intervals. Discrete time representation is widely applied in industrial processes

(Méndez et al., 2006). Although this a simplified version of the original problem, this time formulation is efficient in cases in which a reasonable number of time intervals is sufficient to represent appropriately the problem under study. The size of the mathematical model and the computational time required to solve it depend, among other factors, on the length of the time interval (i.e., the number of time intervals), and the appropriate length of the time interval depends on the characteristics of each problem, such as the duration of the events involved in the problem and the accuracy needed in the solution. Furthermore, the inappropriate length of the time interval may cause the solution to be suboptimal or even unfeasible, since the discrete formulation is an adaptation of the real times to a discrete modelling framework. This drawback can be afforded by introducing variable interval size within the discrete time formulation, in order to obtain a better approximation and to improve the accuracy of the mathematical model (Lee et al., 2001).

2.5.2. Continuous time representation

On the other hand, in continuous time formulations, variables representing the initial and final times of all tasks are really representing the exact times in which each event will take place (Harjunkoski et al., 2014), leading to decisions more accurate and sensitive to small task durations. However, the use of this formulation for large size problems becomes unaffordable in terms of computational time (Méndez et al., 2006).

2.5.3. Hybrid time representation

The limitation to solve large size problems by using the continuous time formulation and the possibility to obtain a suboptimal solution by using the discrete time formulation have led to the development of intermediate formulations between discrete and continuous time representations, classified as hybrid formulations, which combine the presence of discrete and continuous variables under the presence of time intervals. The hybrid time representation takes advantage of the flexibility of the continuous time representation and the management of events that can take place in fixed points, although this formulation requires more computational time than the discrete time formulation. Castro et al. (2012) developed a hybrid time grid sequencing model in order to determine the optimal schedule for a chemical process, incorporating the concept of general precedence instead of the use of sequence variables. Also, Neiro et al. (2014) proposed a hybrid time formulation to minimize the total cost for diesel and distribution blending and distribution scheduling, using time slots of variable length. This work proposes the combination of both discrete and continuous time representations within a new hybrid time formulation, in order to manage appropriately different elements with different time grid in the decision making process.

2.6. Management of scheduling and resources

External sources are essential in industrial processes. This section is focused on the state of the art related to the integration of utilities within the production process, especially the use of water and energy.

The interest related to minimize the use of water has led to the development of several mathematical models to manage the use of water in chemical processes. This work considers the presence of water in the chemical processes for cleaning purposes. This means that wastewater is generated during the cleaning of the equipment units involved in the process. Also, this works takes into account the direct water reuse, which considers recycle and reuse of water. Whereas the recycle is related to the use of and outlet wastewater from a processing unit in the same unit, the concept of reuse is associated to the use of an outlet wastewater from a processing unit in another processing unit (Seid and Majozi, 2014).

Gouws et al. (2010) reviewed water minimization techniques for batch processes based on graphical and mathematical techniques. The main disadvantage of using graphical techniques is that their application is limited to single contaminant cases, whereas mathematical techniques can be applied to multiple contaminant problems (Foo et al., 2005). However, first mathematical optimization-based approaches were focused on optimizing the schedule of water reuse of a single contaminant, considering fixed and variable schedules (Gouws et al., 2008). This kind of formulations usually involves the presence of non-linearities, which introduces more complexity in the decision making processes. Majozi and Gouws (2009) proposed a continuous time MINLP that was solved by linearizing the original problem to a MILP, in order to minimize the wastewater generation for single and multiple contaminants, determining simultaneously process schedule and water minimization. Posteriorly, Adekola and Gouws (2011) extended the work of Majozi and Gouws (2009) by introducing wastewater regenerator for further improvement of the use of water.

Methodologies for heat integration in batch processes can be classified into sequential and simultaneous approaches. Sequential approaches are based on determining the process schedule and posteriorly the heat integration synthesis. The main drawback of this procedure is that the solution may become suboptimal (Adonyi et al., 2003). Wang et al. (1995) developed a sequential graphical-based pinch analysis for batch processes. Foo et al. (2008) developed a sequential approach for the heat exchange network synthesis for batch processes, in order to minimize the heat exchange units involved in the process. Halim and Srinivasan (2009) proposed a sequential MILP approach using direct heat integration in batch process scheduling.

More recent works are focused on the simultaneous optimization of heat integration and process schedule. The main advantages of this methodology is that scheduling and heat integration are taken into account at the same time, which leads to a global optima. However, the complexity of this kind of problem can be unaffordable. In this field, Papageorgiou et al. (1994) developed a simultaneous approach by extended the previous work developed by Kondili et al. (1993), introducing the heat integration within the scheduling problem. Also, a discrete time MILP was formulated by Pinto et al. (2003), in order to design a multipurpose plant with direct heat integration. Posteriorly, Majozi (2006) presented a continuous time MILP approach for the simultaneous management of process schedule and heat integration, which was extended by Majozi (2009), in order to incorporate the presence of heat storage, which introduce more flexibility in the model. A recent review related to energy recovery for batch processes can be found in Fernández et al. (2012).

The simultaneous heat integration and water reuse has been usually studied separately, due to its complexity. Halim and Srinivasan (2011) presented a MINLP approach that solves sequentially the process schedule, water reuse and heat integration. Initially, the optimal production schedule is obtained, and posteriorly, the minimum water and energy necessities are determined. The main drawback of this formulation is that the solution may become suboptimal, since the problem is solved sequentially and not simultaneously.

Posteriorly, Adekola et al. (2013) developed a simultaneous MINLP approach for the management of scheduling, water reuse and heat integration of a multipurpose batch plant. The objective of this approach was to improve the profitability of the production plant by minimizing the wastewater generation and utility usage. The optimization problem was solved by the linearizing the original MINLP problem into a MILP formulation. Furthermore, Seid and Majozi (2012 and 2014) presented a MINLP approach for the simultaneous process schedule and use of water and energy, using a non-global optimizer, such as DICOPT.

2.7. Open issues

Based on the literature review, it is foreseen the need to devote further research efforts in order to solve the main troubles found on tackling the SCM problem, which constitutes future research challenges and are enumerated in the next list:

- Novel optimization strategies should emerge in order to deal with real sized problems. Therefore, methods which may improve the computational performance of the solution process and facilitate the integration function should be studied (Chapter 4).
- The integration of different hierarchical levels represents a big opportunity to solve design and operational planning problems, or strategic and operational planning problems simultaneously in one model (Chapter 7).
- Also, the integration of supply and demand represents a challenge, in order to improve the decision making process, due to the coordination of production and consumption (Chapter 4). Moreover, the integration of all resources within the production process is not fully studied (Chapter 6).
- Another major issue is the handling of internal and external uncertainty associated to industrial processes. A major challenge here is how to best formulate a stochastic optimization model that is meaningful and whose results are easy to interpret and implement.
    - ✓ The consideration of uncertainty is one of the major challenges in this research area. Several works have been exposed integrating demand uncertainty while the analysis of different sources of uncertainty (i.e., resource variability) still remains open. The majority of previous works study product demand and prices. However, the uncertainty associated to suppliers' performance, production processes and financial markets has not been studied enough. Regarding inclusion of third actors involving the SC decision making should be subjected to important improvements focusing on the systematic consideration. It is a fact that the SC of interest should face a global market (Chapter 7).
    - ✓ One of the main considerations to be studied is the development of the dynamics of the SC for enhanced production. In this context, it is important to research and implement dynamic models, incorporating low-level decisions, and the implications of this incorporation for the dynamics of the entire SC (Chapter 8).
- Integration of all data and information associated to an industrial process within a coordinated information technology platform to improve and automate the decision making process:
    - ✓ One important area to be researched is the real time monitoring and diagnosis in integrated SCM to timely provide and update the SC state information needed by the different decision making hierarchical levels, through a data

communication platform. This fact will contribute to improve the efficiency of SC planning (Chapter 8).

- ✓ In order to achieve the integration among the different decision levels through a SC, it is essential the coordination of a common modelling system using, in this particular case, an ontological framework (Chapter 8).

Chapter 3. Methods and tools

3.1. Optimization

The optimization of a chemical process consists in selecting, among all possible alternatives, the most favourable alternative, fulfilling several objectives. Optimization can be applied to numerous areas, including production facilities, processes, transportation, management, and human resources (Edgar et al., 2001). For example, optimization techniques could be used in order to improve profit or production and also to decrease operational costs, energy consumption or generation of pollutants.

In order to perform an optimization, it is first required to identify Key Performance Indicators (KPIs) to build an objective function, which is a measure that indicates the fitness of a particular decision. Different measures of the quality of the solution can be used for optimization problems. Thus, each feasible solution of the problem is any choice of decision variables that satisfies the set of constraints. Moreover, the optimal solution is a feasible solution that optimizes the objective function (Biegler et al., 1997).

The selection of the optimization goal directly affects the quality of the solution as well as the model computational performance. Typical objective functions include the optimization of profit, costs, revenues, makespan, weighted lateness, production costs, inventory costs, social impact or environmental impact. Notice that some objective functions can be very hard to implement for some event representations, requiring additional variables and complex constraints. Moreover, the optimization procedure can take into account one objective, or the consideration of multiple criteria in the decision making process.

The basic steps to execute an optimization process are:

- Analyse all available information.
- Identify an objective function.
- Identify the decision variables.
- Formulate a mathematical model.

3.2. Mathematical models

A mathematical model is a representation or approximation of the reality that allows predicting the behaviour of a system based on the variables of the system. This mathematical model usually includes:

- Balances, including not only mass and energy balances, but also momentum, integral/differential and dynamic/stationary state, and other relevant information.
- Constitutive equations, like chemical properties, transport speed, thermodynamic relations and kinetic expressions.
- Other equations, such as design specifications, incomes and costs, functional relationships and boundary conditions.

The formulation of a mathematical model generally involves discrete and continuous variables. The general formulation of an optimization problem has the following form (Grossmann et al., 2000):

$$\left.\begin{array}{ll} min\ or\ max\ f(x) & \text{Objective function} \\ subject\ to & \\ h(x) = 0 & \text{Equality constraints (e.g. process equations)} \\ g(x) \leq 0 & \text{Inequality constraints (e.g. specifications)} \\ x = (x_1, x_2, \dots, x_n)^T \in \mathbb{R}^n & \text{Decision variables} \end{array}\right\} \quad (3.1)$$

According to this formulation, $f(x)$, $h(x)$ and $g(x)$ are scalar functions of vector x. The function $f(x)$ corresponds to the objective function (to be minimized or maximized), and represents the quantitative measue of the performance of the system under study. The components of vector x are the decision variables, which can be both continuous and discrete variables. The values of these variables are determined in the optimization procedure. Additionally, the mathematical formulation can include different constraints, which represents all restrictions that the decision variables must satisfy. Particularly, $h(x)$ are constraints of equalities, whereas $g(x)$ represents the inequalities of the model. According to the characteristics of the model, the mathematical problem is classified into:

- Linear: if vector x is continuous and the functions $f(x)$, $h(x)$ and $g(x)$ are linear.
- Non-linear: if vector x is continuous and at least one of the functions $f(x)$, $h(x)$ or $g(x)$ is non-linear.
- Mixed integer linear: if vector x requires at least some of the x_i elements to be integer (or binary) and the functions $f(x)$, $h(x)$ and $g(x)$ are linear.
- Mixed integer non-linear: if vector x requires at least some of the x_i elements to be integer (or binary) and at least one of the functions $f(x)$, $h(x)$ or $g(x)$ is non-linear.

Furthermore, mathematical models can be classified in dynamic or static models, depending on whether the variable values change over time or not.

3.2.1. Optimality criteria

A point x which satisfies all the constraints is called a feasible point and therefore is a feasible solution to the problem. The set of all feasible points is called the feasible region. A point x^* is called a strong local maximum of the optimization problem if $f(x)$ is defined in a δ-neighbourhood $N(x^*, \delta)$ and satisfies $f(x^*) > f(u)$ for $\forall u \in N(x^*, \delta)$ where $\delta > 0$ and $u \neq x^*$. If x^* is not a strong local maximum, the inclusion of equality in the condition $f(x^*) \geq f(u)$ for $\forall u \in N(x^*, \delta)$ defines the point x^* as a weak local maximum (see Figure 3.1). The local minima can be defined in the similar manner when $f(x^*) > f(u)$ and $f(x^*) \geq f(u)$ are replaced by $f(x^*) < f(u)$ and $f(x^*) \leq f(u)$, respectively. Figure 3.1 illustrates several local maxima and minima. Point A is a strong local maximum, and point B is a weak local maximum since there exist many different values of x which will lead to the same value of $f(x^*)$. Finally, point C is a global maximum.

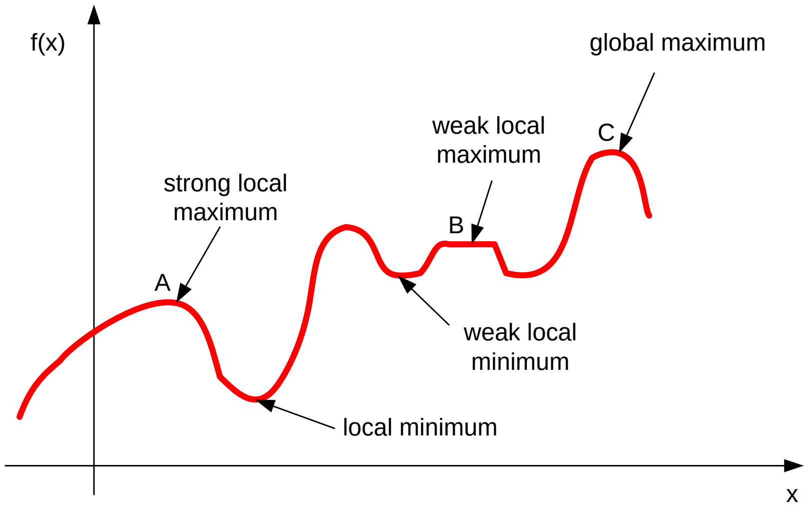

Figure 3.1. Illustrative example for strong and weak maxima and minima.

3.2.2. Convexity

Let ϑ be a set in a real or complex vector space. Set ϑ is convex if, for every pair of points x and y belonging within the set, every point on the straight line segment that connects them is also within the set ϑ, as illustrated in Figure 3.2. This definition is can be mathematically expressed as:

$$\vartheta \; is \; convex \iff \forall(x,y) \in \vartheta \wedge \theta \in \{0,1\}, [(1-\theta)\cdot x + \theta \cdot y] \in \vartheta \quad (3.2)$$

A function $f(x)$ is convex if its epigraph (i.e., the set of points lying on or above its graph) is a convex set, as shown in Figure 3.3. Convexity plays a significant role in mathematical programming due to the following Theorem 3.1:

Theorem 3.1. If a mathematical program is convex then any local (i.e., relative) minimum represents a global minimum.

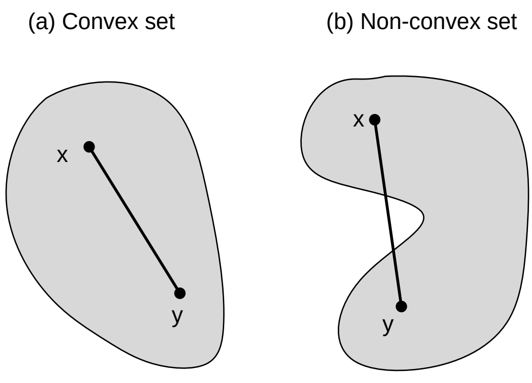

Figure 3.2. Graphical representation of convexity.

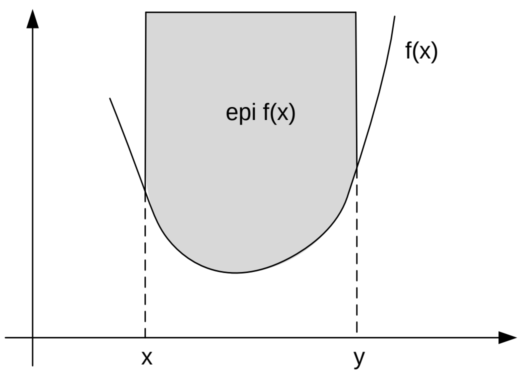

Figure 3.3. Graphical representation of a convex function.

The research subfield that deals with non-convex programs is referred to as global optimization, which aims finding the globally best solution of models in the potential presence of multiple local optima.

3.2.3. Duality

Duality is one of the most fundamental concepts in mathematical programming and establishes a connection between two symmetric programs, namely, the primal and dual problem. Duality is a powerful and widely employed tool in applied mathematics because:

- The dual program is always convex even if the primal is not.
- The number of variables in the dual is equal to the number of constraints in the primal which is often less than the number of variables in the primal program.
- The maximum value achieved by the dual problem is often equal to the minimum of the primal.

Although dual problem usually refers to the Lagrangian dual problem, other dual problems are used, such as the Wolfe dual problem and the Fenchel dual problem. Notice that this section is focused in the Lagrangian dual problem. The dual function is introduced as:

$$\xi(\lambda,\mu) = \ Infimum_x\{f(x) + \lambda^T h(x) + \mu^T g(x)\} \tag{3.3}$$

Then, the dual problem of the primal problem is defined as follows:

$$\begin{aligned} &\min_{\lambda,\mu} \xi(\lambda,\mu) \\ &\mu \geq 0 \end{aligned} \tag{3.4}$$

Hence, using the Lagrangian function, the dual problem can also be rewritten as:

$$\begin{aligned} &\max_{\lambda,\mu}\{Infimum_x\ \mathcal{L}(x,\lambda,\mu)\} \\ &\mu \geq 0 \end{aligned} \tag{3.5}$$

where vectors λ and μ are called Lagrangian multipliers, and the Lagrangian function is defined by:

$$\mathcal{L}(x,\lambda,\mu) = f(x) + \lambda^T \cdot h(x) + \mu^T \cdot g(x) \tag{3.6}$$

Theorem 3.2 establishes an important relationship between the dual and primal problems.

Theorem 3.2 (weak duality). For any feasible solution x of the primal problem (3.1) and for any feasible solution (λ, μ) of the dual problem, the following holds

$$f(x) \geq \xi(\lambda, \mu) \quad (3.7)$$

In addition, Theorem 3.3 is of relevant importance in mathematical programming. It shows that for convex programs the primal problem solution can be obtained by solving the dual problem.

Theorem 3.3. If the primal problem is convex, then $f(x^*) = \xi(\lambda^*, \mu^x)$. Otherwise, one or both of the two sets of feasible solutions is empty.

Note that x^* represents the optimal solution of the primal problem, and (λ^*, μ^x) are the optimal solutions of the dual problem.

$$f(x) \geq \xi(\lambda, \mu) \quad (3.8)$$

In non-convex programs, there is a difference between the optimal objective function values of the dual and primal problems $\left(\xi(\lambda^*, \mu^x) - f(x^*)\right)$ which is called duality gap. In convex programs duality gap is zero. According to Conejo et al. (2002), for nonconvex programs of engineering applications, the duality gap is usually relatively small.

With regard to the Lagrangean function, the Karush, Kuhn and Tucker conditions (KKT conditions, also known as the Kuhn-Tucker conditions) have been one of the most important theoretical results in optimization, since they establish the first order necessary conditions for a solution in a non-linear constrained programming to be optimal. The KKT optimality conditions for a constrained minimum (where vectors λ and μ are the Lagrangian multipliers) are:

- Lagrangean conditions:

$$\nabla L(x^*, \lambda, \mu) = \nabla f(x^*) + \nabla h(x^*)\lambda + \nabla g(x^*)\mu \quad (3.9)$$

- Complementary conditions:

$$\begin{aligned} &\mu^T g(x^*) = 0 \\ &\mu \geq 0 \end{aligned} \quad (3.10)$$

- Feasibility conditions:

$$\begin{aligned} &g(x^*) \leq 0 \\ &h(x^*) = 0 \end{aligned} \quad (3.11)$$

Theorem 3.4. If $f(x)$ is convex and feasible region is convex, then if there exists a local minimum at x^*,

- x^* is a global minimum.
- The KKT conditions are both necessary and sufficient.

3.3. Optimization techniques

The solution technique to solve an optimization problem depends on the characteristics of each problem. Grossmann and Biegler (2004) summarize the application areas in PSE of different optimization methods. Thus, there have been several contributions to review optimization methods in general and in the area of PSE (Kallrath, 2002a; Biegler and Grossmann, 2004; Kallrath, 2005; Méndez et al., 2006; Li and Ierapetritou, 2007; Barbosa-Povoa, 2007).

The application of mathematical programming approaches implies the development of a mathematical framework and the use of an optimization algorithm. Although this thesis has been focused on solution approaches based on mathematical programming techniques (which include both continuous and mixed integer optimization), it is important to note that there are other solution methods for dealing with optimization problems, such as logic-based optimization (e.g., constraint programming), heuristics, meta-heuristics, artificial intelligence and hybrid methods, among other techniques. Moreover, if the optimization procedure involves the presence of more than one objective, multi-criteria optimization can be applied.

3.3.1. Continuous optimization

Continuous optimization is used in order to solve linear and nonlinear problems. The most common methods to solve linear programming (LP) are simplex and interior points. This kind of optimization is used in order to solve linear problems involving only continuous variables and linear constrains and objective function.

In addition, the introduction of any nonlinearity in any equality and inequality constraint or in the objective function transform the LP into a non-linear programming (NLP). The most common algorithms designed for NLP optimization include Newton-Raphon methods, conjugate gradient methods or quasi-Newton methods (Biegler, 2010). For the specific case of quadratic optimization problems, the most useful algorithm is the successive quadratic programming (Alkaya, 2001).

3.3.1.1. Linear programming

LP is a technique used to optimize a linear objective function subject to the presence of linear equality and/or linear inequality constraints. Given a polytope and a real-valued affine function defined on this polytope, a LP method will find a point on the polytope where this function has the optimal value if such point exists, by searching through the polytope vertices. The feasible region of the problem corresponds to the intersection of the hyperplanes and halfspaces of the constraints (Figure 3.4). This is a basic characteristic of a convex polytope.

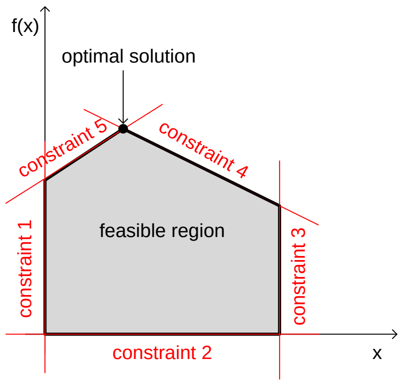

Figure 3.4. Linear programming scheme.

LP problems can be mathematically expressed as follows:

$$\begin{aligned} &max\ f(x) = c^T x \\ &subject\ to \\ &Ax \leq b \\ &x \geq 0 \end{aligned} \tag{3.12}$$

In this mathematical formulation, x represents the vector of decision variables to be taken, whereas c and b are vectors of known coefficients and A is a matrix of known coefficients (i.e., input parameters). The expression to be optimized $f(x)$, is called the objective function. The expression $Ax \leq b$ includes the constraints which identify a convex polytope in which the objective function must be optimized.

LP and the algorithms proposed for solving this kind of problems, such as the simplex method and interior point methods, are based on Theorem 3.5:

Theorem 3.5. If an LP has an optimal solution; there is a vertex of the feasible polytope that is optimal.

3.3.1.1.1. The simplex method

The simplex method is the most used algorithm for solving LP problems. This methodology was first developed by Dantzig (1963), and posteriorly extended by Dantzig and Orchard-Hays. The simplex method algorithm is based in solving linear programs by moving along the boundaries from one vertex of the feasible region to the next.

The algorithm starts with an initial vertex basic feasible solution and tests its optimality. The algorithm terminates, if some optimality condition is verified, otherwise, the algorithm identifies an adjacent vertex, with a better objective value, in which the optimality of this new solution is tested again, and the entire scheme is repeated, until an optimal vertex is finally found (Figure 3.5). It is conditional that the simplex method starts from some initial extreme point, and follows a path along the edges of the feasible region towards an optimal extreme point, such that all the intermediate extreme points visited are not worsening the objective function.

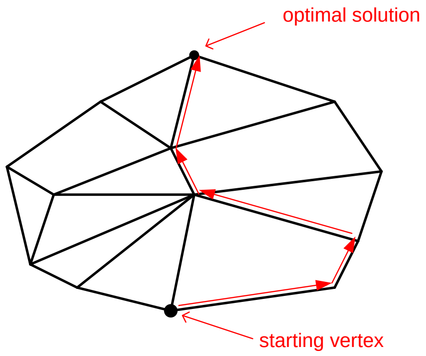

Figure 3.5. Graphical interpretation of the simplex method.

3.3.1.1.2. Interior-points methods

An interior-point algorithm is based on improving a feasible interior solution point of the linear program by steps through the interior feasible region (Wright, 1997). A theoretical breakthrough for interior point methods came in 1979, when L.G. Khachian discovered an ellipsoid algorithm whose running time in its worst case was significantly lower than that of the simplex algorithm. Other theoretical results quickly followed, notably that of N. Karmarkar who discovered an interior-point algorithm whose running time performance in its worst case was significantly lower than that of Kachiyan's (Dantzig and Thapa, 1997 and 2003). While the simplex method looks at the vertex of the feasible region, the interior point methods assume an initial feasible interior point and moves through the feasible region moving in one direction. The stopping rule typically followed is to finish with an approximate optimal solution when the difference between two iterations is sufficiently small in the original space (Figure 3.6).

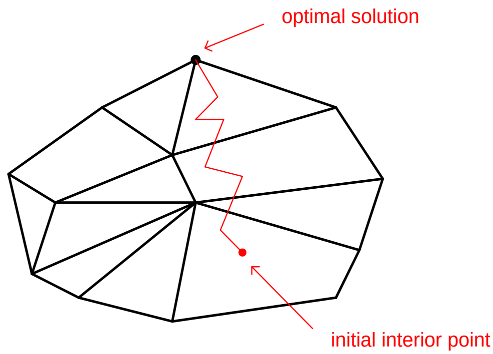

Figure 3.6. Graphical interpretation of the initial interior point.

3.3.1.2. Non-linear programming

NLP corresponds to mathematical models in which all variables are defined as continuous and contains any nonlinearity in the objective function and/or the constraints. Unconstrained and constrained optimization algorithms have been developed to solve this kind of programs.

3.3.1.2.1. Unconstrained optimization

Unconstrained optimization can be mathematically represented as follows:

$$\begin{aligned} &\min f(x) \\ &x = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n \end{aligned} \qquad (3.13)$$

The objective function $f(x)$ is a non-linear function. Algorithms to solve unconstrained non-linear problems can be classified into direct and indirect methods. On the one hand, direct methods do not require the use of derivatives and rely solely on function evaluation. The main advantage of these methods is the simplicity to understand and to execute, whereas the disadvantage is that they are inefficient and not robust enough. This methodology is useful for simple two-variable problems. Some direct methods are random search, grid search, univariate search, conjugate search direction and Powell's method.

On the other hand, indirect methods use derivatives in determining the search solution to move towards and improves solution for optimization. These methods can be classified into:

- First-order indirect methods, which use first derivatives (i.e., steepest descent).
- Second-order indirect methods, which also use second derivatives (i.e., Newton method).

The steepest descent (or gradient) methods is based in the idea in which the gradient of a function $f(x)$ is a vector at a point x that gives the local direction of the greatest increase in $f(x)$ and is orthogonal to the contour of $f(x)$ at x. First of all, it is necessary to establish an initial feasible point x_0. Thereafter at point x_k. In steepest descent, at k-th iteration, the transition from point x_k to another point x_{k+1} can be calculated according to this expression:

$$x_{k+1} = x_k - \lambda_k \nabla f(x_k) \tag{3.14}$$

Where λ_k is a scalar that determines the step length in the direction of steepest descent $\nabla f(x_k)$. Notice that the negative of the gradient gives the direction for minization, not the magnitude, which depends on the choice of λ_k. This procedure must be interatively repeated until the difference between $f(x_{k+1})$ and $f(x_k)$ will be smaller than some tolerance. Termination can occur at any type of stationary point; (i.e., a point where the elements of the gradient are zero) either a local minimum or a saddle point. If a saddle point is obtained, to move away employ a non gradient method, then the minimization may continue as before. Also, this methodology is very scale dependent, and the convergence of this method can be very slow.

Newton's method is based on the idea in which the necessary conditions for stationary point x^* is $\nabla f(x^*) = 0$. This methodology involves the use of the Jacobian matrix of the system. Here, the Jacobian of the above system is the Hessian matrix. Note also, that the Hessian is positive definite at the solution. In this case:

$$x_{k+1} = x_k - \Delta x_k = x_k - [\mathrm{H}(x_k)]^{-1} \nabla f(x_k) \tag{3.15}$$

Then, finish the iteration procedure according to a desired tolerance. This methodology involves quadratic convergence. If an approximated matrix $\overline{H}$ is used instead of Hessian Matrix H, the method is called Quasi-Newton method, and involves superlinear convergence.

Finally, notice that all methods can be reviewed as evolving from Newton's method $H(x_k)\Delta x_k = -\nabla f(x_k)$:

- If H is used, the model corresponds to the Newton method.
- If $H^{-1} = H$, the model is the steepest descent.
- If H is modified, the model is based on the Quasi-Newton method.

3.3.1.2.2. Constrained optimization

Methods to solve constrained programs are methods seeks an approximate solution by replacing the original constrained problem by a sequence of unconstrained sub-problems. Constrained non-linear problems can be represented as follows:

$$\begin{aligned} &\min f(x) \\ &subject\ to \\ &h(x) = 0 \\ &g(x) \leq 0 \\ &x = (x_1, x_2, \dots, x_n)^T \in \mathbb{R}^n \end{aligned} \tag{3.16}$$

Hence, the underlying idea is to construct a closely related, unconstrained problem and apply the algorithms proposed for the unconstrained optimization problems. The main methods to solve constrained non-linear problems are Lagrange multipliers method and Kunh-Tucker optimality conditions.

Lagrange multipliers methodology is used for equality constrained problems, and based on the Theorem 3.6.

Theorem 3.6. Given a non-linear objective function $f(x)$ subject to a set of equality constraint $h(x)$, if $f(x)$ has a constrained extremum at x^*, such that $h_i(x^*) = 0$, $i = 1, \dots, m$, then the gradients of $\nabla f(x^*)$ and $\nabla h_i(x^*)$ are linearly dependent:

$$\begin{aligned} &\nabla f(x^*) + \sum_{i=1}^{m} \lambda_i h_i(x^*) = 0 \\ &h_i(x) = 0 \\ &i = 1, \dots, m \end{aligned} \tag{3.17}$$

Hence, let define the Lagrangian function $L(x, \lambda)$ as follows:

$$L(x, \lambda) = f(x) + \sum_{i=1}^{m} \lambda_i h_i(x^*) \tag{3.18}$$

Consider the stationary conditions of this function, $\nabla L(x, \lambda) = 0$, or:

$$\frac{\partial L}{\partial x} = 0 \Rightarrow \quad \nabla f(x^*) + \sum_{i=1}^{m} \lambda_i h_i(x^*) = 0$$
$$\frac{\partial L}{\partial \lambda_i} = 0 \Rightarrow \quad h_i(x) = 0 \tag{3.19}$$

These conditions are exactly the necessary optimality conditions for the non-linear equality constrained problem. Therefore, the Langrangian function $L(x,\lambda)$ has a stationary point at the minimum of the constrained problem. Notice that λ_i is called the Lagrange multiplier for constant i.

KKT optimality conditions are used when the mathematical formulation includes inequality constraints. In this case, active inequality constraints are treated just like equality constraints with the additional restriction that their Lagrange multipliers must be non-negative. The Lagrange conditions are:

$$\frac{\partial f(x)}{\partial x_j} + \sum_{i=1}^{m} \lambda_i \frac{\partial h_i(x)}{\partial x_j} + \sum_{i=1}^{p} \mu_i \frac{\partial g_i(x)}{\partial x_j} = 0$$
$$j = 1, \dots, n \tag{3.20}$$
$$\mu_i \geq 0$$

Thus, the KKT optimality conditions for a constrained minimum are (see Chapter 3.2.3):

$$\nabla L(x^*, \lambda, \mu) = \nabla f(x^*) + \nabla g(x^*)\lambda + \nabla g(x^*)\mu$$
$$\mu^T g(x^*) = 0$$
$$\mu \geq 0 \tag{3.21}$$
$$g(x^*) \leq 0$$
$$h(x^*) = 0$$

3.3.2. Mixed integer optimization

Discrete optimization or mixed-integer optimization offers a powerful framework for mathematically modelling many optimization problems that include discrete/integer and continuous variables. This kind of optimization is commonly used in process system engineering in order to model discrete decision, such as selection of units in a flowsheet or sequences in scheduling and batch size (Grossmann, 2002). The majority of discrete variables are restricted to the two values 0 and 1 (binary variables), which represents yes/no decisions.

In this context, Mixed Integer Linear Programming (MILP) problems are LP problems which also include integer and/or binary variables. MILP is one of the most extensively explored methods for process scheduling problems due to its rigorousness, flexibility and extensive modelling capability. In a scheduling framework, MILP methods are applied in order to solve from the simplest stage single-unit multiproduct process to the most general multipurpose processes (Floudas and Lin, 2005).

On the other hand, Mixed Integer Non-Linear Programming (MINLP) problems are MILP problems that incorporate nonlinearities in the objective function or in any of the constraints involved. MINLP are widely applied in synthesis and design problems, and in planning and scheduling problems.

A general Mixed Integer Programming (MIP) problem can be expressed as follows:

$$\begin{aligned}
&\min f(x,y) = c^T x + hy \\
&subject\ to \\
&Ax + Gy \leq b \\
&x \geq 0 \\
&x = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^n \\
&y \in \{0,1\}
\end{aligned} \tag{3.22}$$

According to this formulation, $f(x,y)$ represents the objective function, x corresponds to the vector of positive decision variables, y represents the vector of binary variables, c and b are vectors of known coefficients, and A and G are matrices of known coefficients.

Several algorithms have been developed to solve MIP problems. The main methodologies include the branch-and-bound, the cutting-plane, and the branch-and-cut methods. A brief explanation of those methods are next described. Also, disjunctive programs can be applied to solve this kind of problems (Raman and Grossmann, 1994; Lee and Grossmann, 2000). Finally, decomposition techniques can be applied for solving MINLP problems, including the outer-approximation algorithm (Duran and Grossmann, 1986) and the Generalized Benders Decomposition (Biegler and Grossmann, 2004).

3.3.2.1. Branch-and-bound methods

The branch-and-bound method is the basic workhorse technique for solving integer and discrete programming problems. The main idea of branch-and-bound was introduced by Land and Doig (1960), and actually is based on the observation that the enumeration of integer solutions has a tree structure. More specifically, the solution of a problem with a branch-and-bound algorithm is described as a search through a tree (Figure 3.7), wherein the root node corresponds to the relaxed original problem, and each other node corresponds to a subproblem of the original problem. In MIP problems, the branch-and-bound algorithm only branches on the integer variables, therefore the discussion can be restricted to a purely integer problem without loss of generality.

This algorithm consists in generating a sequence of continuous sub-problems, solving them, and analysing and comparing the different solutions until the optimal solution is reached. The algorithm searches the complete space of solutions. The use of bounds for the function to be optimized combined with the value of the current best solution enables the algorithm to implicitly search parts of the solution space.

The main idea in branch-and-bound method is to avoid growing the whole tree as much as possible, because the entire tree is just too big in any real problem. Instead branch-and-bound grows the tree in stages, and grows only the most promising nodes (i.e., partial or complete solutions) at any stage. It determines which node is the most promising by estimating a bound on the best value of the objective function that can be obtained by growing that node to later stages. The name of the method comes from the branching that happens when a bud node (i.e., partial solution, either feasible or infeasible) is selected for further growth and the next generation of children of that node is created. The bounding comes in when the bound on the best value attained by growing a node is estimated. Hope-fully, in the end branch-and-bound will have grown only a very small fraction of the full enumeration tree.

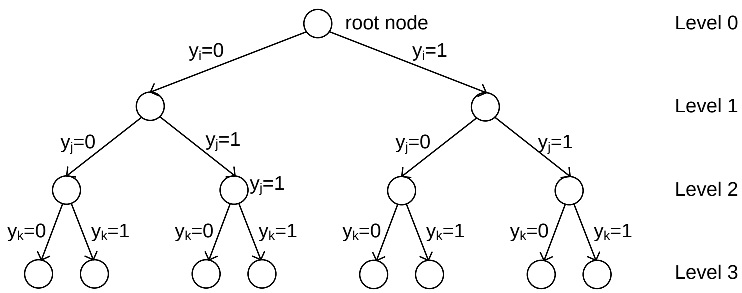

Figure 3.7. An illustrative example of branch-and-bound enumeration tree.

The reduction of the amount of branches can be achieve by following these steps:

- A branch can be eliminated if it can be shown to contain no integer feasible solutions with a better value than the incumbent solution.

- A lower bound for the integer solutions, on any branch, is always the relaxed LP solution for the minimization problem, which ignores the integer requirements.

The end nodes establishes the upper bound for the integer solutions. The optimal (minimum) solution is given by the minimum of the upper bounds. The algorithm terminates when the incumbent solution's objective function value is better than or equal to the bounding function value associated with all of the bud nodes. This means that none of the bud nodes could possibly develop into a better solution than the complete feasible solution already have in hand, so there is no point in expanding the tree any further. All bud nodes in this condition will already have been eliminated, so this terminating rule amounts to saying that branch-and-bound stops when there are no more bud nodes left to consider for further growth. This also proves that the incumbent solution is optimum.

3.3.2.2. Cutting-plane methods

There is an alternative to branch-and-bound methods called cutting planes which can be used to solve mixed integer programs. This methodology was introduced by R.E. Gomory at the end of 1950s. The main idea of cutting-plane methods is to alter the convex set of solutions to the related continuous LP problem (i.e., the LP problem that results by dropping the integer constraints) so that the optimal extreme point to the changed continuous problem is integer-valued. This is accomplished by systematically introducing additional constraints (called cutting planes) that cut off parts of the convex set that do not contain any feasible integer points and solving the resultant problems by the simplex algorithm. Note that an adding cut or constraint to a current fractional solution must assure that every feasible integer solution of the actual program is feasible for the cut, and the current fractional solution is not feasible for the cut. Some techniques to generate these cuts are the Gomory cut methods, the Kelleys method, and the Kelley, Cheney, Goldstein method.

Although initially this methodology was considered as instable and ineffective, it can be effective in combination with branch-and-cut methods and ways to overcome numerical instabilities. Nowadays, all commercial MIP solvers use Gomory cuts in one way or another.

3.3.2.3. Branch-and-cut methods

Branch-and-cut method is a hybrid methods that combines branch-and-bound and cutting-plane methods. The method solves the LP without the integer constraint using the regular simplex algorithm. When an optimal solution is obtained, and this solution has a non-integer value for a variable that is supposed to be integer, a cutting-plane algorithm is used to find further linear constraints which are satisfied by all feasible integer points but violated by the current fractional solution. If such an inequality is found, it is added to the LP, such that resolving it will yield a different solution which is hopefully "less fractional". This process is repeated until either an integer solution is found (which is then known to be optimal) or until no more cutting planes are found.

At this point, the branch-and-bound part of the algorithm begins. The problem is split into two versions, one with the additional constraint that the variable is greater than or equal to the next integer greater than the intermediate result, and another where this variable is less than or equal to the next lesser integer. In this way, new variables are introduced in the basis according to the number of basic variables that are non-integers in the intermediate solution but which are integers according to the original constraints. The new LPs are then solved using the simplex method and the process repeats until a solution satisfying all the integer constraints is found. During the branch-and-bound process, further cutting planes can be separated, which may be either global cuts (i.e., valid for all feasible integer solutions) or local cuts (i.e., satisfied by all solutions fulfilling the side constraints from the currently considered branch-and-bound subtree).

3.3.3. Logic-based optimization techniques

The difficulties to model and to scale mixed integer problems has led to the development of logic-based techniques. The motivations for these logic-based modelling has been to facilitate the modelling, reduce the combinatorial search effort, and improve the handling the non-linearities. A general review of logic-based optimization can be found in Hooker (2000). The most typical logic-based optimization techniques are:

- Generalized Disjunctive Programming (Raman and Grossmann, 1994).
- Mixed Logic Linear Programming (Hooker and Osorio, 1999).
- Constraint Programming.

3.3.3.1. Constraint programming

Constraint programming (CP) is a logic-based approach to discrete and continuous problem solving. It has proved to be successful in several applications, particularly in scheduling problems. The solution of CP models is based on performing constraint propagation at each node by reducing the domains of discrete or continuous variables. Whenever a solution is found, or when a domain of a variable is reduced, new constraints are added. This search finishes when no further nodes must be tested (Kotecha et al., 2010).

Constraint programming is a programming paradigm that was originally developed to solve feasibility problems (Van Hentenryck, 1989 and 2002), but it has been extended to solve optimization problems, particularly scheduling problems. Constraint programming is very expressive since continuous, integer, and Boolean variables are permitted; moreover, variables can be indexed by other variables.

Furthermore, a number of constructs and global constraints have also been developed to efficiently model and solve specific problems, and constraints need neither be linear nor convex. The solution of constraint programming models is based on performing constraint propagation at each node by reducing the domains of the variables. If an empty domain is found the node is pruned. Branching is performed whenever a domain of an integer, binary or Boolean variable has more than one element, or when the bounds of the domain of a continuous variable do not lie within a tolerance. Whenever a solution is found, or a domain of a variable is reduced, new constraints are added. The search terminates when no further nodes must be examined. The effectiveness of constraint programming depends on the propagation mechanism behind constraints. Thus, even though many constructs and constraints are available, not all of them have efficient propagation mechanisms.

For some problems, such as scheduling, propagation mechanisms have been proven to be very effective in solving certain types of scheduling problems, especially those that involve sequencing and resource constraints. However, they are not always effective for solving more general optimal scheduling problems that involve assignments (Méndez et al., 2006).

Some of the most common propagation rules for scheduling are the "timetable" constraint (Le Pape, 1998), the "disjunctive constraint" propagation, the "edge-finding", and the "not-first, not-last" (Baptiste et al., 2001). Finally, Laborie (2003) summarized the main approaches to propagate resource constraints in constraint-based scheduling and identified some of their limitations for using them in an integrated planning and scheduling framework.

3.3.4. Heuristics methods

Heuristics methods are rules or algorithms used in order to obtain good feasible solutions of a given problem, although they do not guarantee optimality. In the area of the short-term planning, these rules use certain empirical criteria to prioritize all the batches that are waiting for processing on a unit. This methodology has demonstrated to have very good performance, although their efficiency is usually evaluated empirically and their applicability is usually very case specific. The main advantage of heuristics is that fact that are considered fast and easy to implement. However, the use of heuristics methods is reduced to limited scheduling problems, because optimality can be proved only in some special cases since these methods cannot guarantee the quality of the solution.

In this field, Lagrangian heuristics consist in iterative methods that try to build feasible solutions from the solution provided by the Lagrangian relaxation of an optimization problem. This process is usually repeated until the gap between the best upper bound and the best lower bound stands below a certain value. The Lagrangian relaxation consists in a relaxation method which converts a constrained optimization problem into a simpler one. The relaxed problem can be usually solved more easily in comparison with the original problem. This method applies penalties in the objective function in case of violation of any constraint, by using Lagrange multipliers (see Chapter 3.2.3). The obtained solution for the relaxed problem will be an approximate solution of the original one, providing useful information to obtain the solution of the original problem.

3.3.5. Metaheuristics methods

Metaheuristics are often inspired by moves arising in natural phenomena. Metaheuristics optimize a problem by iteratively trying to improve a candidate solution with regard to a given measure of quality. This techniques is based on an iterative generation process which guides a subordinate heuristic by combining intelligently different concepts for exploring and exploiting the search space (Blum and Roli, 2003).

While metaheuristics have proved to be very effective in combinatorial problems, their optimality and convergence are not certified; there is no systematic procedure for obtaining good bounds on the attainable optimum values of the objective function (Pekny & Reklaitis, 1998). This means that the use of meta-heuristics do not provide any guarantee on the quality of the solution obtained, and it is often impossible to tell how far the current solution is from optimality. Furthermore, these methods do not formulate the problem as a mathematical program, since they involve procedural search techniques that in turn require some type of discretization or graph representation, and the violation of constraints is handled through ad hoc penalty functions. For this reason, the use of metaheuristics might be problematic for problems involving general processes, complex inequality constraints and continuous decision variables. In this case, the set of feasible solutions might lack nice properties and it might even be difficult to find a feasible solution (Burkard et al., 1998).

Significant research in this field is devoted to incorporate meta-heuristics within mathematical programming techniques. Some of the meta-heuristics methods are genetic algorithms, simulated annealing, tabu search, scatter search and ants colony.

3.3.5.1. Genetic algorithms

Genetic algorithms (GA) are computational models inspired by biological evolution process. These algorithms determine the solution of a problem on a simple chromosome-like data structure and apply recombination, selection and mutation operators to these structures so as to preserve critical information. GAs have increasingly been applied in engineering in the past decade, typically to discrete optimization, since it is considered as a tool for optimization in engineering design. Although these algorithms are not sensitive to local minima, which confers robustness, these methods do not calculate the exact solution of the problem, but make good estimations of the optimal solution.

The genetic algorithm is based on the analogy of improving a population of solutions through modifying their gene pool. Two forms of genetic modification, crossover or mutation, are used and the elements of the optimization vector are represented as binary strings. Crossover deals with random swapping of vector elements (among parents with highest objective function values or other rankings of population) or any linear combinations of two parents. Mutation deals with the addition of a random variable to elements of the vector. In addition, GAs have seen widespread use in process engineering and a wide number of codes are available.

In general, metaheuristics are widely applied in industrial scheduling (Xhafa and Abraham, 2008) for complex problems under deterministic and uncertain conditions (Zamarripa et al., 2012b). For example, He and Hui (2007) present a heuristic approach based on GA for solving large-size multi-stage multi-product scheduling problem in batch plants. Méndez et al. (2006) cite several works related to the application of the aforementioned techniques to the scheduling problem.

3.3.5.2. Simulated annealing

The simulated annealing derives from a class of heuristics with analogies to the motion of molecules in the cooling and solidification of metals. Here, a temperature parameter, can be raised or lowered to influence the probability of accepting points that do not improve the objective function. The method starts with a base point, and objective value. The next point is chosen at random from a distribution. If the objective function improves, the move is accepted with the initial point as the new point. Otherwise, the point is accepted with certain probability.

3.3.6. Artificial Intelligence

Artificial Intelligence techniques have been widely applied to scheduling problems (Metaxiotis et al., 2002). In order to use more efficiently the process information as well as the essential knowledge provided by human schedulers, artificial intelligence mimics human thought and cognitive processes to solve complex problems automatically.

Artificial Intelligence uses techniques for writing computer code to represent and manipulate knowledge. There are different techniques that mimic the different ways that people think and reason. The main artificial intelligence techniques are: rule-based methods, agent-based methods, and expert systems. Rule-based methods can be distinguished into case-based reasoning and model-based reasoning techniques, case-based reasoning is based on previous experiences and patterns of previous or similar experiences to meet the current needs and model-based reasoning concentrates on reasoning about a system’s behaviour from an explicit model of the mechanisms underlying that behaviour. Agent-based approaches are software programs that are capable of autonomous, flexible, purposeful and reasoning action in pursuit of one or more goals. They are designed to take timely action in response to external stimulus from their environment on behalf of a human. Expert systems, also known as knowledge-based approaches, encapsulate the specialist knowledge gained from a human expert and apply that knowledge automatically to make decisions. Some interesting implementations of artificial intelligence technologies into real-world scheduling problems can be found in Zweben and Fox (1994), Sauer and Bruns (1997), Henning and Cerdá (2000) and Strojny et al. (2006).

3.3.7. Hybrid methods

Hybrid methods are based on the combination of different optimization methods, in order to take profit of the advantage of each one of the considered methods. As example of combination of heuristics and MILP methods, Blomer and Gunther (2000) presented a MILP model for scheduling chemical batch processes with a two-stage solution procedure. In the first stage, an initial solution is derived by use of a linear programming-based heuristic. The proposed heuristic relies on a time grid that includes only a limited number of feasible periods in which a processing task is allowed to start. Thus, the size of the original multi-period mixed integer linear programming model is reduced in a controlled manner and optimal solutions to the relaxed model are obtained within reasonable computational time. The second stage consists of an improvement step that aims to compress the initial schedule by left-shifting operations over the time-axis. Burkard and Hatzl (2006) developed a heuristic for batch processing problems occurring in the chemical industry, aiming at makespan minimization, proposing an iterative construction algorithm which alternates between construction and deconstruction phases.

Also, the combination of CP and MILP has received increased attention for their complementarity. Maravelias and Grossmann (2004) developed a hybrid MILP/CP method for the continuous time model and in which different objectives such as profit maximization, cost minimization and makespan minimization can be handled. The proposed method relies on an MILP model that represents an aggregate of the original MILP model. The main advantage of combining both methodologies is to produce order of magnitude reductions in CPU times compared to standalone MILP or CP models (Harjunkoski & Grossmann, 2002; Zeballos et al., 2011).

3.4. Multi-criteria optimization

In chemical engineering problems, it is usual the consideration of multiple criteria decision making, in order to involve multiple considerations in a competitive framework. Multicriteria decision making is a discipline that deals with the methodology and theory to treat complex problems entailing conflicting objectives, such as cost, performance, reliability, safety, sustainability and productivity among others (Wiecek et al., 2008). In presence of multiple criteria, a large number of solutions may be suitable, obtaining a set of solutions (Capón-García et al., 2011 and Zamarripa et al., 2012a).

This kind of problems can be addressed through the use of a priori, interactive and posteriori approaches. Priori approaches are based on establishing initially the objectives, and solving them iteratively. This approach consists on optimizing the first objective, and to use this value as a constraint when solving the next objective. This procedure is repeated iteratively for all the objectives. The main drawback of priori approaches is that the final solution depends on the selected order for optimizing each objective. The iterative approach focuses on directing the search using the information obtained in the optimization process. Finally, posterior approaches consists of producing a set of solutions which covers the trade-off region comprising the best compromise solutions. As a result of the multi-objective optimization problem, a set of solutions are obtained. This thesis applies the latter approach to deal with multi-objective decision problems. A general mathematical representation of multi-objective optimization (MOO) is as follows:

(3.23)

$$\begin{aligned}&subject\ to\\&h(x) = 0\\&g(x) \leq 0\\&x^L \leq x \leq x^U\\&x \in X \subset \mathbb{R}^n\end{aligned}$$

The set of solutions of a MOO problem are known as Pareto solutions. Each Pareto solution is one for which any improvement in one objective can only take place if at least one other objective worsens (Messac et al., 2003).

Considering that Z_p is a scalar that shall be associated to the objective function value $f_p(x)$, a solution x_a, associated to the objective function values $\left\{Z_{1_a}, Z_{2_a}, \dots, Z_{p_a}\right\}$ dominates other solution x_b, with its corresponding point $\left\{Z_{1_b}, Z_{2_b}, \dots, Z_{p_b}\right\}$, if and only if:

$$\begin{gathered}\left[Z_{p_a} \leq Z_{p_b}\ \forall\ p \in \{1 \dots P\}\right] \wedge \left[\exists\ p \in \frac{\{1 \dots P\}}{Z_{p_a}} \leq Z_{p_b}\right]\\ Z_{p_a} = f_p(x_a), \forall p \in \{1 \dots P\}\\ Z_{p_b} = f_p(x_b), \forall p \in \{1 \dots P\}\end{gathered} \tag{3.24}$$

Also, one solution does not dominate another if at least one of the objective criteria of the former is equal or worse than the values for the second solution. Thereby, if a solution x^* is Pareto solution, then it does not exist a different solution $x \in X$ that dominates it.

Given two solutions, if none of them dominates the other, then both of them are non-dominated solutions with respect to one another. In fact, the Pareto optimal solutions are a set of non-dominated solutions. Figure 3.8 presents a set of solutions and the Pareto frontier for a biobjective minimization problem. The set of solutions that are dominated by the solutions are located in the Pareto frontier. Moreover, the anchor points, located at (f_1^*, f_2^{1*}) and (f_1^{2*}, f_2^*), are the result from the optimization problems considering one single criteria at a time. Also, the utopia point $f^u = (f_1^*, f_2^*)$ is defined by the optimal values for each objective function, whereas the nadir point $f^n = (f_1^{2*}, f_2^{1*})$ is given by the worse values of the objective functions.

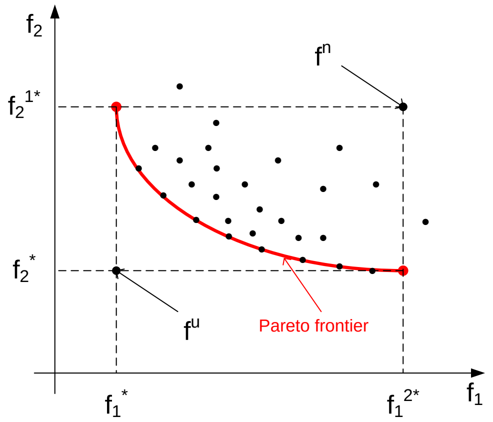

Figure 3.8. Pareto frontier and dominated solutions for a biobjective minimization problem.

There are several approaches to obtain Pareto solutions, which are based on the conversion of the MOO problem into one single objective problem; solving it several times at the same time that each solution represents one feasible point; all the solutions represent the Pareto frontier. These approaches include these methods:

- Physical programming.
- Normal boundary intersection.
- ε-constraint.
- Normal constraint.
- Weighted sum.
- Compromise programming.

3.5. Uncertainty approaches

Although there have been important advances in optimization techniques, decision making in the supply chain management scenario become more complex when the consideration of different sources of uncertainty in the models is essential to ensure solution quality or even its practical feasibility. So, one of the main current challenges consists in integrating the presence of variability in process parameters, including:

- Uncertainty in demand, prices and availability of resources.
- Variability in process parameters (manufacturing time, reaction conditions).
- External uncertainty (errors, strikes…).

The approaches addressed to problems under uncertainty can be classified into reactive and preventive procedures. Reactive approaches are focused on modifying a nominal plan obtained by a deterministic formulation in order to adjust it to different alterations, modifications or updated system data. Some reactive approaches are the multi-parametric programming, the Model Predictive Control (MPC) and the rolling-horizon approach. On the other hand, preventive approaches are based on the consideration of all possible cases, and finding a good solution for all these cases. This approach has the advantage that a feasible solution is found for all considered scenarios. However, the obtained solutions may be too conservative, since the model must take into account all the possibilities. The most frequently adopted approaches as preventive procedure are the stochastic programming, the robust optimization and the fuzzy programming.

3.5.1. Multi-parametric programming

Parametric programming can be used as an analytic tool in order to map the uncertainty in the optimization problem to optimal alternatives. The output of the parametric optimization provides a complete set of profiles of all the optimal inputs to the system as a function of uncertain parameters, and the regions in the space of uncertain parameters where these functions remain optimal. As a result, as the operating conditions fluctuate, one does not have to re-optimize for the new set of conditions since the optimal solution as a function of parameters (or the new set of conditions) is already available (Pistikopoulos et al., 2002). Parametric programming techniques have been developed and proposed as a means of reducing computational effort associated to optimization problems regarding uncertainty.

The general multiparametric programming problem can be written in the following standard form:

$$\begin{aligned}
&\min_{x} f(x,\theta)\\
&subject\ to\\
&h(x,\theta)=0\\
&g(x,\theta)\leq 0\\
&x\in\mathbb{R}^n\\
&\theta\in\Theta\in\mathbb{R}^q/\theta_l^{min}\leq\theta_l\leq\theta_l^{max}, l=1,\dots,q
\end{aligned} \tag{3.25}$$

where x represents the decisions variables (continuous and binary), while θ denotes the vector of uncertain parameters.

The typical multiparametric programming problem is described in terms of the following items:

- A given planning horizon.
- A given performance criterion.
- A set of constraints which cannot be violated.
- A set of parameters.

In an optimization framework with an objective function to minimize, a set of constraints to satisfy and a number of bounded parameters affecting the solution, multi-parametric programming obtains:

- The objective function and the optimization variables as functions of the parameters
- The space of parameters (known as critical regions, CR) where these functions are valid (Figure 3.9).

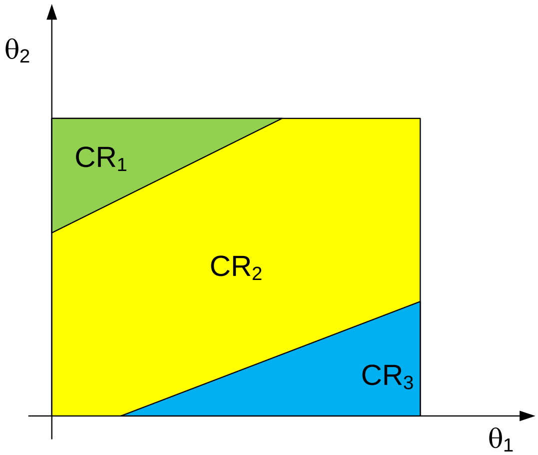

Figure 3.9. Multi-parametric programming: critical regions

$$x(\theta) = \begin{cases} x_1(\theta), if\ \theta \epsilon CR_1 \\ x_2(\theta), if\ \theta \epsilon CR_2 \\ x_3(\theta), if\ \theta \epsilon CR_3 \end{cases} \quad (3.26)$$

Multi-parametric optimization approach is used to generate a complete map of the optimal solutions in the space of the varying internal and external parameters (uncertainty). So, the optimal solution comprises a set of regions, in which there is an optimal and feasible solution, given by analytical expressions. This reactive approach can be used to upload a nominal schedule, which can be continuously updated according to the variations in the parameters and constraints related to internal and external uncertainty sources.

The multiparametric problems can be classified according to the type of mathematical model functions involved in the optimisation problem, including linear, quadratic, nonlinear, dynamic optimisation, global optimisation, MILP and MINLP.

3.5.2. Model Predictive Control

Model Predictive Control (MPC) is a widely academic and industrial technique for advanced multivariable process control, which appeared in the late 1970s (Pistikopoulos, 2009). Although typically this methodology has been applied for production processes, in which empirical models based on experimentation are used, MPC can also be applied to other echelons of the SC (Rivotti et al., 2012).

The objective of MPC is to provide a sequence of control actions over a limited future time horizon, in order to predict the behaviour of the system. Basically, once future behaviour of the process output is predicted, future inputs can be calculated, through manipulated or controlled variables (Figure 3.10, Pistikopoulos, 2009). The basic idea of the MPC implementation is based on the minimization of the difference between the state and control deviation from the set point, by the use control variables. This control method is able to handle multi-variable and constrained systems.

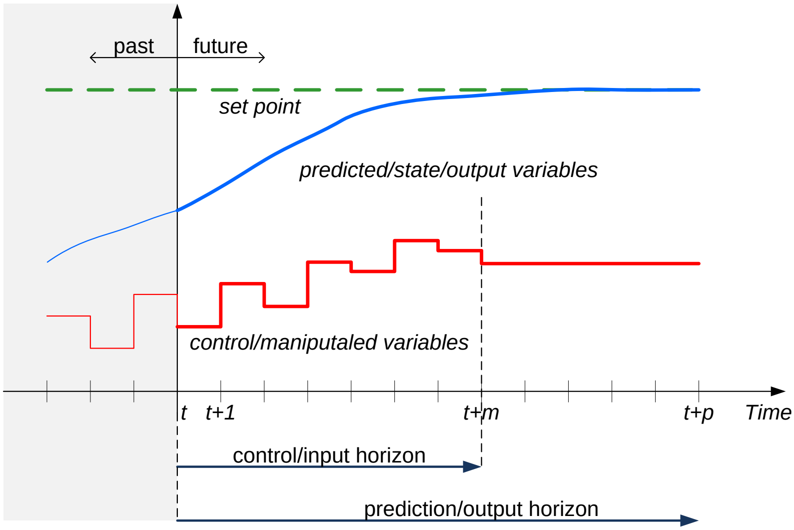

Figure 3.10. Model Predictive Control implementation.

Although control actions are taken in the current time interval taking into account the predicted behaviour, this control sequence is repeated at every sampling instant, including uploaded information (measurements or estimates). The time horizon selected for these predictions must include all significant dynamics related to the process under study, in order to predict appropriately future events.

The main advantage of MPC is that it is model-based, so output predictions are computed using a process model. This means that the model can take into account the constraints on the state and control variables. This model must be accurate to guarantee a good performance of the results (the success of this methodology depends on the precision of the process model), but at the same time, the simplest model that offers precise enough predictions to be solved in a reasonable time.

On the other hand, the most important disadvantage is the computational time required, which means that MPC implementation maybe difficult or even not applicable if sampling time is not large enough to allow for the optimisation problem to be solved in time or if the system includes a large number of process variables.

MPC is usually implemented in discrete time representations. The chosen model depends on the process to be controlled. The most typical models are state-space models, transfer models, finite impulse response models and independent models. All processes inherently include sources of uncertainty, which must be considered in the process control. Therefore, the modelling of MPC includes the presence of disturbances or uncertainty. Hence, the desired output is the set point but the corresponding value of the input variable depends on the unknown disturbance.

3.5.3. Rolling-horizon approach

The rolling-horizon approach is a reactive scheduling method that solves iteratively the deterministic problem by moving forward the optimization horizon in every iteration; assuming that the status of the system cis updated as soon as the different uncertain or not accurate enough parameters became to be known, the optimal schedule for the new resulting scenario (and optimization horizon) may be found. This approach considers: a prediction horizon, in which all the uncertain parameters related to this time horizon are assumed to be known with certainty, due to the fact that the system under study receives feedback related to the unknown parameters, and a control horizon, where the decisions of the optimization for the prediction horizon are applied (Figure 3.11, Kopanos and Pistikopoulos, 2014). Rolling-horizon has been applied to several scheduling problems under uncertainty, and the interested reader can be referred to Kopanos and Pistikopoulos (2014) for a brief review.

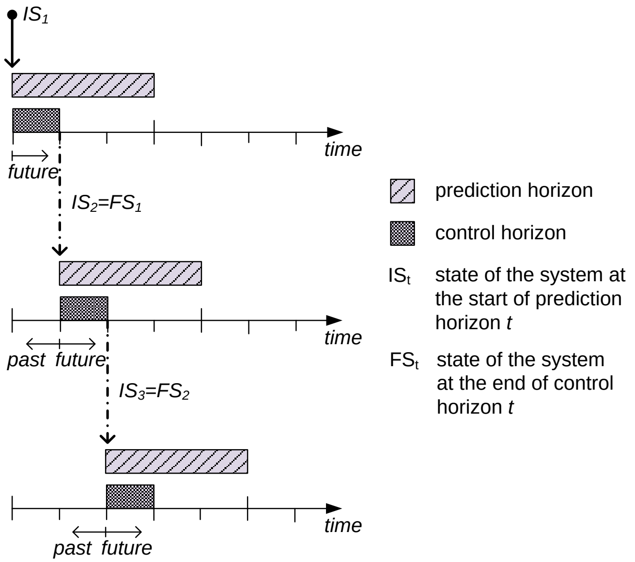

Figure 3.11. Reactive scheduling via a rolling horizon framework.

The rolling horizon algorithm can be applied as follows (Figure 3.12):

- Initially, set the initial conditions of the system, as well as the length of the scheduling, prediction and control horizons.
- Next, establish the first planning period and solve the scheduling problem for the prediction horizon considered.
- Update uncertain parameters and solve again the scheduling problem using data from the last optimization, by the use of linking.
- Then stop, if this new schedule corresponds to the last period of time. Otherwise, fix the values obtained in the optimization problem for that iteration, re-schedule and update the period of time until the last planning period has been reached.

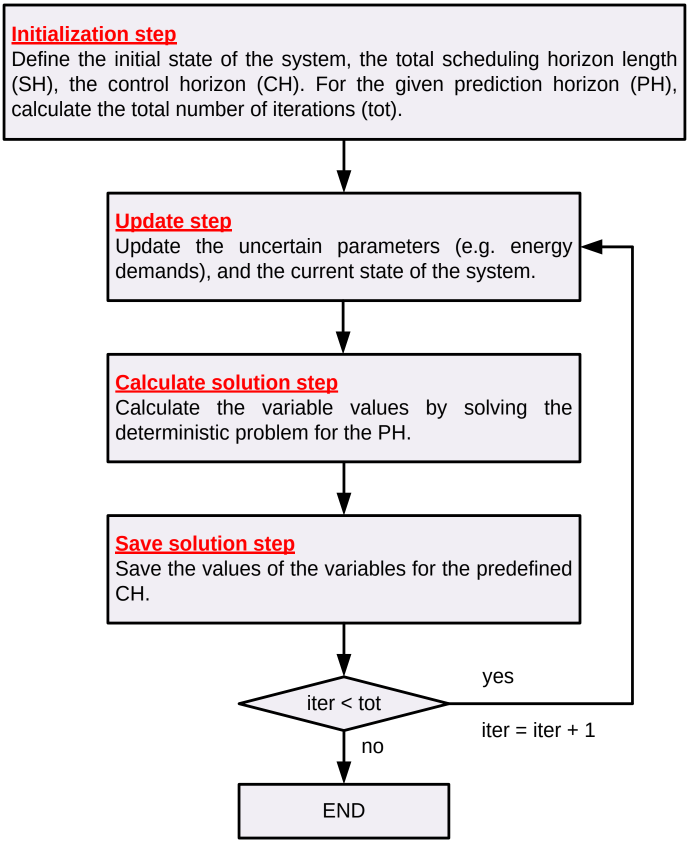

Figure 3.12. Algorithm for the rolling horizon approach.

This reactive approach allows to upload or modify the different uncertain parameters. Note that although the solution obtained in each prediction horizon is expected to be optimal for this period of time, the solution of the overall problem could be suboptimal in practice, since future information outside the current prediction horizon is not taken into account. So, the length of the prediction horizon must be appropriate in order to guarantee the quality of the obtained results. The length of the prediction horizon depends on the characteristics of the problem.

3.5.4. Stochastic programming

Stochastic-based approaches is the most commonly used approach in the literature (Straub and Grossmann, 1992; Terrazas-Moreno et al., 2011). The original deterministic mathematical model is transformed into a stochastic model treating the uncertainties as random variables (Shapiro, 2012 and Shapiro et al, 2013). In a general stochastic optimization problem, it is relevant to distinguish among two set of decision variables:

- On the one hand, first stage decisions are related to those decisions that must be taken before any uncertain parameter is unrevealed. They are also known as "here and now" decisions.
- On the other hand, resource are determined after some or all the uncertain data is revealed. This kind of decisions are also known as the second and so forth stage or "wait and see" decisions.

The most widely used and simplest stochastic program is the two-stage stochastic formulation. Here, the first stage decisions are represented by the vector x, while second stage decisions are represented by the vector y, and the uncertain parameters are represented by the vector ξ. It is worthy to mention that the second stage decisions y are a function of the first stage decisions x and the uncertain events. In order to simplify the problem representation, the recourse function Q is introduced next.

$$\begin{aligned}
&Q(x,\xi) = \min_{x} f_2(y,\xi) \\
&subject\ to \\
&h_2(x,y,\xi) = 0 \\
&g_2(x,y,\xi) \leq 0 \\
&y \in Y \subset \mathbb{R}^{n2} \\
&f_2 : \mathbb{R}^{n2} \to \mathbb{R} \\
&h_2 : \mathbb{R}^{n2} \to \mathbb{R}^{l2} \\
&g_2 : \mathbb{R}^{n2} \to \mathbb{R}^{m2}
\end{aligned} \tag{3.27}$$

All equations involving recourse decisions y are considered in Q. As it can be seen, Q is a mathematical program that minimizes the second-stage variable for a given value of the uncertain parameter $\boldsymbol{\xi}$. Then, the expected recourse function Q, is defined by the expression (3.28):

$$Q(x) = E_{\xi}[Q(x,\xi)] \tag{3.28}$$

Finally, the mathematical representation of a two-stage stochastic formulation can be represented as follows:

$$\min[f_1(x) + Q(x)] \tag{3.29}$$

$$f_1: \mathbb{R}^{n1} \rightarrow \mathbb{R}$$
$$h_1: \mathbb{R}^{n1} \rightarrow \mathbb{R}^{l1}$$
$$g_1: \mathbb{R}^{n1} \rightarrow \mathbb{R}^{m1}$$

Moreover, this formulation is extended to solve complex and real engineering applications to a multistage recourse program. The recursive programming applied to process engineering becomes the most used technique to consider uncertainty in the decision making process. Meanwhile allow to the decision makers to know the expected performance of the system at the same time they are using a robust decision making tool.

In the case that continuous probability function is utilized to represent the uncertain parameter ξ, program (3.29) can be analytically solved just for a few simple problems. However, approximations can be obtained by constructing a discrete number of scenarios which represent the continuous distribution behaviour. In this case, sampling techniques can be used to approximate to discrete functions the continuous probability functions in a stochastic program. The combinatory if the different scenarios that can take place can be represented by using a scenario tree representation (Figure 3.13).

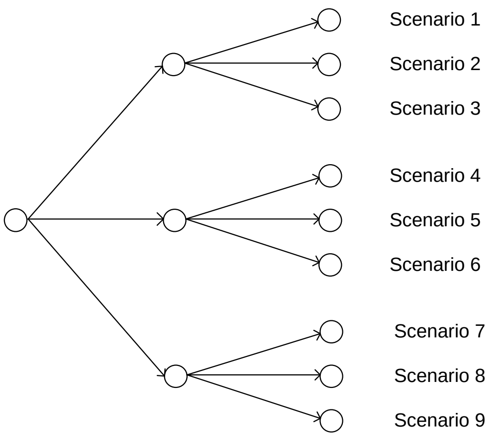

Figure 3.13. Scenario tree representation for a stochastic programming.

3.5.5. Robust optimization

The robust optimization is focused on building the proactive approach to minimize the effects of disruptions on the performance measure. They also try to ensure that the predictive and realized schedule and/or planning do not differ drastically, while maintaining a high level of schedule and/or performance. In mathematics, robust optimization is an approach in optimization to deal with uncertainty. It is similar to the recourse model of stochastic programming, in that some of the parameters are random variables, except that feasibility for all possible realizations (called scenarios) is replaced by a penalty function in the objective. As such, the approach integrates goal programming with a scenario-based description of problem data (Al-Qahtani et al, 2008).

3.5.6. Fuzzy programming methods

The main difference between the stochastic programming and the robust optimization respect to fuzzy optimization approaches is in the way in which uncertainty is modelled. This proactive approach considers random parameters as fuzzy numbers and constraints are treated as fuzzy sets. Some constraint violation is allowed and the degree of satisfaction of a constraint is defined as the membership function of the constraint. Objective functions in fuzzy mathematical programming are treated as constraints with the lower and upper bounds of these constraints defining the decision-makers expectations. Fuzzy logic and probability are different ways of expressing uncertainty. While both fuzzy logic and probability theory can be used to represent subjective belief, fuzzy set theory uses the concept of fuzzy set membership (i.e., how much a variable is in a set), probability theory uses the concept of subjective probability (i.e., how probable do I think that a variable is in a set).

3.6. Modelling frameworks

There are some commercial tools for general optimization purposes, including GAMS (General Algebraic Modeling System, Rosenthal et al., 2012), AMPL (A Mathematical Programming Language, Fourer et al. 2002), AIMMS (Advanced Interactive Multidimensional Modeling System, Roelofs, 2010) or Matlab. All of them render very similar characteristics (general mathematical language, use different solvers to solve the modelled problems, etc.).

3.6.1. GAMS – General Algebraic Modeling System

Optimization problems in this Thesis have been solved using GAMS, which is the most used optimization software in PSE field. GAMS is a programming language that allows modelling and solving optimization problems. Castillo et al. (2001) point out some important characteristics, such as:

- Modelling and solving procedure are completely separated. Once the model is developed; several solvers are available to optimize the problem.
- The model representation in GAMS is analogous to the mathematical description of the problem.
- Models are described in compact and concise algebraic statements which are easy for both humans and machines to read.
- Allows changes to be made in model specifications simply and safely.
- Allows unambiguous statements of algebraic relationships.
- The ability to model small size problems and afterwards transform them into large-scale problems without significantly varying the code.
- GAMS allows to import and export data from/to Microsoft Excel files. Additionally, MATLAB and GAMS could be easily connected.

Moreover, it is worthy to mention that optimization algorithms mentioned above are embedded in some of the different GAMS solvers. Each solver is usually developed to tackle a specific type of program (i.e., LP, NLP, MILP, MINLP, etc.).

3.7. Solvers

3.7.1. CPLEX solver

IBM ILOG CPLEX, often informally referred to simply as CPLEX, is an optimization solver package. GAMS/CPLEX is a GAMS solver that allows to combine the high level modelling capabilities of GAMS with the power of CPLEX optimizers. CPLEX optimizers are designed to solve large, difficult problems quickly. Access is provided (subject to proper licensing) to CPLEX solution algorithms for linear, quadratically constrained and mixed integer programming problems. While numerous solving options are available, GAMS/CPLEX automatically calculates and sets most options at the best values for specific problems. It is worth mentioning that for problems with integer variables CPLEX uses a branch-and-cut algorithm which solves a series of LP subproblems. Because a single mixed integer problem generates many subproblems, even small MIP problems can be very compute intensive and require significant amounts of physical memory.

3.7.2. GloMIQO solver

The Global Mixed-Integer Quadratic Optimizer, GloMIQO (Misener and Floudas, 2013), is a numerical global solver addressed to mixed-integer quadratically-constrained quadratic programs to ε-global optimality. The algorithmic components to solve this kind of MINLP problems are the problem reformulation (by variable elimination and bilinear term disaggregation, which may significantly increase the number of nonlinear terms in the model but may also tighten the linear relaxation), the detection of special structure including convexity and edge-concavity, the generation of tight convex relaxations (by generation MILP relaxations), the partition of the search space through variable branching and finally the reduction of the search space through variable bounding and finding good feasible solutions.

3.8. Information management software

Recent trends in process industries are shifting the focus from controlling the process plant as a stand-alone entity toward managing it as an integral part of a larger system (Klatt & Marquardt, 2009). Such approach aims at exploiting the process and environment dynamics in order to maximize the plant economic indicators. A holistic management of the different elements composing a SC and, in many cases, the relations among them, are necessary to improve resource use, minimize production costs and inventory, enhance economic benefits, increase customer satisfaction or improve process control, among other objectives usually associated to process profitability.

Obviously, such understanding of process management entails the integration of the different decision level functions. The complexity of simultaneously considering the whole decision making process involved, lead to the traditional division of such process in different hierarchical levels (strategic, tactical and operational, as usually recognised even by the ISA standards). Therefore, a current important challenge lies on the coordination of the decision making and the optimization of different decision levels, both vertically across a single process plant, and horizontally along the different geographically distributed subsystems of the SC in a given time horizon.

The process engineer is also frequently responsible for the continuous improvement of the production processes, the products and the associated techniques. (Noakes et al., 2011). Currently, tasks related to management, research and development involves the generation of huge amount of data that must be analysed, interpreted and stored throughout the decision making process, using computer simulation and computer control techniques. In chemical companies, these data are related to design issues, planning and production, coordination, cooperation and attention to customer demands, as well as constraints related to economy, environmental impacts, social policy, ethical topics, health, safety and sustainability (Accreditation Board for Engineering and Technology, ABET, 2008).

One first step toward such integration consists of the sharing of information, which is nowadays being achieved with modern information technology tools, such as SAP and

Oracle, that allow the instantaneous flow of information along the various organizations in a company (Grossmann et al., 2008). The implementation and use of information technology tools involve a huge number of data to handle. For this reason, standardizing information structures and tools to improve the availability and communication of data is essential to integrate these data and use the previously mentioned tools efficiently for Chemical SCs management (Bessiris et al., 2011).

3.8.1. Ontologies

Among the different types of knowledge-based systems which can be applied in complex scenarios to help decision making, ontologies provide structures for the coordination of information sources (Muñoz et al., 2010), and so, they can be used in the process engineering area to coordinate the development of new products, to identify new manufacturing recipes (Singh et al., 2010) and also to integrate different decision levels within a SC (Muñoz et al., 2011). This includes facilitating communication and knowledge, which allow the information exchange among the different modelling paradigms used for the enterprise-wide optimization, and also helps the acquisition, maintenance, access, reuse and sharing of information related to processes, with the aim of increasing the efficiency of cost, time and resources (Fensel, 2003). The use of such systems allows the establishment of common standards and enables the full exploitation of the stored relationships among all available data.

Ontologies are considered a key semantic tool to reduce or eliminate conceptual and terminological confusion and come to a shared understanding of all available information, specifying the structure of a domain of knowledge in a generic way that can be read by a computer and presented in a human readable form (Figure 3.14). Moreover, ontologies incorporate knowledge of processes, incorporating the relationship between different processes into a logical structure. The main advantages of using ontologies are the communication in a shared framework among people and across application systems as well as the conceptualization that describes the semantics of all data in a standard way, using a common language.

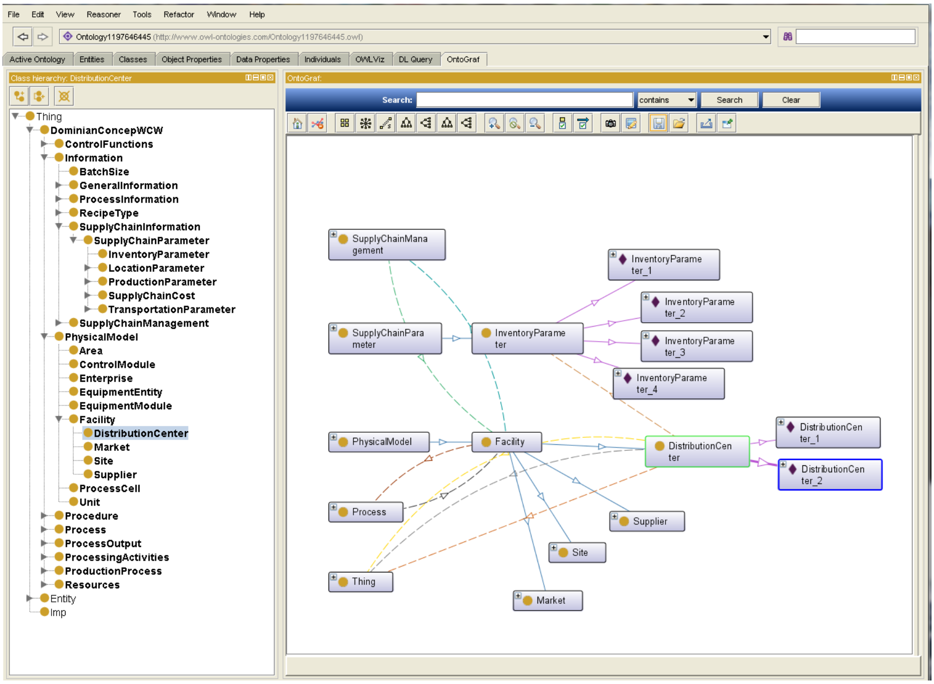

Figure 3.14. Ontology system, representing the relationship between different hierarchies within a supply chain.

3.9. Final remarks

In this chapter, different optimization techniques have been outlined. The main ideas behind each technique have been briefly introduced with the purpose of providing the reader a general understanding of the theory involved into the solution techniques applied in this thesis. In order to implement mathematical formulation in optimization software (i.e., GAMS), one requires to have a good understanding of their principles, to interpret results as well as to debug skills. For that reason, special emphasis has been made to these topics. Particularly in this Thesis, MIP models have been developed using discrete time and hybrid time representations, in order to characterize the system under study, considering both deterministic and uncertain conditions.

Part II – Integrated production and demand management

Chapter 4. Time representation

One of the key points of the scheduling problem of a supply chain concerns the time representation. All existing scheduling formulations can be classified into discrete time models, hybrid time models and continuous time models (see Chapter 2.5).

This second part of this thesis analyses the operational decision making procedures required to address the simultaneous management of supplies and requests, in order to best accommodate arbitrary resource availability profiles, and to extensively exploit the eventual flexibility of the production requirements to be fulfilled. In this Chapter, the optimization of the resulting short term scheduling problem in deterministic scenarios is addressed through a Mixed-Integer Linear Programming (MILP) mathematical model, which includes a new hybrid time formulation developed to take profit of the advantages of the procedures based on discrete time representations, while maintaining the ability to identify solutions requiring a continuous time representation, which might be qualitatively different to the ones constrained to consider a fixed time grid for decision making. The performance of this new time representation has been studied, taking into account the granularity of the model and analysing the associated trade-offs in front of other alternatives.

4.1. Introduction

The simultaneous management of production and demand would introduce an additional degree of freedom to the supply chain management problem, which would permit achieving further benefits. As mentioned in Chapter 2.4 this additional flexibility can be greatly potentiated by storage systems, which may be used to decouple production and demand peaks, and to cope with the uncertain (fluctuating) availability of renewable resources.

For these previous reasons, the development of an efficient production planning and scheduling model is necessary to coordinate generation, storage and use of resources/materials to maximize efficiency by optimally adjusting production and demand. This chapter proposes a general model to solve the operational decision making problem for a supply chain, considering the simultaneous management of production and consumption. Two particular models using discrete and hybrid time representations have been implemented to study the trade-off between both approaches, taking into account the granularity of the problem. The assessment of their performance is presented through a case study addressing the optimal management of the energy generation, storage and consumption of several appliances within a single household served by a simple microgrid.

4.2. Problem statement

The system under study consists of a set of interconnected elements (i.e., producers/generators, storages, consumptions) as well as a set of decisions (when, where, who, how much) that define a typical managerial problem (resource allocation and timing).

The specific problem in this case is to determine the production and storage levels to be established in the supply chain along a given time horizon, as well as to manage the consumption profiles in order to maximize some economic indicators, considering incomes associated to production sales as well as the costs related to production, storage and deviation in the consumptions from the initial targets. In the discrete time representation, decisions in terms of production, storage and consumptions are taken every given time interval. However, in order to represent a continuous demand profile, a hybrid time formulation has been developed, which incorporates the possibility of starting any consumption at any time. This time formulation was chosen in order to represent the different time scales related to production and consumption.

The problem under study is described in the following terms:

(i) A scheduling horizon which is divided into a set of time intervals $t \in T$.
(ii) A set of production sources $i \in I$, which are characterized by a minimum and maximum production capacity and a given operational cost.
(iii) A set of storage systems $k \in K$ in order to accumulate resources/materials, featuring a minimum and maximum storage capacity and a storage cost.
(iv) A set of products, materials, resources or utilities $m \in M$. Notice that although this term can be referred to different items, in order to abbreviate the explanation, only the term product will be used for this set.
(v) A set of consumptions which define the overall demand. A desirable starting time of each consumption and its duration are established, but every consumption is bounded within a time window delimited by a starting time and a maximum completion time, which cannot be exceeded. So, delays in the nominal demands are allowed under associated penalty costs. This

flexibility allows the integration or coordination of production and demand. Then, each consumption can be moved assuming a certain penalty cost.

The mathematical model presented contemplates two main aspects: the material/resource balances describing flows, production, storage, consumption and loses, and the capacity constraints associated to the equipment and technologies involved in the considered SC.

The decisions to be made, so as to maximize the profit of the SC, are related to:

(i) The materials/resources to be produced/purchased from source i at time interval t.
(ii) The storage level to be maintained at the end of each time interval t.
(iii) The specific time to execute a demand.
(iv) The materials/resources to be sold to the external market r at time interval t.

The need to introduce these elements, when applied to real size cases using a continuous time representation, lead to mathematical model sizes which are out of the capacities of currently available optimization solvers (see Chapter 2.5), so only discrete and hybrid time based formulations are considered in this chapter. In the discrete time based model next presented, decisions related to production and consumption are taken at the beginning of each time interval t. However, when the hybrid time representation is used, decisions related to production are taken at the beginning of each time interval t, whereas decisions related to consumption can be taken continuously. This means that both models differ only in the equations related to consumption.

4.3. Mathematical formulation

The constraints associated to sequencing, allocating of consumptions and resources, and distribution of a multi-product supply chain are next presented in the following discrete time and hybrid time MILP formulations. The major part of the model is identical for both formulations, since only equation (4.19) used for discrete time formulations and equations (4.20), (4.21), (4.22), (4.23) and (4.24) differ.

Eq. (4.1) establishes a material balance, considering the raw material and its transformation to products m, by considering a conversion degree between raw materials and products. Although the transformation of raw material are considered, the remaining equations are formulated for situations in which their transformation takes place or not, in order to generalise the proposed formulation. Also, eq. (4.2) restricts the minimum and maximum production level in each source i can supply product m. This value will be zero in case it is not used and it is bounded in case it is active. Thus, the overall production for each product m at each interval t is calculated in eq. (4.3) as the summation of the production in each of the active sources. Notice that these equations can be applied for both production and purchases of product m, since they consider the amount of material to be produced (or purchased) and its production or acquisition cost.

$$\sum_{m \in RM} P_{i,m,t-Tp_m} = \rho_m \cdot \sum_{m \in PR} P_{i,m,t} \qquad \forall i,t \qquad (4.1)$$

$$P_{i,m,t}^{min} \cdot X_{i,m,t} \leq P_{i,m,t} \leq P_{i,m,t}^{max} \cdot X_{i,m,t} \qquad \forall i,m,t \qquad (4.2)$$

$$PT_{m,t} = \sum_{i \in I} P_{i,m,t} \qquad \forall m,t \qquad (4.3)$$

The storage level of product m in each storage k at each time interval t is bounded within a minimum value and a maximum value. In addition, the balance for each storage system k at each interval t is given by the variation of storage level and eventual loses (i.e., product or energy loses) in eq. (4.5), assuming a maximum level of load, given by eq. (4.6). Thus, eq. (4.7) indicates that the storage level variation in each storage k at each time interval t is delimited by a maximum variation level.

$$SE_{k,m,t}^{min} \leq SE_{k,m,t} \leq SE_{k,m,t}^{max} \qquad \forall k,m,t \qquad (4.4)$$

$$SE_{k,m,t} = SE_{k,m,t-1} + \eta_{k,m}^{in} \cdot Ld_{k,m,t} - \frac{SP_{k,m,t}}{\eta_{k,m}^{out}} \qquad \forall k,m,t \qquad (4.5)$$

$$0 \leq \sum_{k \in K} Ld_{k,m,t} \leq PT_{m,t} \cdot DT \qquad \forall m,t \qquad (4.6)$$

$$-\alpha_{k,m} \cdot SE_{k,m,t}^{max} \leq SE_{k,m,t} - SE_{k,m,t-1} \leq \alpha_{k,m} \cdot SE_{k,m,t}^{max} \qquad \forall k,m,t \qquad (4.7)$$

Constraints are also required for the demand-side management, in order to determine the initial time of each consumption jf of each product m. The starting time, $Ts_{j,f,m}$, bounded by eq. (4.8), is required to be greater or equal than minimum starting time $Ts_{j,f,m}^{min}$, and less or equal to the time allowing due completion. Moreover, eq. (4.9) determines the final time of each consumption jf, which is given by the starting time and its duration. For the hybrid time representation model, $Ts_{j,f,m}$ corresponds to the real time in which consumption jf begins, whereas for the discrete time model representation, this term is related to the time interval in which each consumption starts. The same concept is applied to $Tf_{j,f,m}$.

$$Ts_{j,f,m}^{min} \leq \ Ts_{j,f,m} \leq Tf_{j,f,m}^{max} - Dur_{j,f,m} \qquad \forall j, f \in F_j, m \qquad (4.8)$$

$$Tf_{j,f,m} = Ts_{j,f,m} + Dur_{j,f,m} \qquad \forall j, f \in F_j, m \qquad (4.9)$$

In order to locate the initial and final time of each consumption jf of each product m ($Ts_{j,f,m}$ and $Tf_{j,f,m}$), the binary variables $Y_{j,f,m,t}$ and $Z_{j,f,m,t}$ are defined as active when consumptions starts and finishes, respectively, at time period t. These logical restrictions can be reformulated as a set of big-M constraints, where T_t corresponds to time:

$$Ts_{j,f,m} \geq T_t \quad - M \cdot \left(1 - Y_{j,f,m,t}\right) \qquad \forall j, f \in F_j, m, t \qquad (4.10)$$

$$Ts_{j,f,m} \leq T_{t+1} + M \cdot \left(1 - Y_{j,f,m,t}\right) \qquad \forall j, f \in F_j, m, t \qquad (4.11)$$

$$Tf_{j,f,m} \geq T_t \quad - M \cdot \left(1 - Z_{j,f,m,t}\right) \qquad \forall j, f \in F_j, m, t \qquad (4.12)$$

$$Tf_{j,f,m} \leq T_{t+1} + M \cdot \left(1 - Z_{j,f,m,t}\right) \qquad \forall j, f \in F_j, m, t \qquad (4.13)$$

Big-M constraints are methodologies applied to solve mixed integer programming problems. This kind of formulations are used to convert a logic or nonconvex constraint to a set of constraints describing the same feasible set, using auxiliary binary variables and additional constraints. Furthermore, eq. (4.14) forces that a consumption jf cannot start since the previous one in the same consumer unit j has finished, not allowing neither an overlap nor a change in the established consumption sequence in consumer j.

$$Tf_{j,f,m} \leq Ts_{j,f',m} \qquad \forall j, f \in F_j, \forall f' \in F_j, f < f', m \qquad (4.14)$$

Moreover, assignment constraints are implemented to enforce unique starting and finishing times for each consumption jf of product m, according to eq. (4.15) and (4.16), respectively. Since values of $Y_{j,f,m,t}$ and $Z_{j,f,m,t}$ are equal to zero outside the time window, the summation of these binary variables is only considered within such window, in order to improve the efficiency in terms of computational effort. Eq. (4.17) determines when each consumption jf is active. In this equation, $t' \in T$ indicates other elements of the same set T. In the term $\sum_{\substack{t' \in T \\ t' \leq t}} Y_{j,f,m,t'}$, $t' \in T$ must be greater or equal than the element $t \in T$. Moreover, in the term $\sum_{\substack{t' \in T \\ t' < t}} Z_{j,f,m,t'}$, $t' \in T$ must be greater than the element $t \in T$. Notice that both t and t' are elements of the same set T.Finally, eq. (4.18) is used to enforce the condition that all consumptions that start must finish.

$$\sum_{\substack{t \in T \\ T_t \leq Tf_{j,f,m}^{max} - Dur_{j,f,m}}} Y_{j,f,m,t} = 1 \qquad \forall j, f \in F_j, m \qquad (4.15)$$

$$\sum_{\substack{t \in T \\ T_t \leq Tf_{j,f,m}^{max}}} Z_{j,f,m,t} = 1 \qquad \forall j, f \in F_j, m \qquad (4.16)$$

$$W_{j,f,m,t} = \sum_{\substack{t' \in T \\ t' \leq t}} Y_{j,f,m,t'} - \sum_{\substack{t' \in T \\ t' < t}} Z_{j,f,m,t'} \qquad \forall j, f \in F_j, m, t \qquad (4.17)$$

$$\sum_{t \in T} Y_{j,f,m,t} = \sum_{t \in T} Z_{j,f,m,t} \qquad \forall j, f \in F_j, m \qquad (4.18)$$

Using the discrete time representation, the total demand at time interval t is given by all the active consumptions at this time and determined by eq. (4.19). The second term of this equation determines the exact consumption for those time intervals in which the consumption of a consumer will not take place in the overall time interval. Also, this allows to enforce the overall balance of the network.

$$Dem_{m,t} = \sum_{j \in J} \sum_{f \in F_j} Cons_{j,f,m} \cdot DT \cdot \left[W_{j,f,m,t} - Z_{j,f,m,t} \cdot \left(\overline{Dur}_{j,f,m} - Dur_{j,f,m}\right)\right] \qquad \forall m, t \qquad (4.19)$$

However, eq. (4.19) is not valid for the hybrid time representation, since it does not take into account that the consumption can start at any time during the time interval, not only at the beginning. Also, one of the characteristics of this hybrid time formulation is that any consumption can take place in more than one time interval. Therefore, the consumption in the hybrid time representation requires a more complex mathematical model, as the one composed by eq. (4.20), (4.21), (4.22), (4.23) and (4.24). The consumption at each period of time is given by eq. (4.20), where $XDem_{j,f,m,t}$ indicates the time period in which consumption jf of product m is active at time interval t. In order to calculate this term, four different situations have to be taken into account (Figure 4.1):

(i) is produced in the overall interval t, given by eq. (4.21),
(ii) starts during this interval t, indicated by eq. (4.22),
(iii) finishes during interval t, according to eq. (4.23),
(iv) and starts and finishes during interval t, given by eq. (4.24).

$$Dem_{m,t} = \sum_{j \in J} \sum_{f \in F_j} Cons_{j,f,m} \cdot DT \cdot XDem_{j,fm,,t} \qquad \forall m, t \qquad (4.20)$$

$$XDem_{j,f,m,t} \geq (T_{t+1} - T_t) \quad - M \cdot (1 - W_{j,f,m,t} + Y_{j,f,m,t} + Z_{j,f,m,t}) \qquad \forall j, f \in F_j, m, t \qquad (4.21)$$

$$XDem_{j,f,m,t} \geq (T_{t+1} - Ts_{j,f,m}) - M \cdot (2 - W_{j,f,m,t} - Y_{j,f,m,t} + Z_{j,f,m,t}) \qquad \forall j, f \in F_j, m, t \qquad (4.22)$$

$$XDem_{j,f,m,t} \geq (Tf_{j,f,m} - T_t) \quad - M \cdot (2 - W_{j,f,m,t} + Y_{j,f,m,t} - Z_{j,f,m,t}) \qquad \forall j, f \in F_j, m, t \qquad (4.23)$$

$$XDem_{j,f,m,t} \geq (Tf_{j,f,m} - Ts_{j,f,m}) - M \cdot (3 - W_{j,f,m,t} - Y_{j,f,m,t} - Z_{j,f,m,t}) \qquad \forall j, f \in F_j, m, t \qquad (4.24)$$

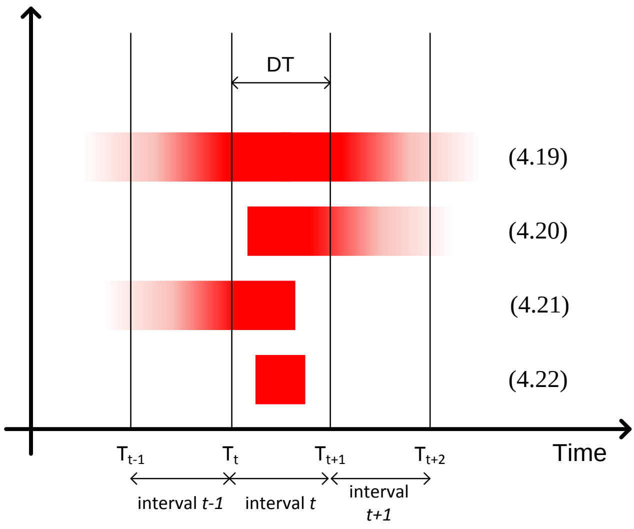

Figure 4.1. Time consumption within a time interval.

Obviously, the use of different time representations does not affect to the global balance, which in any case should include production, charge and discharge of the storage system, consumption and sales, is enforced by eq. (4.25):

$$\sum_{k \in K} SP_{k,m,t} + PT_{m,t} \cdot DT - Dem_{m,t} - \sum_{k \in K} Ld_{k,m,t} - \sum_{r \in R} Pg_{r,m,t} \cdot DT = 0 \qquad \forall m, t \qquad (4.25)$$

Furthermore, the economic aspects related to the management are introduced, considering production, storage and penalty costs in case of deviation from the initial target. The production cost is assumed to be proportional to the real amount of production, and according to the different production sources, eq. (4.26). In the same way, the storage cost is calculated as proportional to the real storage expected for each time period, according to eq. (4.27). Finally, the flexibility in the demand profile is tuned through the introduction of an additional term in the usual cost-based objective function penalizing the deviation from given initial consumption targets, eq. (4.28). The introduction of this penalty term and the flexibility to consider any arbitrarily availability profile in the generation systems previously described in eq. (4.1), (4.2) and (4.3) are the basic elements to allow the simultaneous management of production and consumption. The value selected for the penalty coefficient of each requirement depends on the specific characteristics of this requirement: small values are associated to high flexibility, while high values will lead to very strict requirements. Hence, it is important to choose appropriate values for each one of the penalty coefficients to guarantee the adequate management of the demand. Also, eq. (4.29) establishes the transport cost, taking into account the amount of material and the distance between production and markets.

$$CostPro = \sum_{t\in T}\sum_{m\in M}\sum_{i\in I} cpro_{i,m,t} \cdot P_{i,m,t} \cdot DT \tag{4.26}$$

$$CostSto = \sum_{t\in T}\sum_{m\in M}\sum_{k\in K} csto_{k,m,t} \cdot SE_{k,m,t} \tag{4.27}$$

$$CostPen = \sum_{m\in M}\sum_{j\in J}\sum_{f\in F_j} cpen_{j,f,m} \cdot (Ts_{j,f,m} - Ts_{j,f,m}^{min}) \tag{4.28}$$

$$CostTrp = \sum_{m\in M}\sum_{j\in J}\sum_{i\in I} ctrp_{i,j,m} \cdot P_{i,m,t} \cdot d_{i,j} + \sum_{m\in M}\sum_{r\in R}\sum_{i\in I} ctrp_{i,r,m} \cdot P_{i,m,t} \cdot d_{i,r} \tag{4.29}$$

Also, sales from external markets r have been taken into account. No maximum limits on the products m that can be sold to external markets r have been considered. Thus, incomes are computed as linear from the materials/resources sold and its selling price to the external market eq. (4.30), although this term may be modified according to applicable the market regulations.

$$Incomes = \sum_{t\in T}\sum_{m\in M}\sum_{r\in R} Price_{r,m,t} \cdot Pg_{r,m,t} \cdot DT \tag{4.30}$$

The profit of the network, which corresponds to the objective function to be maximized, is calculated considering incomes and costs in eq. (4.31).

$$Profit = Incomes - (CostPro + CostSto + CostPen) \tag{4.31}$$

To sum up, two models are defined based on the presented formulation, namely:

- Discrete time model
    - ✓ Objective function: equation (4.31)
    - ✓ Subject to constraints (4.1) to (4.19) and constraints (4.25) to (4.30)

- Hybrid time model
  - ✓ Objective function: equation (4.31)
  - ✓ Subject to constraints (4.1) to (4.18) and constraints (4.20) to (4.30)

Only linear constraints are included in the present formulation, since one of the objectives of this chapter is to study the difference between the discrete and the hybrid time formulations, in terms of results and computational effort. The presented formulations can be extended by introducing more complex constraints associated to the features of the scheduling problems, which can lead to the introduction of non-linear constraints. Also, the model does not consider the presence of fixed costs associated to the investment and installation of production sources, since the design of the network has not been taken into account and only short-term decisions are contemplated.

4.4. Case study

Both proposed MILP formulations have been applied to a case study based on a microgrid, in which the objective is the simultaneous management of energy supply and demand. Although the proposed formulations can be used to consider simultaneously multi-products, only one product (energy) is going to be taken into account. Additionally, the considered value of the conversion degree is 1, without considering a high degree of detail in the energy production process. This microgrid includes a photovoltaic panel ($i1$) and a micro-wind turbine ($i2$) as renewable energy sources, as well as a bidirectional connection to the power grid ($i3$) to purchase and to sell energy. The possibility to purchase energy to the power grid ensures the feasibility of the optimization problem, disregarding weather conditions and abnormal demand requirements. Also, an energy storage system k has been considered. The distances between all elements are neglected, so transport costs are not taken into account.

Moreover, 30 different appliances or consumers j have been taken into account, with different energy requirements $Cons_{j,f}$, which are assumed to admit a certain degree of flexibility in their respective targets, in terms of accepting some delay from their expected schedule. Each consumption has associated a penalty cost, to be applied in case of that such deviations from their respective targets are introduced. The power required by each consumer is assumed to be constant during each consumption. Data related to minimum/maximum initial time, duration and penalty cost associated to each energy consumption can be found in Table 4.5 (see the Appendix of this chapter). A penalty cost has been assigned according to the characteristics of each energy consumption. A schematic representation of the considered microgrid can be found in Figure 4.2.

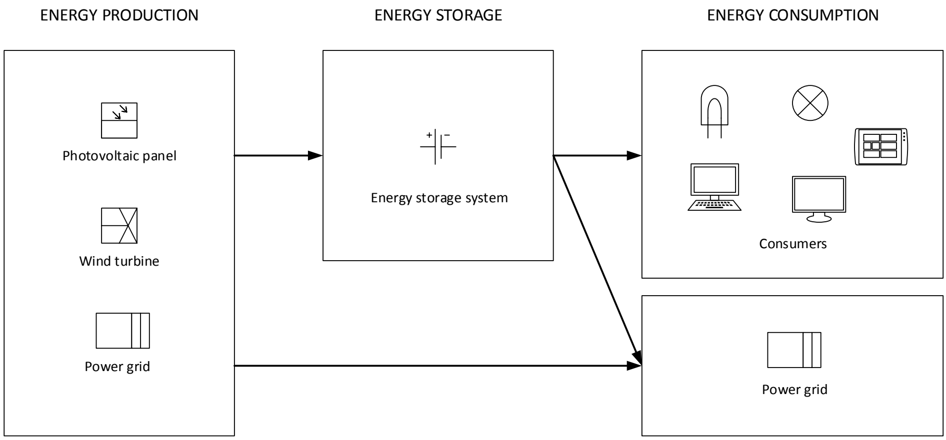

Figure 4.2. Schematic representation of the case study.

The results of the optimization procedure includes energy production, storage and consumption patterns. Decisions related to energy production are given every 15 minutes, according to the expected energy demand requirements and the anticipated energy availability resulting from the specific weather forecast. The considered time horizon extents to 24 hours, thus resulting in 96 time slots. According to the described discrete time model, decisions related to the consumption schedule are considered to be taken according to the indicated time grid (i.e., every 15 minutes), whereas in the hybrid time model, these decisions can be scheduled at any moment along the continuous time horizon.

Data related to energy production cost for each generator and energy storage cost are presented in Table 4.1. Also, the same table displays the minimum/maximum values for power supply and energy storage as well as other economic data. Variable production costs related to the energy production through solar panels and wind turbines are considered to be zero.

Table 4.1. Economic data and capacity constraints.

Unit	Description	$cpro_{i,t}$ or $csto_{k,t}$ (m.u. / kWh)	P_i^{min} (kW)	SE_k^{min} (kWh)	SE_k^{max} (kWh)	α_k (-)
i1	Photovoltaic panel	0	0	-	-	-
i2	Wind turbine	0	0	-	-	-
i3	Power grid	0.153	0	-	-	-
k1	Energy storage system	$1{\cdot}10^{-4}$	-	13.44	16.80	0.0

4.5. Results

Different scenarios and solution approaches have been considered in order to compare, analyse and highlight the characteristics of the proposed models, including:

(i) the absence of demand management opportunities (energy demands cannot be shifted),
(ii) demand management using the discrete time model and,
(iii) demand management using the hybrid time model.

The resulting MILP models have been implemented in GAMS 24.1 (Rosenthal, 2012) and solved using CPLEX 12, in a Pentium Intel® Core™ i7 CPU 2600 @ 3.40 GHz, with 8.00 GB of installed memory (RAM).

The same power availability (Figure 4.3) has been assumed for the three solution approaches. Also, the energy storage level has been forced to be equal at the beginning and at the end of the scheduling horizon in order to ensure a fair comparison among the different obtained solutions.

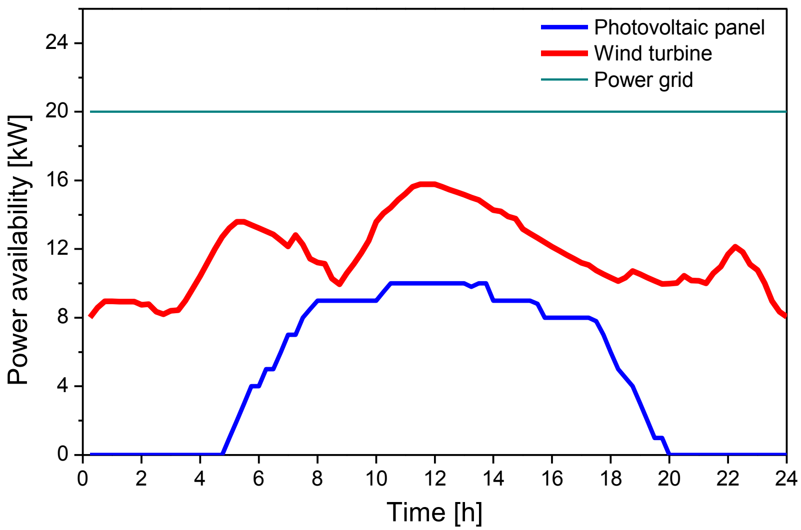

Figure 4.3. Power availability.

In the first situation (i), only production management is considered. The energy storage system is the only resource to be used in order to optimize the match between production and demand, since energy requirements do not match energy availability. The resulting energy storage level profile is represented in Figure 4.5. The solution in this case shows that the generation (and storage) of energy from renewable sources is insufficient to timely satisfy the set of fixed energy consumptions, so the purchase of energy from the power grid is required (Figure 4.4a). Figure 4.7a shows the optimum energy consumptions schedule obtained with this model.

The characteristics of the model proposed for the second situation (ii) allows to consider the possibility of delaying energy consumptions at the expense of a penalty cost for each delay. The optimum decisions in this case would lead to the independence from the power grid, so external energy purchases are not required to satisfy the energy demand (Figure 4.4b and Table 4.3). In this case, some energy consumptions have been delayed one or more complete time intervals (15 minutes). The total accumulate delay is up to 19.35 hours (Table 4.2). These are delays are due to:

- The granularity of the model: The discrete time model forces all consumptions to start at the beginning of one time interval. Thus, all consumptions have been delayed to start in the boundary of the corresponding time interval, involving solutions qualitatively different. In this particular case study, this represents almost 40 % of the total accumulated delay.
- The decision making process itself which, in order to optimize the matching between production and demand, and the associated penalties, introduces additional changes. These quantitative differences results in about 60 % of the total accumulated time delay in this case study.

The third approach (iii) corresponds to the proposed hybrid time representation. Also with this model, the simultaneous management allows to satisfy the overall energy demand without acquiring energy from the grid, at the expense of introducing consumption delays. Actually, the same energy production profile from the renewable (cheap) sources is obtained in all cases (Figure 4.4b and Table 4.3), since the microgrid should use all the available energy from renewable sources at their maximum capacity, and to sell the excess to the power grid (Figure 4.6). Although energy purchases from the power grid are shown in Figure 3, this acquisition takes place only in the case with non demand-side management, but not in the cases with demand- side management, which do not require external purchases. But in this case the value of the objective function is improved since the delays in the consumptions may be better adjusted (Figure 4.7c), and the penalty cost may be reduced accordingly. Now the total delay in the optimum case was 11.97 hours (Table 4.2). Obviously, and unlike the discrete model, only delays due to the decision making process are introduced.

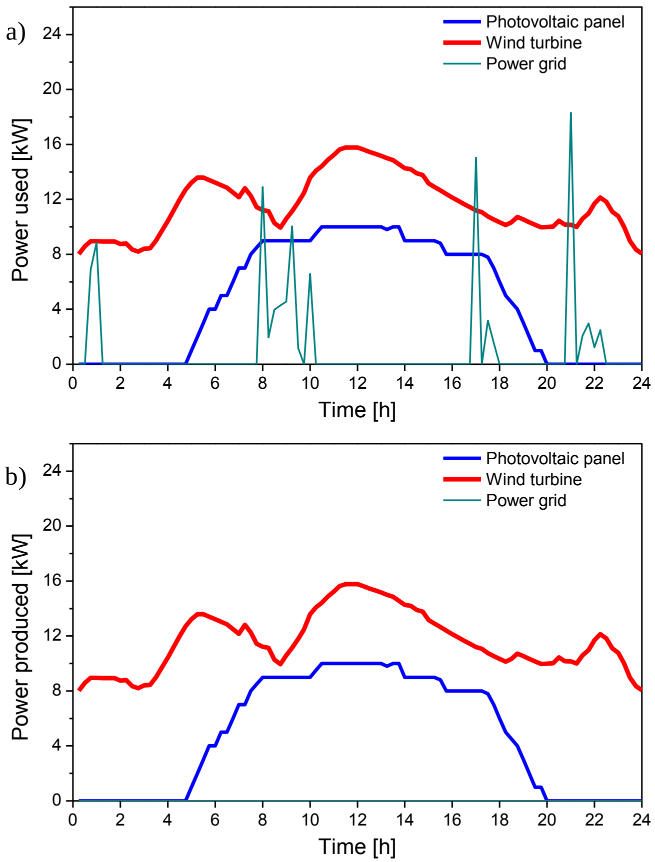

Figure 4.4. Power source in each time period
a) no-demand side management, b) demand side management using both the discrete and the hybrid time model.

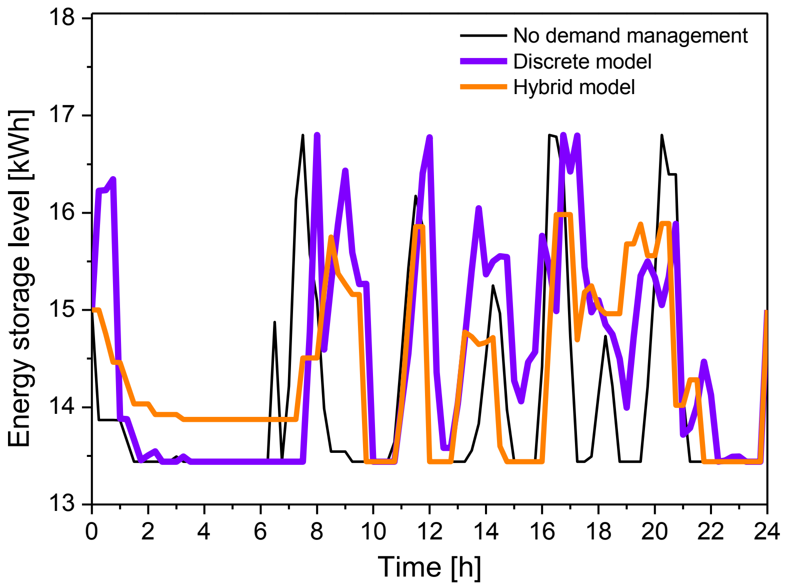

Figure 4.5. Energy storage level.

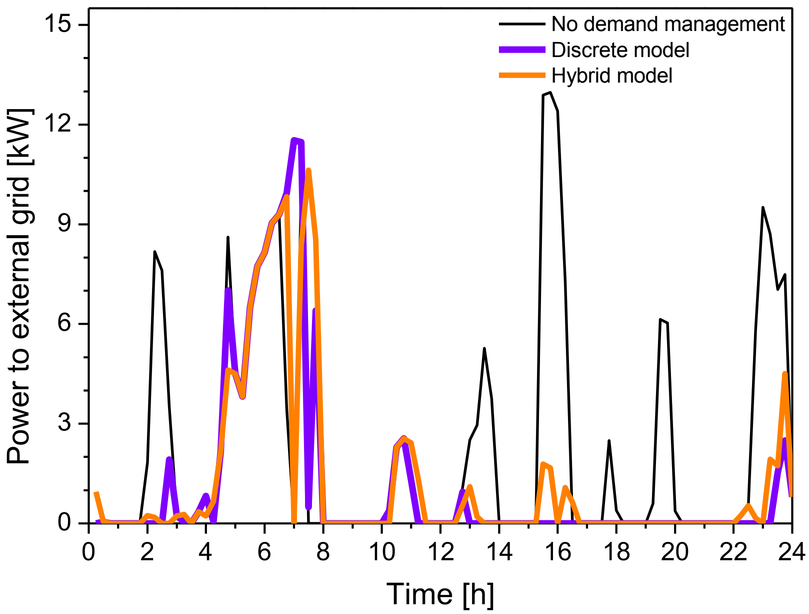

Figure 4.6. Power to the external power grid.

Table 4.2. Delays produced in each energy consumption.

Energy consumer *j*	Energy demand *f*	Delay using discrete time formulation with time interval of 15 minutes (h)		Delay using hybrid time formulation (h)
		Granularity	Decision	Decision
j5	f10	0.075	0.00	0.004
j5	f12	0.125	0.00	0.035
j6	f1	0.075	0.00	0.184
j7	f1	0.225	0.50	0.785
j7	f2	0.125	0.00	0.125
j7	f6	0.000	0.00	0.012
j7	f9	0.050	0.00	0.118
j7	f10	0.125	0.00	0.070
j11	f1	0.125	0.50	0.576
j14	f1	0.000	0.25	0.000
j15	f1	0.075	1.75	1.797
j16	f1	0.050	0.50	0.484
j19	f1	0.225	0.50	0.475
j19	f2	0.025	0.00	0.030
j20	f3	0.225	0.25	0.000
j21	f1	0.150	0.25	0.475
j22	f1	0.200	1.25	1.346
j22	f2	0.125	1.00	1.024
j23	f1	0.150	1.00	0.964
j24	f1	0.225	0.25	0.090
j24	f2	0.000	0.25	0.130
j25	f1	0.125	0.25	0.400
j27	f1	0.175	0.25	0.000
j28	f1	0.025	0.25	0.000
j29	f1	0.075	1.50	1.575
j29	f2	0.000	0.50	0.356
j30	f1	0.075	0.25	0.239
j31	f1	0.175	0.50	0.675
Other		4.575	0.00	0.000
Total delay (h)		7.600	11.750	11.696
		19.350		

The absence of energy demand management involves energy purchases in order to satisfy power peaks which can be avoided by the non-shifted demand. However, in this particular case study (Table 4.3), the simultaneous energy production and demand management would allow the independence of the microgrid from the power grid, since energy purchases are not required to satisfy the global energy demand. Not surprisingly, all renewable sources (photovoltaic panel and wind turbine) are always switched on, in order to satisfy the energy demand, to store energy or to sell energy to the power grid. This management will lead to purchase energy only if using renewable sources (which involve less production cost) and the energy storage system are not enough. Delays are introduced in the demand side management models as much as costs related to the production through renewable and the penalty associated to the initial target are below energy purchase costs.

Table 4.3. Comparison of the obtained results through the different solution approaches.

Unit	No demand management	Discrete time model	Hybrid time model
Profit (m.u.)	2.63	3.08	3.51
Incomes (m.u.)	6.60	3.41	3.66
Production cost (m.u.)	3.97	0.00	0.00
Penalty cost (m.u.)	0.00	0.33	0.15
Consumed energy (kWh)	359.0	359.0	359.0
Energy produced or purchased (kWh)	417.9	391.9	391.9
Energy from photovoltaic panels (kWh)	112.7	112.7	112.7
Energy from wind turbines (kWh)	279.2	279.2	279.2
Energy from power grid (kWh)	26.0	0.0	0.0
Energy from storage systems (kWh)	17.1	19.3	10.7
Energy sold to the power grid (kWh)	55.0	28.5	30.5
Energy loses and load the energy storage system (kWh)	21.0	23.7	13.1

Figure 4.7 summarizes the main optimum decisions obtained using each one of the 3 presented solution approaches. In general, the introduction of delays is proposed in those energy requirements expected to start in the time slots in which the energy from less expensive sources is not enough, but the need to match decisions with a pre-stablished time grid (discrete time formulation) may introduce some unexpected behaviour.

Some of these cases can be analysed and compared in more detail in Figure 4.8: As an example, using the discrete time formulation a significant deviation from its initial target was proposed to consumer $j27$ since the consumption cannot start until the beginning of the next time interval (due to the granularity of the model) and at this boundary of the time interval the optimal decision is to delay the consumption again because the lack of availability in the energy generation system. On the contrary, using the hybrid time model the possibility to satisfy this particular consumption according to its target is recognized so no delay was proposed at all.

Table 4.4 shows that, although the two time-representations involve the same number of discrete variables, the hybrid time representation model requires more equations and more continuous variables, as well as a substantial increase in the computational effort in order to determine the optimal solution. Moreover, in order to study how the length of the time interval affects the solution and the computational time, the same problem has been solved using different time interval sizes (Table 4.4). The solution using the discrete time formulation is improved when the length of the time interval decreases, since the model becomes more sensitive and delays due to the granularity of the model are reduced. But obviously, the computational effort increases when the duration of the time interval is reduced, since more binary variables are required in order to define the model. It is worthy to mention that the solution for the discrete time model using a time interval of 1 minute could not be obtained because the memory requirements exceeded that capacity of the computational system used for these tests. This was also the case of the hybrid model with time intervals of 5 and 3 minutes.

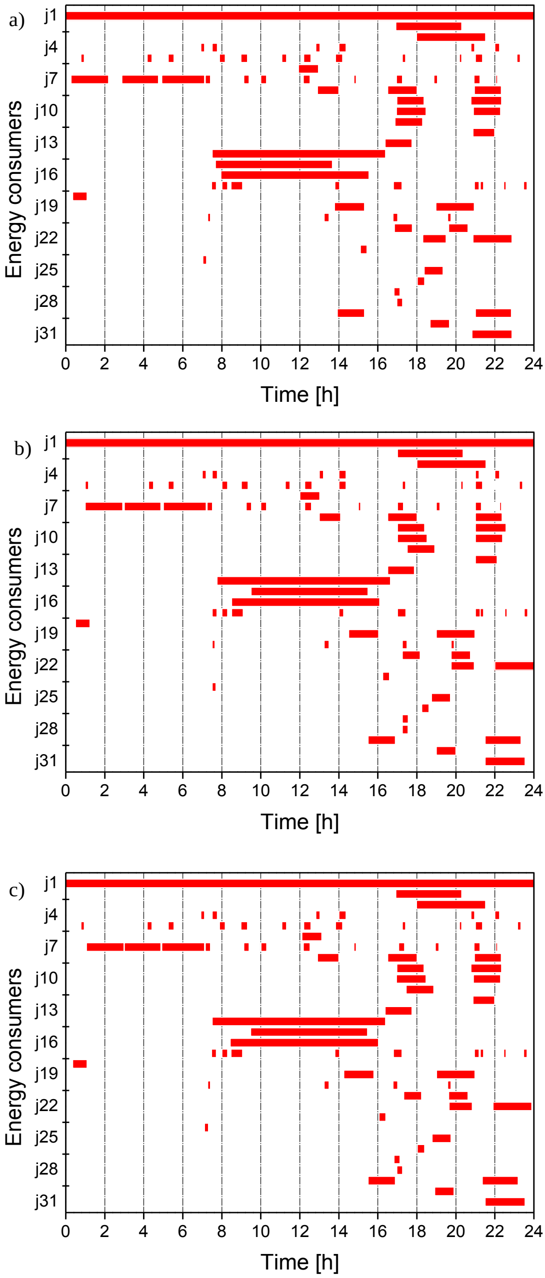

Figure 4.7. Active energy consumers in each time period
a) no-demand side management and the demand side management using b) discrete model and c) hybrid model.

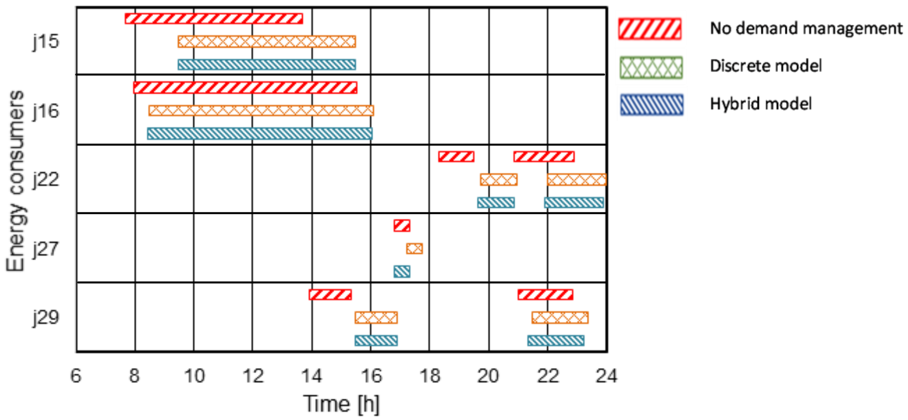

Figure 4.8. Comparison of the consumption schedule for some energy consumptions.

Table 4.4. Comparison of optimal solution and model statistics.

Key performance indicator	dt = 15 min		dt = 5 min	dt = 3 min
	Discrete time model	Hybrid time model	Discrete time model	Discrete time model
Profit (economic units)	3.30	3.51	3.42	3.50
Equations	93,606	312,978	582,726	1,477,350
Continuous variables	54,615	76,626	328,599	823,767
Binary variables	33,468	33,468	210,554	535,034
Generation time (CPU, s)	4.1	6.1	71.5	302.5
Resource time (CPU, s)	0.8	242.7	10.5	31.8
Total computational time (CPU, s)	4.9	248.8	82.0	334.3
Memory required (Mb)	128	176	2,086	8,581
Relative gap (%)	0	< 1	0	0
Requirements	GAMS 24.1 / CPLEX 12 Pentium Intel® Core™ i7 CPU 2600 @ 3.40 GHz			

4.6. Concluding remarks

This chapter addresses the short-term scheduling problem of a supply chain in order to determine optimal decisions in terms of both energy production and demand. This is achieved by maximizing an economic objective function including penalties for the delayed fulfilment of the demand requirements. In order to solve the inconveniences shown by traditional discrete and continuous time representations to manage the decision making process at both the production and at the demand sides simultaneously, a new hybrid time formulation, combining elements from both discrete and continuous time representations, is presented, and the resulting discrete and hybrid MILP formulations have been presented and discussed.

The obtained results demonstrate that the proposed model is able to address, with high level of confidence, the short-term daily scheduling problem of a supply chain for a given horizon using both time representations, and to take profit of the advantages of the potential flexibility in the energy demand-side, which would allow enhancing the efficiency and autonomy of the supply chain. In the proposed case-study, the obtained results show how the introduction of flexibility in the demand-side allows an improvement in the value of the objective up to 17% and 33% through the use of the discrete and hybrid time formulations, respectively, when a time interval of 15 minutes are considered to solve its daily horizon. In addition, the hybrid time representation proposed improves the results due to a better adjust of the required starting time of consumptions, which improves the robustness of the model and the value of the optimal solution. This improvement is achieved at the expense of an increase in the complexity of the model, which results in an affordable increase in the required computational effort. Furthermore, as the length of the time interval in the discrete time formulation decreases, the value of the objective function is improved and closes the gap from the hybrid time representation.

The presented formulations can be extended by incorporating uncertainty related to weather conditions effects in energy suppliers and energy demand variations, through the implementation of the rolling horizon approach and the stochastic programming (see Chapter 5).

4.7. Nomenclature

Indexes and sets

$i \in I$	*Production sources*
$j \in J$	*Consumers*
$f \in F$	*Demands*
$jf \in F_j$	*Subset of demands associated to a consumer* j
$k \in K$	*Storage systems*
$m \in M$	*Products, materials, utilities or resources (product)*
$m \in PR$	*Subset of manufactured products* m
$m \in RM$	*Subset of raw material products* m
$r \in R$	*External market*
$t \in T$	*Time intervals included in the overall scheduling horizon*

Parameters

$Cons_{j,f,m}$	*Individual consumption* jf *of product* m
$cpen_{j,f,m}$	*Penalty cost associated to consumption* jf *of product* m
$cpro_{i,m,t}$	*Production (or purchase) cost of product* m *in source* i *at time* t
$csto_{k,m,t}$	*Storage cost of product* m *in storage system* k *at time* t
$ctrp_{i,j,m}$	*Transport cost of product* m *from production location* i *to consumer* j
$ctrp_{i,r,m}$	*Transport cost of product* m *from production location* i *to market* r
DT	*Duration of the time interval*
$Dur_{j,f,m}$	*Duration of consumption* jf *of product* m
$\overline{Dur}_{j,f,m}$	*Round up value of the duration of consumption* jf *of product* m
$P_{i,m,t}^{min}$	*Minimum supply of product* m *from source* i *at interval* t
$P_{i,m,t}^{max}$	*Maximum supply of product* m *from source* i *at interval* t
$Price_{r,m,t}$	*Price to be sold product* m *to the external market* r *at interval* t
$SE_{k,m,t}^{min}$	*Minimum storage level of product* m *in storage system* k *at interval* t
$SE_{k,m,t}^{max}$	*Maximum storage level of product* m *in storage system* k *at interval* t
$SE_{0k,m,t}$	*Initial storage level of product* m *in system* k *at interval* t
Tp_m	*Processing time to obtain product* m
$Ts_{j,f,m}^{max}$	*Maximum initial time of consumption* jf *of product* m
$Ts_{j,f,m}^{min}$	*Target initial time of consumption* jf *of product* m
ρ_m	*Conversion degree of product* m
$\eta_{k,m}^{in}$	*Charging efficiency of storage system* k *of product* m
$\eta_{k,m}^{out}$	*Discharging efficiency of storage system* k *of product* m

Continuous and positive variables

$Benefit$	*Supply chain benefit*
$CostPen$	*Supply chain penalty cost*
$CostPro$	*Supply chain production cost*
$CostSto$	*Supply chain storage cost*
$CostTrp$	*Supply chain transport cost*
$Dem_{m,t}$	*Total consumption at interval* t *of product* m
$Incomes$	*Supply chain incomes*
$Ld_{k,m,t}$	*Amount of product* m *supplied to load system* k *during interval* t
$P_{i,m,t}$	*Amount of product* m *supplied from source* i *at interval* t
$Pg_{r,m,t}$	*Amount of product* m *supplied to external market* r *at interval t*
$Profit$	*Total profit along the scheduling horizon (objective function)*

$PT_{m,t}$	*Amount of product m supplied at interval t*
$SE_{k,m,t}$	*Storage level of product m in system k at the end of the interval t*
$SP_{k,m,t}$	*Amount of product m supplied by storage system k during interval t*
$Tf_{j,f,m}$	*Finishing time of consumption jf of product m*
$Ts_{j,f,m}$	*Starting time of consumption jf of product m*
T_t	*Time corresponding to time interval t*
$XDem_{j,f,m,t}$	*Period of time in which consumption jf of product m is active at interval t*

Binary variables

$X_{i,m,t}$	*= 1, if production source i is used at interval t to supply product m*
$Y_{j,f,m,t}$	*= 1, if consumption jf of product m starts at interval t*
$Z_{j,f,m,t}$	*= 1, if consumption jf of product m finishes at interval t*
$W_{j,f,m,t}$	*= 1, if consumption jf of product m is active at interval t*

4.8. Appendix

Table 4.5. Input parameters.

Energy consumer *j*	Energy demand *f*	$Cons_{j,f}$ (kW)	$Ts_{j.f}^{min}$ (h)	*Dur$_{j,f}$* (h)	$Tf_{j.f}^{max}$ (h)	Penalty cost (m.u./h)
j1	f1	2.557	0.000	0.250	0.250	40
j1	f2	1.012	0.250	0.250	0.500	40
j1	f3	0.957	0.500	0.250	0.750	40
j1	f4	0.916	0.750	0.250	1.000	40
j1	f5	0.955	1.000	0.250	1.250	40
j1	f6	1.693	1.250	0.250	1.500	40
j1	f7	1.705	1.500	0.250	1.750	40
j1	f8	0.520	1.750	0.250	2.000	40
j1	f9	0.605	2.000	0.250	2.250	40
j1	f10	0.728	2.250	0.250	2.500	40
j1	f11	0.683	2.500	0.250	2.750	40
j1	f12	0.174	2.750	0.250	3.000	40
j1	f13	0.157	3.000	0.250	3.250	40
j1	f14	1.187	3.250	0.250	3.500	40
j1	f15	1.341	3.500	0.250	3.750	40
j1	f16	1.606	3.750	0.250	4.000	40
j1	f17	1.143	4.000	0.250	4.250	40
j1	f18	1.843	4.250	0.250	4.500	40
j1	f19	1.684	4.500	0.250	4.750	40
j1	f20	1.719	4.750	0.250	5.000	40
j1	f21	1.776	5.000	0.250	5.250	40
j1	f22	1.686	5.250	0.250	5.500	40
j1	f23	1.672	5.500	0.250	5.750	40
j1	f24	1.070	5.750	0.250	6.000	40
j1	f25	1.008	6.000	0.250	6.250	40
j1	f26	0.565	6.250	0.250	6.500	40
j1	f27	0.565	6.500	0.250	6.750	40
j1	f28	0.945	6.750	0.250	7.000	40

Energy consumer *j*	Energy demand *f*	$Cons_{j,f}$ (kW)	$Ts_{j.f}^{min}$ (h)	$Dur_{j,f}$ (h)	$Tf_{j.f}^{max}$ (h)	Penalty cost (m.u./h)
j1	f29	0.335	7.000	0.250	7.250	40
j1	f30	0.492	7.250	0.250	7.500	40
j1	f31	0.560	7.500	0.250	7.750	40
j1	f32	0.233	7.750	0.250	8.000	40
j1	f33	0.288	8.000	0.250	8.250	40
j1	f34	0.260	8.250	0.250	8.500	40
j1	f35	0.230	8.500	0.250	8.750	40
j1	f36	0.348	8.750	0.250	9.000	40
j1	f37	0.386	9.000	0.250	9.250	40
j1	f38	0.163	9.250	0.250	9.500	40
j1	f39	0.481	9.500	0.250	9.750	40
j1	f40	0.168	9.750	0.250	10.000	40
j1	f41	0.600	10.000	0.250	10.250	40
j1	f42	1.129	10.250	0.250	10.500	40
j1	f43	1.311	10.500	0.250	10.750	40
j1	f44	0.400	10.750	0.250	11.000	40
j1	f45	0.200	11.000	0.250	11.250	40
j1	f46	0.655	11.250	0.250	11.500	40
j1	f47	0.694	11.500	0.250	11.750	40
j1	f48	0.494	11.750	0.250	12.000	40
j1	f49	0.681	12.000	0.250	12.250	40
j1	f50	0.436	12.250	0.250	12.500	40
j1	f51	0.723	12.500	0.250	12.750	40
j1	f52	1.195	12.750	0.250	13.000	40
j1	f53	0.212	13.000	0.250	13.250	40
j1	f54	0.295	13.250	0.250	13.500	40
j1	f55	0.342	13.500	0.250	13.750	40
j1	f56	0.209	13.750	0.250	14.000	40
j1	f57	0.421	14.000	0.250	14.250	40
j1	f58	0.179	14.250	0.250	14.500	40
j1	f59	0.296	14.500	0.250	14.750	40
j1	f60	0.236	14.750	0.250	15.000	40
j1	f61	0.174	15.000	0.250	15.250	40
j1	f62	0.155	15.250	0.250	15.500	40
j1	f63	0.423	15.500	0.250	15.750	40
j1	f64	0.734	15.750	0.250	16.000	40
j1	f65	0.075	16.000	0.250	16.250	40
j1	f66	0.680	16.250	0.250	16.500	40
j1	f67	0.573	16.500	0.250	16.750	40
j1	f68	0.171	16.750	0.250	17.000	40
j1	f69	0.465	17.000	0.250	17.250	40
j1	f70	0.461	17.250	0.250	17.500	40
j1	f71	0.479	17.500	0.250	17.750	40
j1	f72	0.010	17.750	0.250	18.000	40
j1	f73	0.457	18.000	0.250	18.250	40
j1	f74	0.077	18.250	0.250	18.500	40
j1	f75	0.224	18.500	0.250	18.750	40
j1	f76	0.632	18.750	0.250	19.000	40
j1	f77	0.441	19.000	0.250	19.250	40
j1	f78	0.028	19.250	0.250	19.500	40
j1	f79	0.088	19.500	0.250	19.750	40

Energy consumer *j*	Energy demand *f*	$Cons_{j,f}$ (kW)	$Ts_{j.f}^{min}$ (h)	$Dur_{j,f}$ (h)	$Tf_{j.f}^{max}$ (h)	Penalty cost (m.u./h)
j1	f80	0.743	19.750	0.250	20.000	40
j1	f81	0.931	20.000	0.250	20.250	40
j1	f82	0.792	20.250	0.250	20.500	40
j1	f83	0.906	20.500	0.250	20.750	40
j1	f84	1.299	20.750	0.250	21.000	40
j1	f85	0.918	21.000	0.250	21.250	40
j1	f86	0.894	21.250	0.250	21.500	40
j1	f87	0.572	21.500	0.250	21.750	40
j1	f88	0.193	21.750	0.250	22.000	40
j1	f89	0.725	22.000	0.250	22.250	40
j1	f90	0.187	22.250	0.250	22.500	40
j1	f91	0.443	22.500	0.250	22.750	40
j1	f92	0.259	22.750	0.250	23.000	40
j1	f93	0.689	23.000	0.250	23.250	40
j1	f94	0.631	23.250	0.250	23.500	40
j1	f95	0.862	23.500	0.250	23.750	40
j1	f96	0.312	23.750	0.250	24.000	40
j2	f1	1.500	16.675	3.375	20.250	0.4
j3	f1	1.500	17.725	3.550	21.500	0.4
j4	f1	0.350	6.675	0.200	7.000	0.04
j4	f2	0.350	7.250	0.275	7.750	0.04
j4	f3	0.350	12.575	0.213	13.000	0.04
j4	f4	0.350	13.750	0.375	14.250	0.04
j4	f5	0.350	20.525	0.198	21.000	0.04
j4	f6	0.350	21.750	0.250	22.000	0.04
j5	f1	2.000	0.525	0.175	1.000	0.04
j5	f2	2.000	3.925	0.250	4.250	0.04
j5	f3	2.000	5.000	0.300	5.500	0.04
j5	f4	2.000	7.625	0.300	8.250	0.04
j5	f5	2.000	8.725	0.350	9.250	0.04
j5	f6	2.000	10.825	0.250	11.250	0.04
j5	f7	2.000	11.950	0.375	12.500	0.04
j5	f8	2.000	13.575	0.375	14.250	0.04
j5	f9	2.000	17.000	0.175	17.250	0.04
j5	f10	2.000	19.925	0.125	20.250	0.04
j5	f11	2.000	20.750	0.375	21.250	0.04
j5	f12	2.000	22.875	0.175	23.250	0.04
j6	f1	2.640	11.675	1.025	13.000	0.04
j7	f1	8.000	0.025	1.925	2.750	0.04
j7	f2	8.000	2.625	1.875	5.000	0.04
j7	f3	8.000	4.675	2.200	7.250	0.04
j7	f4	8.000	6.900	0.275	7.500	0.04
j7	f5	8.000	8.875	0.275	9.500	0.04
j7	f6	8.000	9.750	0.300	10.250	0.04
j7	f7	8.000	11.925	0.350	12.500	0.04
j7	f8	8.000	14.525	0.125	15.000	0.04
j7	f9	8.000	16.700	0.313	17.250	0.04
j7	f10	8.000	18.625	0.188	19.000	0.04
j7	f11	8.000	20.675	0.313	21.250	0.04
j7	f12	8.000	21.800	0.088	22.750	0.04
j8	f1	0.400	12.650	1.100	14.250	0.02

Energy consumer *j*	Energy demand *f*	$Cons_{j,f}$ (kW)	$Ts_{j.f}^{min}$ (h)	$Dur_{j,f}$ (h)	$Tf_{j.f}^{max}$ (h)	Penalty cost (m.u./h)
j8	f2	0.400	16.250	1.525	18.250	0.02
j8	f3	0.400	20.700	1.375	22.750	0.02
j9	f1	0.240	16.725	1.400	18.500	0.02
j9	f2	0.240	20.525	1.575	23.000	0.02
j10	f1	0.240	16.700	1.525	18.750	0.02
j10	f2	0.240	20.650	1.400	22.750	0.02
j11	f1	12.000	16.625	1.425	19.250	0.02
j12	f1	2.000	20.625	1.125	22.250	0.02
j13	f1	8.000	16.125	1.375	18.000	0.02
j14	f1	7.000	7.250	8.900	16.750	0.02
j15	f1	7.000	7.425	6.000	15.750	0.02
j16	f1	7.000	7.700	7.600	16.250	0.02
j17	f1	2.000	7.225	0.250	7.750	0.02
j17	f2	2.000	7.750	0.300	8.250	0.02
j17	f3	2.000	8.225	0.600	9.250	0.02
j17	f4	2.000	13.550	0.250	14.500	0.02
j17	f5	2.000	16.550	0.438	17.500	0.02
j17	f6	2.000	20.700	0.250	21.000	0.02
j17	f7	2.000	21.000	0.175	21.750	0.02
j17	f8	2.000	22.200	0.125	22.750	0.02
j17	f9	2.000	23.225	0.188	23.500	0.02
j18	f1	7.500	0.100	0.750	1.500	0.02
j19	f1	1.500	13.525	1.550	16.250	0.02
j19	f2	1.500	18.725	1.975	21.000	0.02
j20	f1	0.240	7.025	0.150	7.750	0.004
j20	f2	0.240	13.000	0.250	13.500	0.004
j20	f3	0.240	16.525	0.250	17.250	0.004
j20	f4	0.240	19.325	0.175	19.750	0.004
j21	f1	0.350	16.600	0.925	18.000	0.004
j21	f2	0.350	19.375	1.000	20.500	0.004
j22	f1	5.000	18.050	1.200	20.750	0.004
j22	f2	5.000	20.625	2.000	23.750	0.004
j23	f1	10.000	14.850	0.350	16.750	0.004
j24	f1	20.000	6.775	0.200	7.500	0.004
j24	f2	20.000	7.750	0.250	10.000	0.004
j25	f1	4.000	18.125	0.975	19.750	0.004
j26	f1	0.192	17.775	0.375	18.750	0.004
j27	f1	0.440	16.575	0.313	17.500	0.004
j28	f1	0.660	16.725	0.300	17.500	0.004
j29	f1	4.000	13.675	1.400	17.000	0.004
j29	f2	4.000	20.750	1.850	23.500	0.004
j30	f1	0.200	18.425	1.000	19.750	0.004
j31	f1	1.500	20.575	2.050	23.750	0.004

Chapter 5. Reactive scheduling for uncertainty management

Chapter 4 describes a methodology to manage simultaneously production and demand under deterministic conditions. However, the decision making process associated becomes more complex as the model considers eventual variabilities within the process. This fact involves that the complexity in the decision making process arises by the need to consider a certain degree of uncertainty in the models used to forecast the events that should be considered. Many published works in this area explicitly addressed the problem associated with uncertainty in the available data.

This chapter continues the development of optimization-based scheduling strategies for the coordination of production networks started in the previous section. The main novelty there (the simultaneous management of production and demand) is now integrated within a reactive and/or proactive scheduling approach to deal with the presence of uncertainty associated to production and consumption. Delays in the nominal demands are still accepted under associated penalty costs to tackle flexible and fluctuating demand profiles.

This methodology is again applied to a case study based on a microgrid structure studied consists of renewable energy generators and energy storage units that alleviate the main drawback of such systems which is the mismatch between energy production and demand. Consequently, a MILP formulation is presented and used in a stochastic rolling horizon scheme that periodically updates input data information.

5.1. Introduction

The operations management of production processes is affected by several types of uncertainty, such as demand variations. Therefore, the uncertainty must be consider in order to ensure the generation of feasible solutions of good quality and practical interest. The decision making process become more complex when the consideration of different sources of uncertainty in the models is essential to ensure the quality of the solution or even its practical feasibility. Different types of uncertainty sources can be found, including:

(i) External sources, including uncertainty in demand, prices and availability of resources.
(ii) Internal sources, like fluctuations in process parameters.
(iii) Other sources, such as measurements errors or strikes.

The approaches to address scheduling problems under uncertainty could be classified into reactive and proactive. On one hand, reactive approaches focus on modifying a nominal schedule obtained by a deterministic formulation in order to adjust it to different alterations, modifications or updated system data. On the other hand, proactive approaches are based on the consideration of all possible cases, and finding a good solution for all these cases. These approaches have the advantage that a feasible solution is found for all considered scenarios. However, this solution may be too conservative, since the model must take into account all the possibilities even the ones that do not occur eventually. The most broadly used proactive approaches are stochastic programming (Shapiro et al., 2013) and robust optimization (Li et al., 2011).

In this chapter, a discrete time MILP mathematical formulation is presented to cope with the underlying uncertainty through a rolling horizon approach with the purpose to optimally manage a SC (i.e., schedule the production and consumption). This approach will allow to update all input parameters and to react to any variation from the nominal or expected conditions. One of the main elements for the optimization of the SC operation problem is scheduling. But the term scheduling actually embraces several decisions (degrees of freedom), as unit assignment or timing decisions. The resulting optimization models may be different in terms of their capacity to manage a generalized SC network structure, their capacity to manage several technical constraints, and also the way in which the different types of uncertainty are addressed in the problem of interest. This chapter focuses on this last point. This approach considers: a prediction horizon, in which all the uncertain parameters related to this time horizon are assumed to be known with certainty, due to the fact that the system under study receives feedback related to the unknown parameters, and a control horizon, where the decisions of the optimization for the prediction horizon are applied. Although the use of rolling horizon strategies to scheduling problems in uncertain scenarios is well-known, its application to SCs and also the exploitation of the demand side flexibility to improve the matching between production and demand constitute a challenge in this area. For this reason, this chapter emphasizes on the simultaneous optimization of production and demand side management as a means for improved decision making of scheduling problems in supply chains.

5.2. Problem statement

As in Chapter 4, the system under study consists of a set of interconnected elements (i.e., producers/generators, storages, consumptions) as well as a set of decisions (when, where, who, how much) that define a managerial problem (resource allocation and timing). Unlike the Chapter 4, the problem is formulated under uncertain conditions.

The proposed formulation takes into account not only the production and storage levels to be managed by the supply chain, but also the possibility to modify the timing of any consumption within a certain time window, if this is considered acceptable. The proposed formulation contemplates that the consumption can take place within the supply chain as well as sales to external markets. Costs involved in the process are considered, including production and storage costs, as well as penalty costs in case of deviations from the consumers' target, in order to maximize the profit. The mathematical model includes both the balance constraints required to describe the flows (generation, storage and consumption), and the constraints associated to the equipment and technologies involved in the supply chain. Consequently, the problem under study is described in terms of the following items:

(i) A given scheduling horizon SH, which is divided into a number of equal-size time intervals $t \in T$. Also, a given Prediction Horizon PH and a Control Horizon CH.

(ii) A set of producers/generators $i \in I$, characterized by a minimum and maximum production capacity, $P_{i,t}^{min}$ and $P_{i,t}^{max}$, and a given operational cost $cpro_{i,t}$.

(iii) A set of storage systems $k \in K$, having a minimum and a maximum storage capacity, $SE_{k,t}^{min}$ and $SE_{k,t}^{max}$, and cost $csto_{k,t}$.

(iv) A set of products, materials, resources or utilities $m \in M$. Notice that although this term can be referred to different items, in order to abbreviate the explanation, only the term product will be used for this set.

(v) A set of demands, given by the amount of requirements related to different consumption tasks jf, where $f \in F_j$ denotes the number of times that a consumer j can be active. For any consumption, its duration $Dur_{0,j,f}$ and a target starting time $Ts_{j,f}^{min}$ are provided, although consumption tasks can be delayed within certain time limits generating a penalty cost $cpen_{j,f}$.

(vi) All consumption tasks which might be active during each iteration of the rolling horizon approach are included in the dynamic set F_jRH.

(vii) A given set of external markets $r \in R$, to sell the produced materials/resources.

The proposed reactive scheduling problem has been introduced into an iterative approach based on a rolling horizon framework (see Chapter 3.5.3), which allows to upload or modify the different parameters related to the uncertainty, including both internal and external variability. As previously mentioned (Chapter 3.5.3), the solution obtained in each prediction horizon is expected to be optimal for this period of time. However, this solution can be suboptimal since future information outside the current prediction horizon is not considered. Hence, the length of the prediction horizon, which depends on the characteristics of each problem, must be adequate to guarantee high quality in the results.

Thus, the main decisions to be made in order to maximize the profit of the supply chain, are:

- (i) The production level P_t to be produced (or purchased) in each time interval t.
- (ii) The producers/generators that are in operation $X_{i,t}$ in each time interval t.
- (iii) The storage level $SE_{k,t}$ during time interval t.
- (iv) The specific (nominal) time to execute a consumption.
- (v) The amount of materials/resources $Pg_{r,t}$ to be sold to the external market r in each time interval t.

It is worth noting that the presented formulation is based on a discrete time representation, in which the scheduling horizon is divided in a finite number of identical time intervals. This representation of time forces the tasks to start at the beginning of each time interval. The computational time to solve discrete time models depends on the size of the problem, which strongly depends on the number of time intervals of the prediction horizon PH. The length of the time interval depends on the characteristics of the problem under consideration, since long time intervals could lead to suboptimal solutions, and short time intervals could imply an unaffordable computational effort to reach the optimal solution.

5.3. Mathematical formulation

The discrete time mathematical formulation proposed in Chapter 4 is extended to incorporate the rolling horizon approach within the formulation, which introduces equations that allow to solve the problem iteratively. Despite the similarities with the mathematical model explained in Chapter 4, the full mathematical formulation is detailed, in order to avoid any misunderstood.

The constraints associated to sequencing, allocating of consumptions and resources, and distribution of a multi-product supply chain are next presented in the following discrete time and hybrid time MILP formulations.

Eq. (5.1) establishes a material balance, considering the raw material and its transformation to products m, by considering a conversion degree ρ_m between raw materials and products. Although the transformation of raw material are considered, the remaining equations are formulated for situations in which their transformation takes place or not, in order to generalise the proposed formulation. One of the limitations of this formulation is that the duration of the processing time Tp_m must be lower to the duration of the prediction horizon, which is the common situation, since the duration of the production horizon must be long enough to guarantee quality solutions. Production bounds for every producer/generator i (including material/resource purchases) are specified by eq. (5.2). For each source i of product m and time interval t included in the prediction horizon the binary variable $X_{i,m,t}$ indicates if this source is being used or not. Thus, the total amount of product m produced (or purchased) at each interval t is given by eq. (5.3):

$$\sum_{m \in RM} P_{i,m,t-Tp_m} = \rho_m \cdot \sum_{m \in PR} P_{i,m,t} \qquad \forall i, t \in TRH \qquad (5.1)$$

$$P_{i,m,t}^{min} \cdot X_{i,m,t} \leq P_{i,m,t} \leq P_{i,m,t}^{max} \cdot X_{i,m,t} \qquad \forall i, m, t \in TRH \qquad (5.2)$$

$$PT_{m,t} = \sum_{i \in I} P_{i,m,t} \qquad \forall m, t \in TRH \qquad (5.3)$$

The amount of product m in each storage k at each time interval t is bounded within a minimum value and a maximum value, which corresponds to the full storage level, as given by eq. (5.4). Eq. (5.5) represents the balance at a specific storage system and time for each product m. This equation considers the storage level $SE_{k,m,t}$, the requirements covered by the storage $SP_{k,t}$, the supply flows arriving to the storage $Ld_{k,m,t}$ and the input and output efficiency of the storage system η. The maximum level of flow arriving to the storage system k is bounded by eq. (5.6). Also, material/resource constraints related to the charge and discharge of the storage systems must be considered. Thus, eq. (5.7) indicates that the storage level variation in each storage k at each time interval t is bounded by a maximum variation level.

$$SE_{k,m,t}^{min} \leq SE_{k,m,t} \leq SE_{k,m,t}^{max} \qquad \forall k, m, t \in TRH \qquad (5.4)$$

$$SE_{k,m,t} = SE_{k,m,t-1} + \eta_{k,m}^{in} \cdot Ld_{k,m,t} - \frac{SP_{k,m,t}}{\eta_{k,m}^{out}} \qquad \forall k, m, t \in TRH \qquad (5.5)$$

$$0 \leq \sum_{k \in K} Ld_{k,m,t} \leq PT_{m,t} \cdot DT \qquad \forall m, t \in TRH \qquad (5.6)$$

$$-\alpha_{k,m} \cdot SE_{k,m,t}^{max} \leq SE_{k,m,t} - SE_{k,m,t-1} \leq \alpha_{k,m} \cdot SE_{k,m,t}^{max} \qquad \forall k, m, t \in TRH \qquad (5.7)$$

The proposed mathematical formulation allows to start the consumption tasks within a time window. Thus, the demand side management involves the determination of the starting time of each consumption jf of product m. Hence, some constraints are required regarding the time window within consumers j are allowed to consume for the f-th time. According to eq. (5.8), the starting time is bounded by a minimum (target) and a maximum initial time. Moreover, the final time of each consumption task jf is given by the starting time plus its duration, according to eq. (5.9).

$$Ts_{j,f,m}^{min} \leq Ts_{j,f,m} \leq Ts_{j,f,m}^{max} \qquad \forall j, f \in F_jRH, m \qquad (5.8)$$

$$Tf_{j,f,m} = Ts_{j,f,m} + Dur_{j,f,m} \qquad \forall j, f \in F_jRH, m \qquad (5.9)$$

The binary variable $Y_{j,f,m,t}$ is active (i.e., equal to 1) when the consumption jf of product m starts at time interval t. Accordingly, $Z_{j,f,m,t}$ is active if its consumption finishes its consumption at time interval t. These logical restrictions can be reformulated as a set of Big-M constraints, given by eq. (5.10)-(5.13):

$$Ts_{j,f,m} \geq T_t \quad - M \cdot \left(1 - Y_{j,f,m,t}\right) \qquad \forall j, f \in F_jRH, m, t \in TRH \qquad (5.10)$$

$$Ts_{j,f,m} \leq T_{t+1} - M \cdot \left(1 - Y_{j,f,m,t}\right) \qquad \forall j, f \in F_jRH, m, t \in TRH \qquad (5.11)$$

$$Tf_{j,f,m} \geq T_t \quad - M \cdot \left(1 - Z_{j,f,m,t}\right) \qquad \forall j, f \in F_jRH, m, t \in TRH \qquad (5.12)$$

$$Tf_{j,f,m} \leq T_{t+1} - M \cdot \left(1 - Z_{j,f,m,t}\right) \qquad \forall j, f \in F_jRH, m, t \in TRH \qquad (5.13)$$

Furthermore, any consumption of a given consumer cannot overlap in the same unit time:

$$Tf_{j,f,m} \leq Ts_{j,f',m} \qquad \forall j, f \in F_jRH, f' \in F_jRH, f < f', m \qquad (5.14)$$

Moreover, eq. (5.15) and (5.16) ensure a unique starting time for consumption jf. The binary variable $Y_{j,f,m,t}$ determines if consumption task jf starts during the current time interval included in the prediction horizon, and $\hat{Y}_{j,f,m}$ determines if this consumption starts outside this time interval, forcing that all consumptions must start in the scheduling horizon.

In the same way, eq. (5.17) and (5.18) determine the final time for consumption task jf. Also, eq. (5.19) establishes when each consumption task jf is active at time t.

$$\sum_{\substack{t \in T \\ T_t \leq Ts_{j,f}^{max}}} Y_{j,f,m,t} \leq 1 \qquad \forall j,f \in F_jRH, m \tag{5.15}$$

$$\hat{Y}_{j,f,m} + \sum_{t \in TRH} Y_{j,f,m,t} = 1 \qquad \forall j,f \in F_jRH, m \tag{5.16}$$

$$\sum_{\substack{t \in T \\ T_t \leq Tf_{j,f,m}^{max}}} Z_{j,f,m,t} \leq 1 \qquad \forall j,f \in F_jRH, m \tag{5.17}$$

$$\hat{Z}_{j,f,m} + \sum_{t \in TRH} Z_{j,f,m,t} = 1 \qquad \forall j,f \in F_jRH, m \tag{5.18}$$

$$W_{j,f,m,t} = \hat{Y}_{j,f,m} + \sum_{\substack{t' \in TRH \\ t \geq t'}} Y_{j,f,m,t'} - \hat{Z}_{j,f,m} - \sum_{\substack{t' \in TRH \\ t > t'}} Z_{j,f,m,t'} \qquad \forall j,f \in F_jRH, m, t \in TRH \tag{5.19}$$

The total demand of the supply chain at time interval t, determined by all the active consumption tasks jf of at this time interval t, is given by eq. (5.20). The second term of this equation determines the exact consumption for those time intervals in which the consumption will not take place during the overall time interval.

$$Dem_{m,t} = \sum_{j \in J} \sum_{f \in F_j} Cons_{j,f,m} \cdot DT \cdot \left[W_{j,f,m,t} - Z_{j,f,m,t} \cdot \left(\overline{Dur}_{j,f,m} - Dur_{j,f,m}\right)\right] \qquad \forall m, t \in TRH \tag{5.20}$$

Eq. (5.21) establishes the overall balance of the supply chain, considering the production, the consumption, the charge and discharge of the storage unit and the sales to external markets r.

$$\sum_{k \in K} SP_{k,m,t} + PT_{m,t} \cdot DT - Dem_{m,t} - \sum_{k \in K} Ld_{k,m,t} - \sum_{r \in R} Pg_{r,m,t} \cdot DT = 0 \qquad \forall m, t \in TRH \tag{5.21}$$

Hence, economic aspects related to the management of the supply chain are studied, taking into account production, storage and penalty costs. The production cost is calculated in eq. (5.22) as the amount of the costs associated to each producer/generator, given by the unitary production cost multiplied by the units produced. The storage cost for each interval t is the amount of costs associated to each period, which are the same as the unitary storage cost multiplied by the storage, according to eq. (5.23). The penalty cost is determined as a function of the delay in satisfying each demand, and given by eq. (5.24).

Also, eq. (5.25) determines the transport cost, taking into account the amount of material and the distance between production and markets.

The total operating cost of the supply chain is given by eq. (5.26), which takes into account the previous costs.

$$CostPro = \sum_{t\in TRH}\sum_{m\in M}\sum_{i\in I} cpro_{i,m,t}\cdot P_{i,m,t}\cdot DT \tag{5.22}$$

$$CostSto = \sum_{t\in TRH}\sum_{m\in M}\sum_{k\in K} csto_{k,m,t}\cdot SE_{k,m,t} \tag{5.23}$$

$$CostPen = \sum_{j\in J}\sum_{m\in M}\sum_{f\in F_jRH} cpen_{j,f,m}\cdot (Ts_{j,f,m} - Tin_{j,f,m}) \tag{5.24}$$

$$CostTrp = \sum_{m\in M}\sum_{j\in J}\sum_{i\in I} ctrp_{i,j,m}\cdot P_{i,m,t}\cdot d_{i,j} + \sum_{m\in M}\sum_{r\in R}\sum_{i\in I} ctrp_{i,r,m}\cdot P_{i,m,t}\cdot d_{i,r} \tag{5.25}$$

$$Costs = CostPro + CostSto + CostPen + CostTrp \tag{5.26}$$

Also, revenues to external markets r have been taken into account. Thus, incomes are given by eq. (5.27) considering the product m sold and its selling price to each external market.

$$Incomes = \sum_{t\in TRH}\sum_{m\in M}\sum_{r\in R} Price_{r,m,t}\cdot Pg_{r,m,t}\cdot DT \tag{5.27}$$

The profit of the supply chain (which is the objective function), subject to the previous constraints, is calculated considering incomes and costs in eq. (5.28).

$$Profit = Incomes - Costs \tag{5.28}$$

In order to use the proposed model in a rolling horizon scheme, the following set of variables and equations are used to link past decisions with the current prediction horizon. Minimum and maximum starting times for these consumptions at each iteration are given by eq. (5.29) and (5.30), considering the minimum/maximum starting time of the previous iteration and the duration of the control horizon (CH). The duration of the consumptions is also updated at each iteration, as indicated by eq. (5.31). And finally, the storage level of the previous control horizon is linked to the initial storage level of the current prediction horizon by eq. (5.32). The optimization problem will be iteratively solved according to the rolling horizon approach. As previously mentioned, the introduction of this reactive approach will be used to adjust all input parameters to the current available information.

$$Ts_{j,f,m}^{min} = Ts_{0,j,f,m}^{min} - CH \cdot it \qquad \forall j, f \in F_j RH, m \qquad (5.29)$$

$$Ts_{j,f,m}^{max} = Ts_{0,j,f,m}^{max} - CH \cdot it \qquad \forall j, f \in F_j RH, m \qquad (5.30)$$

$$Dur_{j,f,m} = Dur_{0,j,f,m} - \left(CH \cdot it - Ts_{j,f,m}\right) \cdot \hat{Y}_{j,f} \qquad \forall j, f \in F_j RH, m \qquad (5.31)$$

$$SE_{k,m,t-1} = \widehat{SE}_{k,m,t'} \qquad \forall k, m, t \in TRH, t' = T_t \cdot DT \qquad (5.32)$$

This mathematical formulation involves a MILP model. Moreover, the discrete time representation has been chosen instead of the hybrid or the continuous time formulation. Although the optimal solution could be improved by the use of hybrid or continuous time representations, the resulting models involve more computational time. Also, the proposed model does not consider the presence of fixed costs associated to the investment and installation of producers/generators, since the design of the supply chain has not been taken into account and only short-term decisions are addressed.

5.4. Case study

The proposed MILP formulation have been applied to a case study, based on a microgrid. The same values of the input parameters considered in Chapter 4 have been taken into account. The only difference is the value of the starting time of each consumption, since only discrete values are considered. Thus, only delays associated to the decision making process are going to be obtained. In other words, there are no delays associated to the granularity of the model. The values of the staring times of each consumption are detailed in Table 5.1.

The underlying scheduling problem includes energy production, storage and consumption tasks to be optimized. Data and decisions related to energy production are given for every 15 min, according to energy demand and the current weather forecast. Also, decisions related to energy demand are considered for every 15 min, as well as production decisions. The total scheduling horizon considered is 24 h, and the duration of each time interval is 15 min (i.e., 96 time intervals in total). Prediction Horizons (PHs) of 5, 10, 20 and 30 time intervals have been considered. It has been considered that input data (e.g., energy demands, weather conditions, etc.) are updated at the beginning of each time interval, so the control horizon has been set also equal to 15 min (i.e., one time interval).

Table 5.1. Starting times.

Energy consumer *j*	Energy demand *f*	$Ts_{j.f}^{min}$ (h)
j1	f1	0.000
j1	f2	0.250
j1	f3	0.500
j1	f4	0.750
j1	f5	1.000
j1	f6	1.250
j1	f7	1.500
j1	f8	1.750
j1	f9	2.000
j1	f10	2.250
j1	f11	2.500
j1	f12	2.750
j1	f13	3.000
j1	f14	3.250
j1	f15	3.500
j1	f16	3.750
j1	f17	4.000
j1	f18	4.250
j1	f19	4.500
j1	f20	4.750
j1	f21	5.000
j1	f22	5.250
j1	f23	5.500
j1	f24	5.750
j1	f25	6.000
j1	f26	6.250
j1	f27	6.500
j1	f28	6.750
j1	f29	7.000
j1	f30	7.250
j1	f31	7.500
j1	f32	7.750
j1	f33	8.000
j1	f34	8.250
j1	f35	8.500
j1	f36	8.750
j1	f37	9.000
j1	f38	9.250
j1	f39	9.500
j1	f40	9.750
j1	f41	10.000
j1	f42	10.250
j1	f43	10.500
j1	f44	10.750
j1	f45	11.000
j1	f46	11.250
j1	f47	11.500
j1	f48	11.750
j1	f49	12.000
j1	f50	12.250

Energy consumer *j*	Energy demand *f*	$Ts_{j.f}^{min}$ (h)
j1	f51	12.500
j1	f52	12.750
j1	f53	13.000
j1	f54	13.250
j1	f55	13.500
j1	f56	13.750
j1	f57	14.000
j1	f58	14.250
j1	f59	14.500
j1	f60	14.750
j1	f61	15.000
j1	f62	15.250
j1	f63	15.500
j1	f64	15.750
j1	f65	16.000
j1	f66	16.250
j1	f67	16.500
j1	f68	16.750
j1	f69	17.000
j1	f70	17.250
j1	f71	17.500
j1	f72	17.750
j1	f73	18.000
j1	f74	18.250
j1	f75	18.500
j1	f76	18.750
j1	f77	19.000
j1	f78	19.250
j1	f79	19.500
j1	f80	19.750
j1	f81	20.000
j1	f82	20.250
j1	f83	20.500
j1	f84	20.750
j1	f85	21.000
j1	f86	21.250
j1	f87	21.500
j1	f88	21.750
j1	f89	22.000
j1	f90	22.250
j1	f91	22.500
j1	f92	22.750
j1	f93	23.000
j1	f94	23.250
j1	f95	23.500
j1	f96	23.750
j2	f1	16.675
j3	f1	17.725
j4	f1	6.675
j4	f2	7.250
j4	f3	12.575
j4	f4	13.750

Energy consumer *j*	Energy demand *f*	$Ts_{j.f}^{min}$ (h)
j4	f5	20.525
j4	f6	21.750
j5	f1	0.525
j5	f2	3.925
j5	f3	5.000
j5	f4	7.625
j5	f5	8.725
j5	f6	10.825
j5	f7	11.950
j5	f8	13.575
j5	f9	17.000
j5	f10	19.925
j5	f11	20.750
j5	f12	22.875
j6	f1	11.675
j7	f1	0.025
j7	f2	2.625
j7	f3	4.675
j7	f4	6.900
j7	f5	8.875
j7	f6	9.750
j7	f7	11.925
j7	f8	14.525
j7	f9	16.700
j7	f10	18.625
j7	f11	20.675
j7	f12	21.800
j8	f1	12.650
j8	f2	16.250
j8	f3	20.700
j9	f1	16.725
j9	f2	20.525
j10	f1	16.700
j10	f2	20.650
j11	f1	16.625
j12	f1	20.625
j13	f1	16.125
j14	f1	7.250
j15	f1	7.425
j16	f1	7.700
j17	f1	7.225
j17	f2	7.750
j17	f3	8.225
j17	f4	13.550
j17	f5	16.550
j17	f6	20.700
j17	f7	21.000
j17	f8	22.200
j17	f9	23.225
j18	f1	0.100
j19	f1	13.525
j19	f2	18.725

Energy consumer *j*	Energy demand *f*	$Ts_{j.f}^{min}$ (h)
j20	f1	7.025
j20	f2	13.000
j20	f3	16.525
j20	f4	19.325
j21	f1	16.600
j21	f2	19.375
j22	f1	18.050
j22	f2	20.625
j23	f1	14.850
j24	f1	6.775
j24	f2	7.750
j25	f1	18.125
j26	f1	17.775
j27	f1	16.575
j28	f1	16.725
j29	f1	13.675
j29	f2	20.750
j30	f1	18.425
j31	f1	20.575

5.5. Results

The resulting MILP model has been implemented in GAMS 24.1 and solved using CPLEX 12, to zero optimality in a Pentium Intel® Core™ i7 CPU 2600 @ 3.40 GHz. The resolution of the model provides the daily optimal schedule for energy generation and consumption in order to maximize the profit of the given microgrid. The rolling horizon approach, used to address the presence of uncertainty, has allowed to update input information related to weather conditions and consumption durations. Figure 5.1 displays the daily schedule for energy production and energy consumptions for a prediction horizon of 20 time intervals. Some energy consumption tasks have been delayed (i.e., energy demand has right-shifted). According to this figure, the microgrid produce the maximum energy capacity from energy renewable sources, in order to satisfy the energy demand and to sell this energy to the power grid. The purchases of energy from the power grid are required if the use of both renewable energy systems and the energy storage system is not enough to meet the energy demand.

The application of the rolling horizon, in which the problem formulation is solved iteratively, can produce constant changes in the expected schedule (Figure 5.2). This is caused because the input information is updated and future information is introduced in the system. To highlight these changes, only some consumption tasks have been plotted. At the beginning, some consumption tasks do not appear in the plot because in the current time there is no information related to the mentioned consumptions.

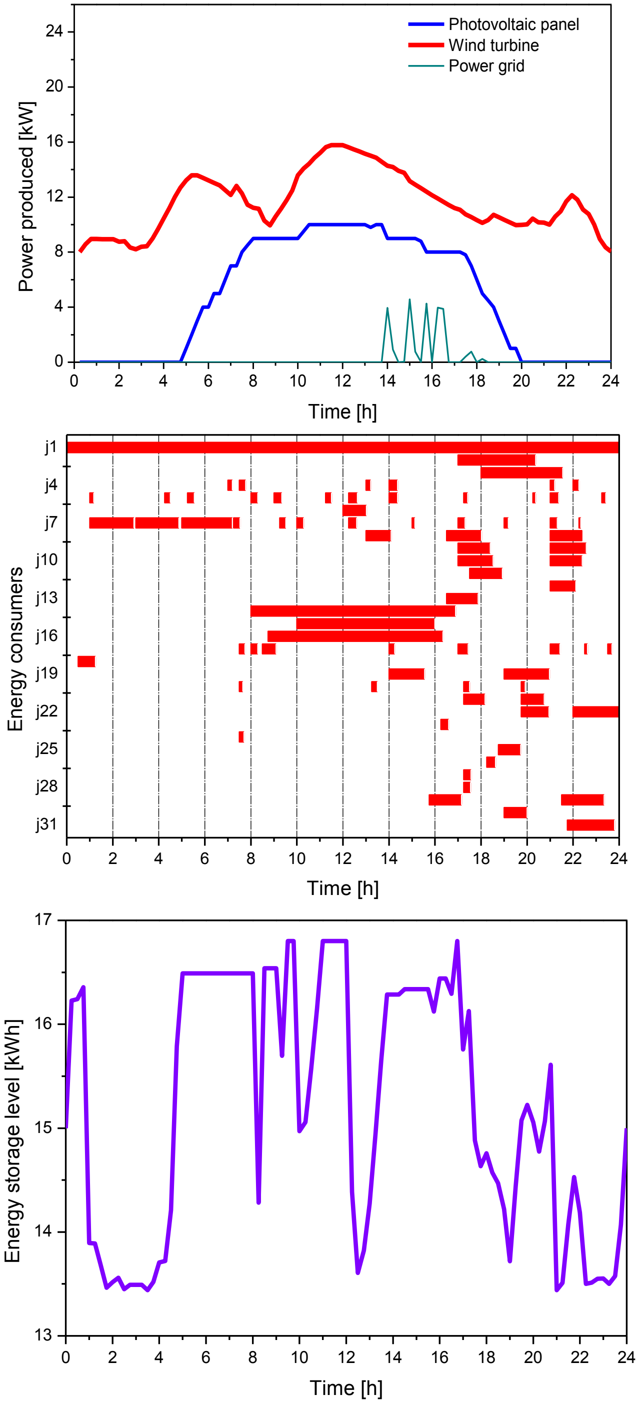
Photovoltaic panel
Wind turbine
Power grid
Power produced [kW]
Time [h]
Energy consumers
j1
j4
j7
j10
j13
j16
j19
j22
j25
j28
j31
Time [h]
Energy storage level [kWh]
Time [h]

Figure 5.1. Daily schedule for energy production, consumption and storage (PH=20).

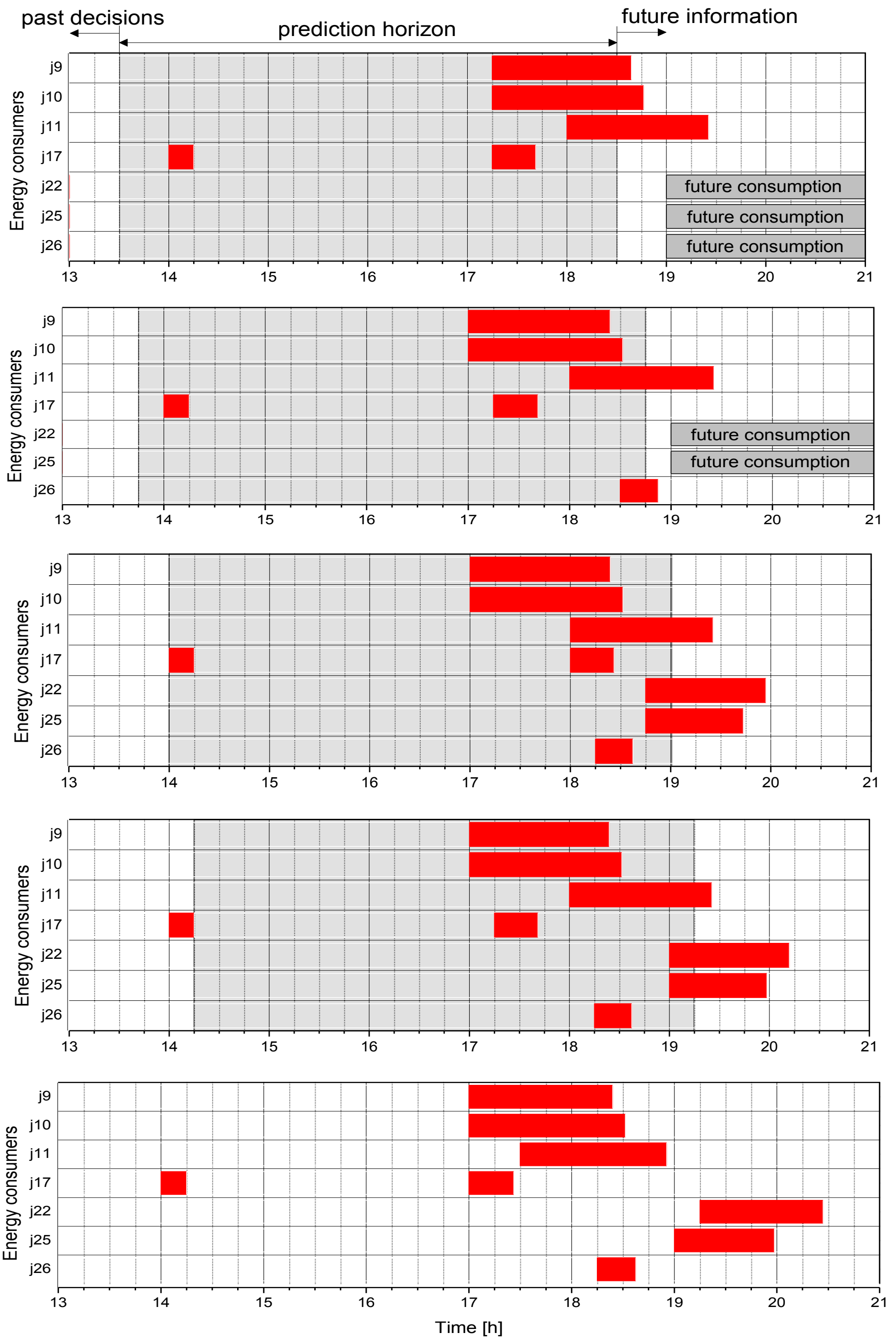

Figure 5.2. Evolution of the energy consumption scheduling for PH=20 in iterations 54, 55, 56, 57 and final iteration.

Different lengths of the prediction horizon have been considered, in order to compare, analyse and highlight the characteristics of the proposed rolling horizon and the simultaneous management of energy production and demand. Thus, prediction horizons of 5, 10, 20 and 30 time intervals has been taken into account. Moreover, the perfect information case (PH=96), which corresponds to the situation in which the length of the prediction horizon is equal to the length of the scheduling horizon, has been considered.

In all these situations, the control horizon is equal to one time interval. According to the obtained results, longer prediction horizons involve a significant reduction in the use of the power grid to satisfy the demand (Figure 5.3), since more future information is received to solve the optimization problem. As a consequence, the profit increases for longer prediction horizons (Figure 5.4 and Table 5.2). In order to compare how the simultaneous energy production and demand management affects the final solution, Table 5.3 shows the obtained results in the case of managing only the energy production, in which energy consumptions cannot be shifted. As expected, the obtained profit decreases in comparison with that of the simultaneous management. Also, notice that the values of the decision variables are the same for the PH=96 in comparison with the discrete time model formulated in Chapter 4. The difference in the value of the profit is due to the fact that input parameters related to the desired staring times are located in the boundaries of time intervals. In the previous chapter, this times could be located inside the time interval.

Table 5.2. Comparison of the obtained results for the scenario 1 (demand side management).

Unit	PH=5	PH=10	PH=20	PH=30	PH=96
Profit (m.u.)	3.12	3.17	3.19	3.27	3.30
Consumed energy (kWh)	359.0	359.0	359.0	359.0	359.0
Total delays (h)	18.25	12.75	12.75	12.50	11.75
Energy produced or purchased (kWh)	401.6	398.0	397.8	394.5	391.9
Energy from photovoltaic panels (kWh)	112.7	112.7	112.7	112.7	112.7
Energy from wind turbines (kWh)	279.2	279.2	279.2	279.2	279.2
Energy from power grid (kWh)	9.7	6.1	5.9	2.6	0.0
Energy from energy storage systems (kWh)	15.4	17.5	16.9	18.0	19.3
Energy sold to the power grid (kWh)	40.4	35.3	35.3	31.7	28.5
Energy to load the storage system (kWh)	33.9	21.6	20.8	22.2	24.1
Energy loses (kWh)	16.2	0.3	0.3	0.3	0.3

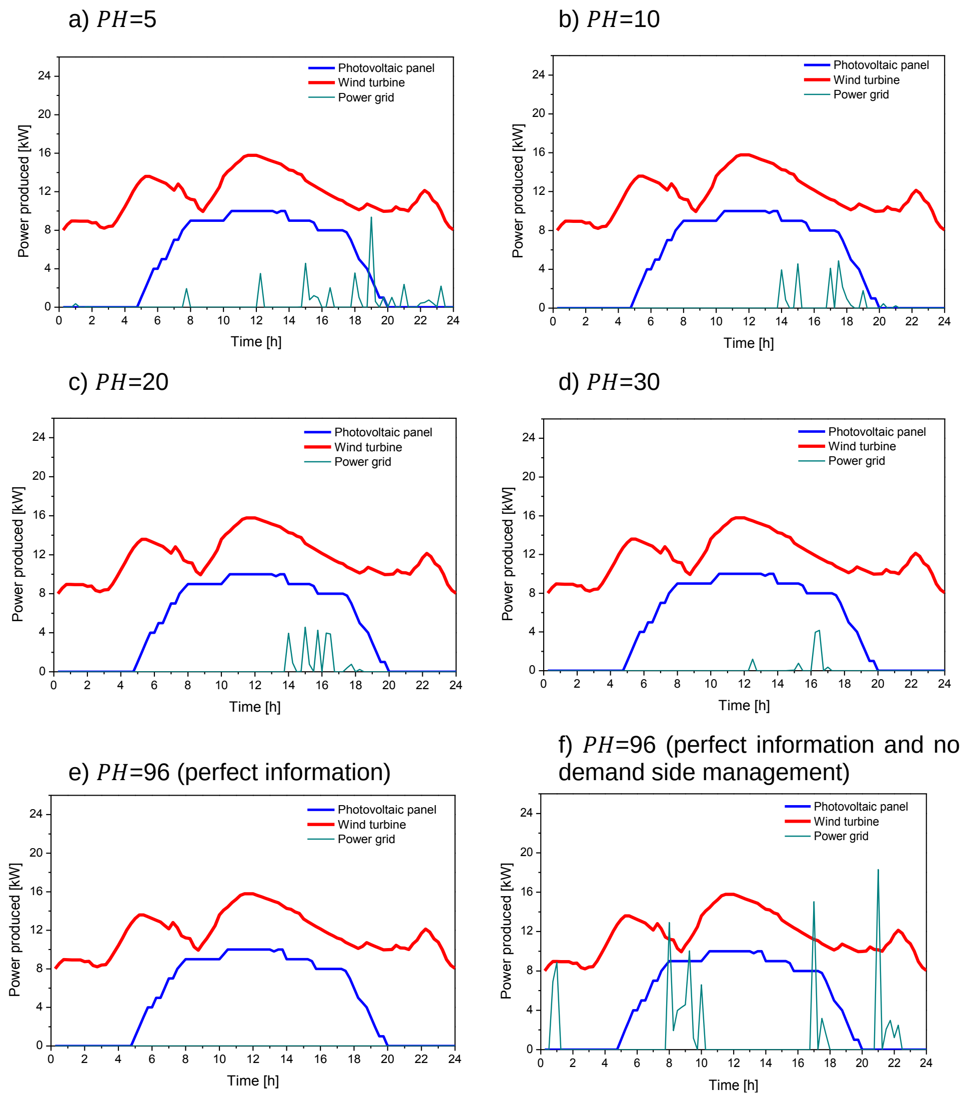

Figure 5.3. Power source in each time period for different PH lengths.

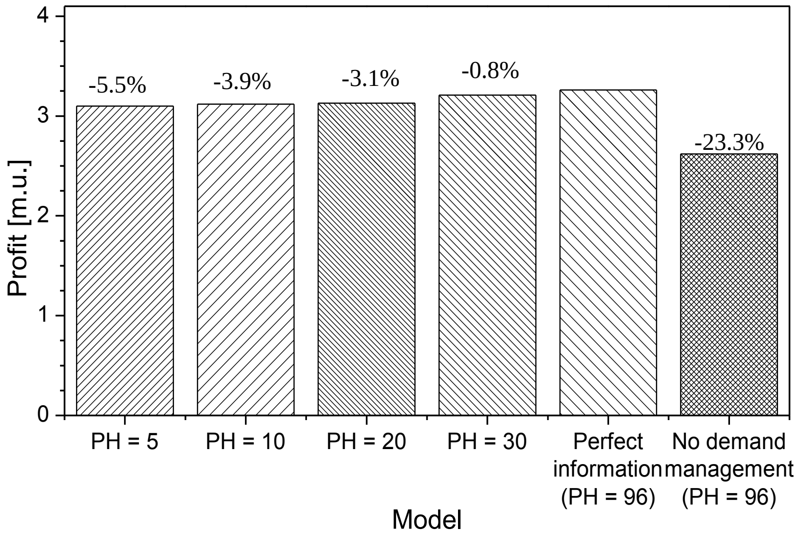

Figure 5.4. Profit for different PHs, perfect information and no demand management case.

Table 5.3. Comparison of the obtained results for the scenario 2 (non-demand side management).

Unit	PH=5	PH=10	PH=20	PH=30	PH=96
Profit (m.u.)	2.61	2.62	2.62	2.62	2.62
Consumed energy (kWh)	359.0	359.0	359.0	359.0	359.0
Total delays (h)	0.00	0.00	0.00	0.00	0.00
Energy produced or purchased (kWh)	422.1	420.8	420.8	420.8	420.8
Energy from photovoltaic panels (kWh)	112.7	112.7	112.7	112.7	112.7
Energy from wind turbines (kWh)	279.2	279.2	279.2	279.2	279.2
Energy from power grid (kWh)	30.3	28.9	28.9	28.9	28.9
Energy from energy storage systems (kWh)	18.2	19.5	19.5	19.5	19.5
Energy sold to the power grid (kWh)	60.2	58.5	58.5	58.5	58.5
Energy to load the storage system (kWh)	21.1	22.8	22.8	22.8	22.8
Energy loses (kWh)	0.1	0.1	0.1	0.1	0.1

Figure 5.5 shows the aggregated objective value for the rolling horizon approach under different prediction horizons in comparison with the perfect information case. Not surprisingly, as the length of the prediction horizon increases, the total objective is improved and closes the gap from the perfect information solution. Shorter prediction horizon involve more energy sales to the power grid (Figure 5.6), because there is no information about future energy demand, requiring energy purchases from the power grid and more delays in the energy consumptions. Model statistics for the proposed model using different lengths for the prediction horizon can be found in Table 5.4.

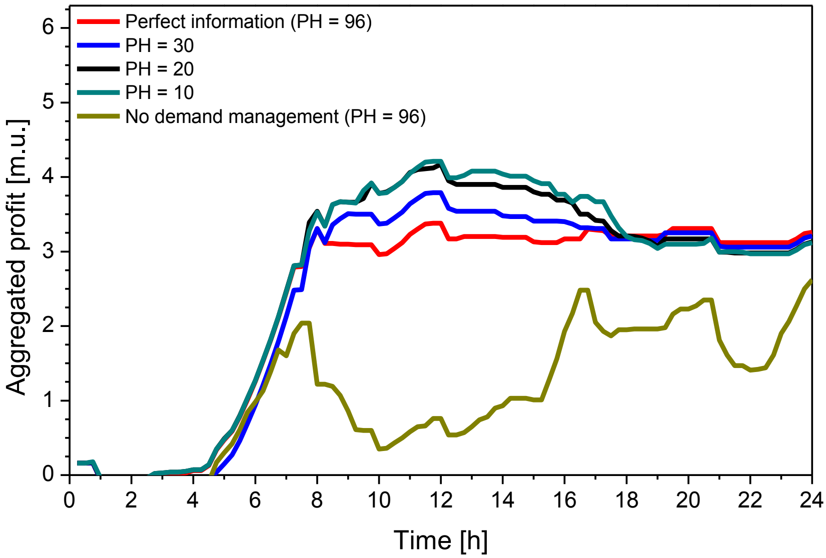

Figure 5.5. Aggregated profit for different PHs, perfect information and no demand management case.

Table 5.4. Comparison of optimal solution and model statistics.

Unit	PH=5	PH=10	PH=20	PH=30	PH=96
Number of iterations	92	87	77	67	1
Equations per iteration	481	1,216	3,726	8,016	93,604
Continuous variables per iteration	360	855	2,424	5,004	54,615
Discrete variables per iteration	80	260	1,001	2,411	33,468
Computational time per iteration	0.1	0.3	0.3	0.4	0.8
Relative gap (%)	0.0	0.0	0.0	0.0	0.0

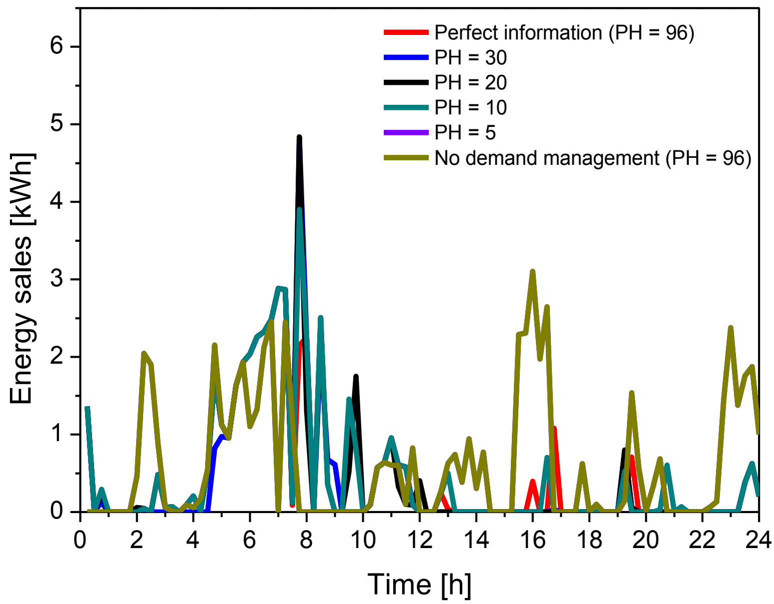

Figure 5.6. Energy sales for different PHs, perfect information and no demand management case.

Finally, in order to show how the energy production is managed, a variation from the initial model was solved. This model variation minimizes the total cost of the microgrid, without taking into account possible energy sales. Thus, the objective function will be to minimize eq. (5.26) subject to constraints (5.1) to (5.24). This fact explains that in specific time intervals, all energy generators can be switched off, in order to match energy production and consumption. However, if the energy generator cannot be controlled (i.e., if produces, the production corresponds to the maximum power availability for this source), the excess of energy will be dissipated to an external load. For example, Figure 5.7 shows the schedule of energy production that will be used to satisfy all energy consumptions for a prediction horizon equal to 20 time intervals. However, this figure indicates just the power used from each energy generator to perform all energy consumption tasks, without taking into account energy dissipations. Notice that in this case in contrast to the previous solution approach, the energy production does not reach the maximum energy production capacity, since only the energy to be consumed or stored is produced. In this case, 365.8 kWh were produced (30.3% produced from the photovoltaic panel and 69.7% from the wind turbine), reducing the energy requirements by 8.0%.

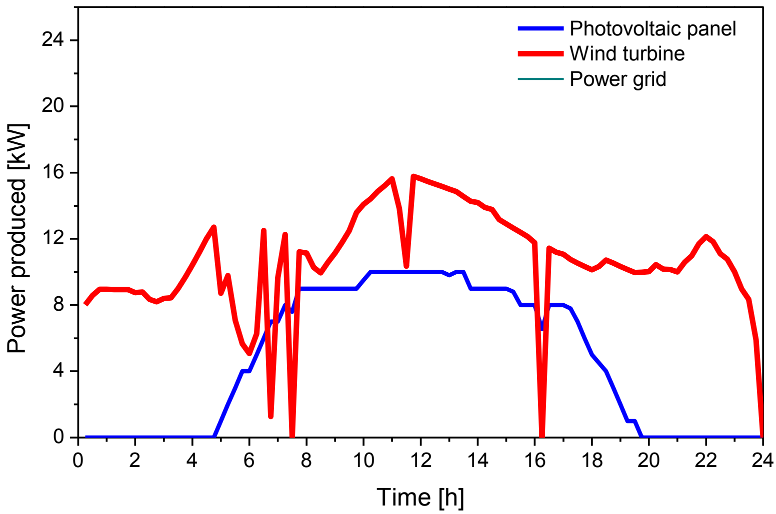

Figure 5.7. Schedule of power produced where no sales to the power grid are allowed (PH=20).

Moreover, the reactive scheduling approach allows updating input parameters to react to variations from the nominal/initial plan, including alterations in the power availability or in the duration of energy consumptions. This means that this approach is able to handle the types of uncertainty associated to the microgrid (i.e., prediction in the wind turbine and photovoltaic panel forecasts and energy consumption predictions). For instance, Figure 5.8 shows an unexpected scenario in which there is a reduction in the power availability as well as an increased duration of some duration consumptions, with the objective of maximizing the profit of the microgrid. This variation is due to the uncertainty to predict accurately the weather forecast which directly affects the power availability.

The rolling horizon approach allows to react to any eventual alteration from the initial conditions. Table 5.5 compares the results for the simultaneous energy production and demand management, for PH=20 and the perfect information case. According to the results, energy purchases are required in both cases to satisfy the energy demand. However, the use of the rolling horizon approach allows the benefit to be more than 3% higher compared with the perfect information case.

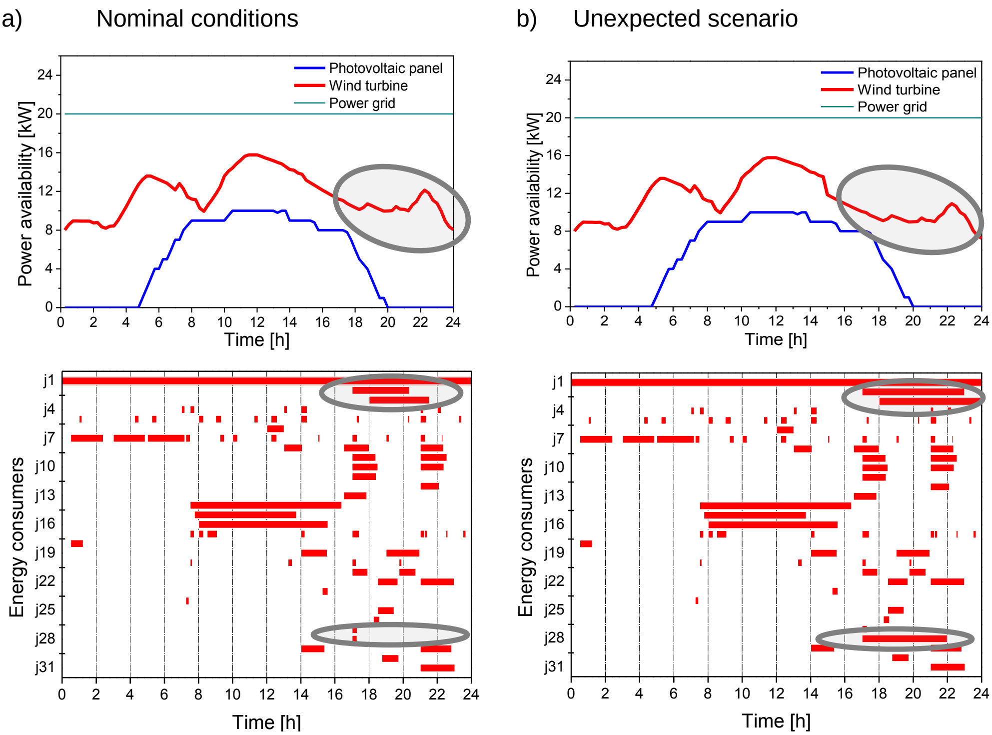

Figure 5.8. Power availability and target schedule for the nominal conditions scenario and the unexpected scenario.

Table 5.5. Comparison of the obtained results for the demand side management for the unexpected scenario.

Unit	PH=20	PH=96
Profit (m.u.)	0.47	0.45
Consumed energy (kWh)	368.6	368.6
Total delays (h)	12.25	11.75
Energy produced or purchased (kWh)	405.0	399.4
Energy from photovoltaic panels (kWh)	112.7	112.7
Energy from wind turbines (kWh)	269.2	269.2
Energy from power grid (kWh)	23.0	17.5
Energy from energy storage systems (kWh)	16.9	19.3
Energy sold to the power grid (kWh)	34.2	27.0
Energy to load the storage system and energy loses (kWh)	19.0	23.1

5.6. Concluding remarks

In this chapter, a discrete time MILP formulation applicable to the simultaneous optimization of production and demand within a supply chain under uncertain conditions has been presented, with the objective of maximizing the profit. The modelling approach proves the advantages of managing the demand, by optimizing the management of the supply chain, which allows enhancing its flexibility and autonomy.

A rolling horizon approach has been introduced in the formulation to address the presence of uncertainty. As expected, longer prediction horizons favour the generation of better solutions, under the assumption of accurate demand predictions. This approach allows updating input parameters, in order to react to variations from the nominal schedule, which allows to adapt energy production and energy demand to update parameters.

The proposed approach has been used to solve a case study based on a microgrid and also it could be used as the basis for solving further problems with higher complexity (i.e., scheduling of an industrial process), by combining a reactive and proactive treatment to take into account the presence of uncertainty, as well as the simultaneous consideration of different factors (i.e., costs, environmental impact) through the implementation of multi-objective optimization approaches. Finally, rescheduling actions penalties could be included to the proposed optimization framework to avoid major changes in the initial schedule after the occurrence of an unexpected event.

5.7. Nomenclature

Indices and sets

$i \in I$	*Production sources*
$j \in J$	*Consumers*
$f \in F_j$	*Demand included in the overall scheduling horizon*
$f \in F_jRH$	*Demand included in the current prediction horizon*
$k \in K$	*Storage systems*
$m \in M$	*Products, materials, utilities or resources (product)*
$m \in PR$	*Subset of manufactured products* m
$m \in RM$	*Subset of raw material products* m
$r \in R$	*External markets*
$t \in T$	*Time intervals included in the overall scheduling horizon*
$t \in TRH$	*Time intervals included in the current prediction horizon*

Parameters

CH	*Length of the control horizon*
$Cons_{j,f,m}$	*Individual consumption* jf *of product* m
$cpen_{j,f,m}$	*Penalty cost associated to consumption* jf *of product* m
$cpro_{i,m,t}$	*Production (or purchase) cost of product* m *in source* i *at time* t

$csto_{k,m,t}$	*Storage cost of product m in storage system k at time t*
$ctrp_{i,j,m}$	*Transport cost of product m from production location i to consumer j*
$ctrp_{i,r,m}$	*Transport cost of product m from production location i to market r*
DT	*Duration of the time interval*
$Dur_{j,f,m}$	*Remaining time consumption of task jf of product m in the current prediction horizon*
$\overline{Dur}_{j,f,m}$	*Round up value of the remaining time consumption of task jf of product m in the current prediction horizon*
$Dur_{0,j,f,m}$	*Duration of consumption jf of product m in the overall scheduling horizon*
it	*Iteration*
$P_{i,m,t}^{min}$	*Minimum supply of product m from source i at interval t*
$P_{i,m,t}^{max}$	*Maximum supply of product m from source i at interval t*
PH	*Length of the prediction horizon*
$Price_{r,m,t}$	*Price to be sold product m to the external market r at interval t*
$SE_{k,m,t}^{min}$	*Minimum storage level of product m in storage system k at interval t*
$SE_{k,m,t}^{max}$	*Maximum storage level of product m in storage system k at interval t*
$SE_{0k,m,t}$	*Initial storage level of product m in system k at interval t*
SH	*Length of the scheduling horizon*
Tp_m	*Processing time to obtain product m*
$Ts_{j,f,m}^{max}$	*Maximum initial time of consumption jf of product m in the current prediction horizon*
$Ts_{j,f,m}^{min}$	*Target initial time of consumption jf of product m in the current prediction horizon*
$Ts_{0,j,f,m}^{max}$	*Maximum initial time of consumption jf of product m in the overall scheduling horizon*
$Ts_{0.j,f,m}^{min}$	*Target initial time of consumption jf of product m in the overall scheduling horizon*
$\alpha_{k,m}$	*Percentage of variation of product m in storage system k*
ρ_m	*Conversion degree of product m*
$\eta_{k,m}^{in}$	*Charging efficiency of storage system k of product m*
$\eta_{k,m}^{out}$	*Discharging efficiency of storage system k of product m*

Continuous and positive variables

$CostPen$	*Supply chain penalty cost*
$CostPro$	*Supply chain production cost*
$CostSto$	*Supply chain storage cost*
$CostTrp$	*Supply chain transport cost*
$Costs$	*Supply chain operating cost of the supply chain*
$Dem_{m,t}$	*Total consumption at interval t of product m*
$Incomes$	*Supply chain incomes*
$Ld_{k,m,t}$	*Amount of product m supplied to load system k during interval t*
$P_{i,m,t}$	*Amount of product m supplied from source i at interval t*
$Pg_{r,m,t}$	*Amount of product m supplied to external market r at interval t*
$Profit$	*Total profit along the scheduling horizon (objective function)*
$PT_{m,t}$	*Amount of product m supplied at interval t*
$SE_{k,m,t}$	*Storage level of product m in system k at the end of the interval t*
$\widehat{SE}_{k,m,t}$	*Linking variable determining the storage level of product m in storage system k at the end of interval t in the current prediction horizon*
$SP_{k,m,t}$	*Amount of product m supplied by storage system k during interval t*
$Tf_{j,f,m}$	*Finishing time of consumption jf of product m*

$Ts_{j,f,m}$ *Starting time of consumption jf of product m*
T_t *Time corresponding to time interval t*

Binary variables

$X_{i,m,t}$ *= 1, if production source i is used at interval t to supply product m*
$Y_{j,f,m,t}$ *= 1, if consumption jf of product m starts at interval t during the current prediction horizon*
$\hat{Y}_{j,f,m}$ *= 1, if consumption jf of product m starts outside the current prediction horizon*
$Z_{j,f,m,t}$ *= 1, if consumption jf of product m finishes at interval t during the current prediction horizon*
$\hat{Z}_{j,f,m}$ *= 1, if consumption jf of product m finishes outside the current prediction horizon*
$W_{j,f,m,t}$ *= 1, if consumption jf of product m is active at interval t during the current prediction horizon*

Chapter 6. Integrated management of resources in the decision making process

Chapters 4 and 5 describe the simultaneous management of production and demand using different time representations under deterministic and uncertain conditions. This chapter extends this holistic point of view in order to consider the management of common production resources, which can be external (i.e., materials, energy consumption, water management) or internal (i.e., process equipment units). Hence, this chapter presents a MINLP formulation to globally address the optimization of the short term use of common production resources, either dedicated or shared. This approach considers all constraints associated to the production as well as the limitations in the use of resources in a general way in a common formulation, instead of using different mathematical formulation for each considered resource. Moreover, delays in the nominal demand are allowed under associated penalty costs to tackle flexible demand profiles, which provides a better adaptation of production and use of resources. A well-known case study is presented to test this methodology, which considers the production schedule and the use of water and energy as utilities. The obtained results show that this formulation allows to determine the global optimum operating conditions in an affordable computational time.

6.1. Introduction

The need to improve process management efficiency has led to the formulation of different mathematical models to solve process scheduling problems. Usually, these models consider limitations in common resources availability (Castro et al., 2009). More recently, these models have been expanded to take into account broader scopes through the supply chain in which the process of interest is embedded, but nowadays the proposed solution approaches tackle either the availability or the integration of resources (Seid and Majozi, 2013).

Thus, this chapter addresses the integrated management of production resources, either external (i.e., materials, energy consumption, water management) and internal (i.e., process equipment units, manpower), within the operation of a production plant, to determine the overall production strategy to best fit a specified demand, optimizing the use of these resources through their integration and through the adaptation of their consumption to their availability. Some of the most common production resources are water and energy. However, the proposed formulation can be applied to manage the use of all resources, not only to water or energy.

The main objectives of managing water and energy systems are to reduce costs, to reduce the environmental impact and to better satisfy the water and energy demand in terms of time, quality and quantity. For instance, factories use large amounts of process water, for example as mass separating agent, reactant, utility or cleaning agent. The scarcity, the diverse quality requirements, and the strict discharge policies related to the use of water in the industry, motivated by the concern associated to the limitation of this natural source, are significant forces to investigate ways to reduce the use of water. This reduction in the use of freshwater and the reduction of wastewater generation is possible by reusing and recycling water. In the same context, the rational use of energy is essential. Energy Systems Engineering involves all the decision making procedures associated to energy supply chain from the primary energy source to the final energy delivery to the process.

Regarding these two particular resources, in the framework of production plants, the reduction of water and energy consumption is given by the reuse of water and energy (i.e., heat integration). Whereas in continuous process the water reuse and heat integration are limited by concentration and temperature constraints, the difficulty associated to batch process is that also time constraints must be considered. This means that, for example, direct water reuse associated to batch cleaning operations requires that all the operations involved in the integration must follow very strict time constraints: each one must start just immediately after a previous cleaning operations finishes. In the case of semi-continuous operations this can be performed only in periods of time in which the cleaning operations are simultaneously required.

Moreover, flexibility in the resources demand is considered, by applying a penalty term in the economic objective function. The consideration of this kind of flexibility in the product demand would introduce an additional degree of freedom to the management problem.

This objective is met using an extended mathematical formulation of the traditional integration approach (pinch analysis) to consider a generic view of common resources, and to integrate the availability point of view. The proposed approach is illustrated through its application to optimize the batch-size and the sequence of operations of an extended version of a multipurpose batch chemical process case study. The results are analysed in order to show the main benefits of the proposed approach in front of a less integrated management in the use of common resources.

Although this chapter is focused on one echelon of the supply chain (i.e., production plant), the proposed formulation can be extended to enlarge the scope of the problem, taking into account the overall supply chain.

6.2. Problem statement

The development of a mathematical model to manage this multipurpose batch production plant will allow us to optimize its profit. One feature of the presented mathematical model is the management of the product demand, by the introduction of a flexible profile in the demand, which allows to delay the delivery of final products to the customer, as well as the reduction of the environmental impact, since the integrated management of all resources (for example, water or energy) may lead to decrease its use. The mathematical formulation is described in terms of the following items:

(i) A given scheduling horizon, which is divided into a number of equal-size time intervals $t \in T$.
(ii) A set of operations $i \in I$.
(iii) A set of equipment units $j \in J$ to perform operations i.
(iv) A set of resources $k \in K$ to perform all operations.
(v) A set of states $m \in M$, including raw materials, intermediate products and final products.
(vi) A set of quality parameters $c \in C$, which characterize each resource k.
(vii) The initial amount of all states m and resources k.
(viii) The production recipes.
(ix) The process unit configuration.
(x) The operation processing times.
(xi) The characteristics of the stored materials.
(xii) The required time to use any resource k.
(xiii) The variation of the quality of each resource k in each operation i.
(xiv) The input and output quality limits of each resource k in each operation i.
(xv) The costs and prices of all states m and resources k.

The main decisions to be made in order to maximize the profit are:

(i) The production schedule, including allocation of operations, timing and sequence, production level and batch size.
(ii) The use of resources (i.e., fresh utilities).
(iii) The reuse of resources.

The following assumptions are considered:

(i) All states m and resources k can be stored in the production facility.
(ii) Intermediate materials can be stored in finite capacity units with unlimited waiting time.
(iii) Product delivery to the customer can be delayed incurring into a penalty cost.
(iv) Transfer times between process units are considered negligible.
(v) Time to use each resource is assumed to be constant.
(vi) The quantity of each resource k used in each in each equipment unit j is proportional to the batch size.
(vii) Only direct reuse without intermediate storage of any resource is considered.
(viii) No limitation on fresh resources (not used previously) that can be supplied to the system are considered.
(ix) Resource losses are negligible.

6.3. Mathematical formulation

The constraints associated to the sequencing and the allocation of operations to dedicated resources and utilities are next presented in the following discrete time formulation. According to the stated objectives, the main constraints of this mathematical formulation take into account:

- The production schedule.
- The use of resources.
- The demand side management.

Regarding the scheduling constraints, the main relations are associated to allocation constraints, capacity constraints and material balances. Eq. (6.1) forces that, at most, one operation can start at equipment unit j at any time t, which avoids any overlap in any equipment unit. Eq. (6.2) are used to force that an operation i cannot start in an equipment unit j until the previous operation is finished. This equation implies the use of the big-M formulation, where M is a sufficient large positive number. Also, eq. (6.3) and (6.4) are used to limit the minimum and maximum batch size in each operation $B_{i,t}$ and amount of material stored $S_{m,t}$ of all states in each period of time t. Moreover, eq. (6.5) establishes the material balance of raw material, intermediate and final products. This balance is given by the stoichiometry of the chemical process as well as sales of final products and purchases of raw material.

$$\sum_{i\epsilon JI_j} X_{i,t} \leq 1 \qquad \forall j,t \qquad (6.1)$$

$$\sum_{\substack{t\leq t'\epsilon T \\ t'<t+fd_i+UT_i-1}} \sum_{i'\epsilon JI_j} X_{i',t'} - 1 \leq M \cdot \left(1 - X_{i,t}\right) \qquad \forall i,j,t \qquad (6.2)$$

$$X_{i,t} \cdot B_i^{min} \leq B_{i,t} \leq X_{i,t} \cdot B_i^{max} \qquad \forall i,t \qquad (6.3)$$

$$S_m^{min} \leq S_{m,t} \leq S_m^{max} \qquad \forall m,t \qquad (6.4)$$

$$S_{m,t} + SS_{m,t} = S0_m\big|_{t=1} + S_{m,t-1}\big|_{t>1} + \sum_{i\epsilon IO_m} \rho_{i,m} \cdot B_{i,t-fd_i} - \sum_{i\epsilon II_m} \rho_{i,m} \cdot B_{i,t} + P_{m,t} \qquad \forall m,t \qquad (6.5)$$

The use of resources in discontinuous operations is modelled according to the following equations. Eq. (6.6) corresponds to the inlet resource balance in operation i. The total inlet resource k at time t is given by the summation of all the reuses from previous operations and the requirement of fresh resource (resource which has not been used previously in the process). In the same manner, eq. (6.7) establishes the outlet resource balance for operation i, where the total outlet at time t is given by the amount of resource k to be reused and the resource discarded to be treated/removed posteriorly. Also, eq. (6.8) forces the overall resource balance of an operation, which considers that the outlet resource k at time t in operation i corresponds to the amount of inlet resource k in this operation plus the generated resource during this operation.

$$Ui_{k,i,t} = U_{k,i,t} + \sum_{i'\epsilon I} Ur_{k,i',i,t} \qquad \forall i,k\epsilon DU_k,t \qquad (6.6)$$

$$Uo_{k,i,t} = Ue_{k,i,t} + \sum_{i'\epsilon I} Ur_{k,i,i',t} \qquad \forall i,k\epsilon DU_k,t \qquad (6.7)$$

$$Ui_{k,i,t-UT_i} + Ug_{k,i,t} = Uo_{k,i,t} \qquad \forall i,k\epsilon DU_k,t \qquad (6.8)$$

Next equations introduce the quality parameters of each resource used in discontinuous operations. These parameters are modelled to manage the use of each resource according to availability or environmental limitations. Some examples of quality parameters can be the concentration of a contaminant, in terms of water consumption, or the temperature, in terms of use of energy. Regarding the quality parameters, eq. (6.9) corresponds to the each quality parameter c balance over each operation in the equipment unit in which operation i is carried out. This equation establishes the value of the quality parameter at the end of each operation, which is given by the inlet value of the above mentioned quality parameter and its generation/consumption during operation i. Moreover, eq. (6.10) establishes the value of the quality parameter c in an operation, which is given by the value of this quality parameter from previous operations.

$$Uo_{k,i,t} \cdot Co_{c,k,i,t} = Ui_{k,i,t-UT_i} \cdot Ci_{c,k,i,t-UT_i} + CL_{c,k,i} \cdot Wi_{k,i,\,t-UT_i} \qquad \forall i, c, k\epsilon DU_k, t \qquad (6.9)$$

$$Ui_{k,i,t} \cdot Ci_{c,k,i,t} = \sum_{i'\epsilon I} Ur_{k,i',i,t} \cdot Co_{c,k,i',t} \qquad \forall i, c, k\epsilon DU_k, t \qquad (6.10)$$

Eq. (6.11) establishes the initial time to use a discontinuous resource. This allows to use the resource a specific period of time (i.e., at the beginning of an operation/reaction, just immediately the previous chemical reaction will be finished), as a function of the starting time t of an operation i and a period of time D_i. Notice that if the resource is used at the beginning of operation i, the value of D_i corresponds to 0. This formulation requires the use of the binary variable $Wi_{k,i,t}$, which determines if each resource is being used at time t or not. Also, eq. (6.12) and (6.13) restricts the minimum/maximum inlet and outlet quality parameter c for each operation. Furthermore, eq. (6.14) and (6.15) constricts the minimum/maximum inlet and reused quality parameter of each resource k in each operation i, respectively. Hence, binary variable determines if the reuse of resource k can take place. According to eq. (6.16), the reuse of each resource k can be possible only if this resource is used in an operation i.

$$Wi_{k,i,t} = X_{i,t-D_i} \qquad \forall i, k\epsilon DU_k, t \qquad (6.11)$$

$$Ci^{min}_{c,k,i} \cdot Wi_{k,i,t} \leq Ci_{c,k,i,t} \leq Ci^{max}_{c,k,i} \cdot Wi_{k,i,t} \qquad \forall i, c, k\epsilon DU_k, t \qquad (6.12)$$

$$Co^{min}_{c,k,i} \cdot Wi_{k,i,t+UT_i} \leq Co_{c,k,i,t} \leq Co^{max}_{c,k,i} \cdot Wi_{k,i,t+UT_i} \qquad \forall i, c, k\epsilon DU_k, t \qquad (6.13)$$

$$Ui^{min}_{k,i} \cdot Wi_{k,i,t} \leq Ui_{k,i,t} \leq Ui^{max}_{k,i} \cdot Wi_{k,i,t} \qquad \forall i, k\epsilon DU_k, t \qquad (6.14)$$

$$Ur^{min}_{k,i',i} \cdot Wr_{k,i',i,t} \leq Ur_{k,i',i,t} \leq Ur^{max}_{k,i',i} \cdot Wr_{k,i',i,t} \qquad \forall i, i', k\epsilon DU_k, t \qquad (6.15)$$

$$Wr_{k,i',i,t} \leq Wi_{k,i,t} \qquad \forall i, i', k\epsilon DU_k, t \qquad (6.16)$$

Moreover, the use of resources in continuous (or semi-continuous) operations is modelled according to the following equations (i.e., heat integration of continuous processes). This kind of resources are used in a continuous way if a given operation is performed. Whereas the use of discontinuous resources is delimited by the initial and final conditions, the limitations in the flow of the continuous resources are analysed in each period of time. Hence, eq. (6.17) establishes the value of the any characteristic of a given operation i (i.e., pressure, temperature, flow) at beginning of each time interval t. This equation takes into account the initial conditions of the system, given by the term Ti_i or the conditions of the previous period of time, given by $Tr_{i,t-1}\big|_{t>1}$. It is assumed that the evolution of this term is given by a linear temperature ramp in the overall operation i. If the process associated to operation i is active, the value will be given by the term $\sum_{\substack{t'\epsilon T \\ t'<t \\ t\leq t'+dur_i}} \frac{(Ti_i - To_i)}{\frac{dur_i}{DT}}$, whereas final conditions will be given by $\sum_{\substack{t'\epsilon T \\ t'<t \\ t\leq t'+dur_i}} To_i$. The evolution of the process will determine the necessity of resources in each period of time.

$$Tr_{i,t} = Ti_i \cdot X_{i,t} + Tr_{i,t-1}\big|_{t>1} + \sum_{\substack{t'\epsilon T \\ t'<t \\ t\leq t'+dur_i}} \frac{(Ti_i - To_i)}{\frac{dur_i}{DT}} \cdot X_{i,t'} + \sum_{\substack{t'\epsilon T \\ t'<t \\ t\leq t'+dur_i}} To_i \cdot X_{i,t'} \qquad \forall i,t \quad (6.17)$$

Also, in eq. (6.18) the big-M formulation is proposed to determine if the flow of the continuous (or semi-continuous) resource can take place or not, according to the value of the quality parameter. This formulation involves the presence of the binary variable $We_{i,t}$, which determines/evaluates if the above resource can be used. This is very useful, for example, in heat integration processes, where this binary variable would indicate if the heat integration can take place or not, according to the temperature of each process. Eq. (6.19) restricts the value of the reused flow of the resource. Eq. (6.20) is implemented to determine the necessity of resource k to perform operation i. The term Cp_i represents a characteristic parameter of operation i (regarding the heat integration example, this term would represent the heat capacity). Moreover, eq. (6.21) establishes the resource balance in each operation i, taking into account the necessity of the resource in each process, and the reused resource from other operations $Ur_{k,i',i,t}$ or to other operations $Ur_{k,i,i',t}$.

$$Tr_{i',t} - Tr_{i,t} - \left(We_{k,i,i',t} - 1\right) \cdot M \geq 0 \qquad \forall i,i',k\epsilon CU_k,t \quad (6.18)$$

$$Ur_{k,i',i}^{min} \cdot We_{k,i',i,t} \leq Ur_{k,i',i,t} \leq Ur_{k,i',i}^{max} \cdot We_{k,i',i,t} \qquad \forall i,i',k\epsilon CU_k,t \quad (6.19)$$

$$Un_{k,i,t} = \sum_{\substack{t'\epsilon T \\ t'\leq t \\ t\leq t'+dur_i}} B_{i,t'} \cdot Cp_i \cdot \left(Tr_{i,t} - Tr_{i,t+1}\right) \qquad \forall i,k\epsilon CU_k,t \quad (6.20)$$

$$U_{k,i,t} = Un_{k,i,t} - \sum_{\substack{i'\epsilon I \\ i'\neq i}} Ur_{k,i',i,t} + \sum_{\substack{i'\epsilon I \\ i'\neq i}} Ur_{k,i,i',t} \qquad \forall i,k\epsilon CU_k,t \quad (6.21)$$

The proposed approach may also consider the exploitation of the eventual flexibility in the demand duedates, which might be delayed from their initial targets, but at a cost associated to a penalty term in case of not satisfying a given demand. This is useful to alleviate the apparent mismatch between production and demand. For this purpose, the total demand takes into account not only the current demand but also the unsatisfied demand from previous periods of time, which can be calculated from eq. (6.22). Eq. (6.23) establishes that sales of final products are delimited by the total demand, and eq. (6.24) determines that the unsatisfied demand is given by the difference between the demand and the product sales.

$$TDem_{m,t} = Dem_{m,t} + UDem_{m,t-1}\big|_{t>1} \qquad \forall m,t \qquad (6.22)$$

$$SS_{m,t} \leq TDem_{m,t} \qquad \forall m,t \qquad (6.23)$$

$$UDem_{m,t} = TDem_{m,t} - SS_{m,t} \qquad \forall m,t \qquad (6.24)$$

The profit of the production plant, which is the objective function, is given by eq. (6.25). The profit takes into account incomes related to the final products, as well as costs associated to raw material, storage material cost, penalties due to unsatisfied demand, freshwater consumption, wastewater generation and use of energy.

$$Profit = \sum_{m \epsilon F_m} \sum_{t \epsilon T} SS_{m,t} \cdot prm_{m,t} - \sum_{m \epsilon R_m} \sum_{t \epsilon T} P_{m,t} \cdot rmc_{m,t} - \sum_{m \epsilon M} \sum_{t \epsilon T} S_{m,t} \cdot stc_{m,t} - \sum_{m \epsilon M} \sum_{t \epsilon T} UDem_{m,t} \cdot pnc_m - \sum_{k \epsilon K} \sum_{i \epsilon I} \sum_{t \epsilon T} U_{k,i,t} \cdot cu_k \qquad (6.25)$$

Two significant characteristics of this mathematical formulations are the presence of both discrete and continuous variables, and the presence of non-linearities in the model, which lead to a MINLP problem. Particularly, eq. (6.9) and (6.10) contain bilinear terms, requiring the use of non-convex non-linear programming procedures, and introducing more complexity in the optimization procedure. This kind of non-linearity can be solved by the linearization of bilinear terms (Quesada and Grossmann, 1995; Majozi and Gouws, 2009). Linear approximations lead to optimal solution for the approximation, but not necessarily to the optimum of the non-linear problem. However, close solutions can be found with better approximations. Nevertheless, this approach proposes the solution of the problem by using a non-linear solver.

6.4. Case study

The underlying scheduling problem includes production, use of water and heat integration to be optimized. Different utilities have been considered, which are freshwater for cleaning purposes, steam to heat the required chemical reactions and refrigerant fluid to cool some processes. Also, in the considered case study, no constraints on the number of heat exchangers that can operate are considered. Furthermore, only direct heat integration with co-current scheme is considered without heat storage.

Particularly, the proposed case study considers the presence of water in the chemical processes for cleaning purposes. This means that wastewater is generated during the cleaning of the equipment units involved in the process. Also, this work takes into account the direct water reuse.

The proposed MINLP formulation has been applied to a case study based on the widely used scheduling example originally proposed by Kondili et al. (1993), which has been extended in different research works in order to study the use of utilities, such as water and energy (Halim and Srinivasan, 2011). This case study involves 5 operations (heating, reaction 1, reaction 2, reaction 3 and separation), 9 states, which corresponds to three raw material (Feed A, Feed B, Feed C), four intermediate products (Hot A, Int AB, Int BC, Imp E) and two final products (Prod 1 and Prod 2) and 4 equipment units (heater, reactor 1, reactor 2 and distiller). The production of the two final products from feedstocks FeedA, FeedB and FeedC is given as follows:

- Heating: Raw material Feed A is heated from 50 ºC to 70 ºC for 1 hour, forming the intermediate product Hot A. This task requires the use of steam. This task is performed in the heater.
- Reaction 1: A mixture of 50% Feed B and 50% Feed C reacts for 2 hours, forming the intermediate product Int BC. This reaction can take place in reactor 1 or in reactor 2. Cooling water is required to decrease the temperature from 100 ºC to 70 ºC. Also, water is needed for washing.
- Reaction 2: A mixture of 40% Hot A and 60% Int BC reacts for 2 hours, forming Int AB (60%) and Prod 1 (40%). This reaction, which can be performed in reactor 1 and reactor 2, requires steam to be heated from 70 ºC to 100 ºC. Washing water is also needed for washing purposes.
- Reaction 3: A mixture of 20% Feed C and 80% Int AB reacts for 2 hours in order to produce intermediate product Imp E. This task is performed in both reactor 1 and reactor 2. This reaction requires the use of steam in order to heat the mixture from 100 ºC to 130 ºC.

- Separation: Imp E is distil in order to separate Prod 2 (90%) and Int AB (10%), which is recycled, after 2 hours. The separation takes place in the distiller, and the temperature decrease from 130 ºC to 100 ºC.

The model has been discretized in equal time intervals of 15 minutes, considering a scheduling horizon of 10 hours (40 time intervals). Figure 6.1 shows the flowsheet of the chemical process. Table 6.1 shows information related to processing times of all operations as well as information related to process units, Table 6.2 and Table 6.3 show all processing constraints related to water utility management (i.e., maximum inlet and outlet contaminant concentration, contaminant loading). Table 6.4 shows equivalent information for energy management, whereas Table 6.5 contains data related to the initial, minimum and maximum storage, price of final products and raw material and storage costs. Table 6.6 indicates the cost of each utility. Notice that water utility includes freshwater consumption as well as wastewater treatment and finally Table 6.7 shows the demand of each final product.

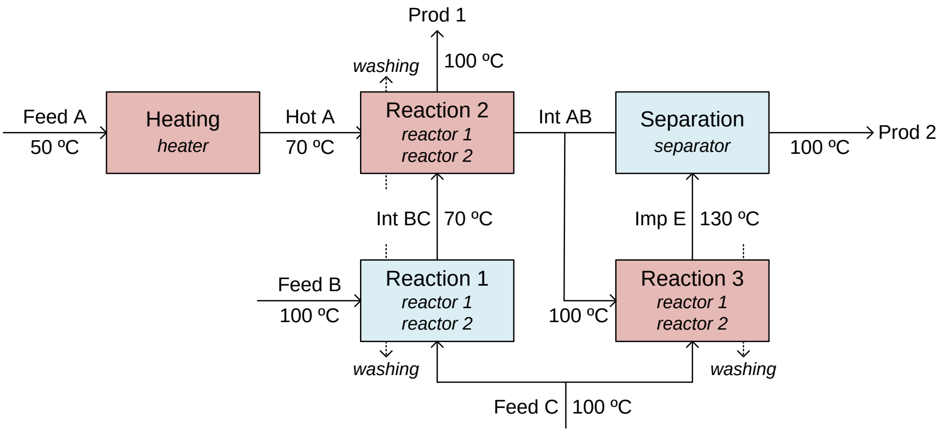

Figure 6.1. Flowsheet of the chemical process.

Table 6.1. Production data.

Task i	Unit j	Minimum batch size, B_i^{min} (kg)	Maximum batch size, B_i^{max} (kg)	Processing time, dur_i (h)	Washing time, WT_i (h)
Heating	Heater	10	100	1.00	0.00
Reaction 1	Reactor 1	10	50	2.00	0.50
	Reactor 2	10	80	2.00	0.25
Reaction 2	Reactor 1	10	50	2.00	0.25
	Reactor 2	10	80	2.00	0.50
Reaction 3	Reactor 1	10	50	1.00	0.25
	Reactor 2	10	80	1.00	0.50
Separation	Distiller	10	200	2.00	0.00

Table 6.2. Inlet and outlet concentration limitations.

Task i	Unit j	Maximum inlet concentration, $Ci_{i,c}^{max}$ (mg/L)			Maximum outlet concentration, $Co_{i,c}^{max}$ (mg/L)		
		Cont A	Cont B	Cont C	Cont A	Cont B	Cont C
Heating	Heater	0.00	0.00	0.00	0.00	0.00	0.00
Reaction 1	Reactor 1	0.50	0.50	2.30	1.00	0.90	3.00
	Reactor 2	0.05	0.20	0.15	0.20	0.40	12.00
Reaction 2	Reactor 1	0.01	0.05	0.30	0.30	0.10	1.20
	Reactor 2	0.18	0.10	0.95	0.40	1.20	1.15
Reaction 3	Reactor 1	0.15	0.20	0.35	0.30	1.00	1.20
	Reactor 2	0.30	0.60	1.50	2.00	1.50	2.50
Separation	Distiller	0.00	0.00	0.00	0.00	0.00	0.00

Table 6.3. Contaminants loading.

Task i	Unit j	Contaminants loading, $CLoad_{i,c}$ (mg contaminant/kg batch)		
		Cont A	Cont B	Cont C
Heating	Heater	0.00	0.00	0.00
Reaction 1	Reactor 1	4.00	80.00	10.00
	Reactor 2	15.00	24.00	358.00
Reaction 2	Reactor 1	28.50	7.50	135.00
	Reactor 2	9.00	2.00	16.00
Reaction 3	Reactor 1	15.00	80.00	85.00
	Reactor 2	22.50	45.00	36.50
Separation	Distiller	0.00	0.00	0.00

Table 6.4. Data for heat integration.

Task i	Unit j	Inlet temperature, Ti_i [ºC]	Outlet temperature, To_i [ºC]	Heat capacity, Cp_i [kJ·kg^{-1}·K^{-1}]
Heating	Heater	50	70	2.5
Reaction 1	Reactor 1	100	70	3.5
	Reactor 2	100	70	3.5
Reaction 2	Reactor 1	70	100	3.2
	Reactor 2	70	100	3.2
Reaction 3	Reactor 1	100	130	2.6
	Reactor 2	100	130	2.6
Separation	Distiller	130	100	2.8

Table 6.5. Scheduling data.

Material state m	Initial inventory, $S0_m$ [kg]	Minimum storage, S_m^{min} [kg]	Maximum storage, S_m^{max} [kg]
Feed A	100	0	1000
Feed B	100	0	1000
Feed C	100	0	1000
Hot A	0	0	100
Int AB	0	0	200
Int BC	0	0	150
Imp E	0	0	200
Prod 1	0	0	1000
Prod 2	0	0	1000

Table 6.6. Revenues and costs.

Material state m	Revenue, $Pr_{m,t}$ [m.u.·kg^{-1}]	Raw material cost, $rmc_{m,t}$ [m.u.·kg^{-1}]	Storage cost, $stc_{m,t}$ [m.u.·kg^{-1}·h^{-1}]	Penalty cost [m.u.·kg^{-1}·h^{-1}]
Feed A	0	10	0.10	0.0
Feed B	0	10	0.10	0.0
Feed C	0	10	0.10	0.0
Hot A	0	0	0.01	0.0
Int AB	0	0	0.01	0.0
Int BC	0	0	0.01	0.0
Imp E	0	0	0.50	0.0
Prod 1	20	0	1.00	2.0
Prod 2	20	0	0.20	0.5

Table 6.7. Demand.

Time interval	Demand of product 1 [kg]	Demand of product 2 [kg]
t18	20	0
t20	32	0
t31	0	46
t36	30	0
t39	0	40
t40	2	0

6.5. Results

The resulting MINLP model has been implemented in GAMS 24.1 (Rosenthal, 2012) and solved using GloMIQO 2.1 (Misener and Floudas, 2013), to optimality (gap of 0.1%) in a Pentium Intel® Core™ i7 CPU 2600 @ 3.40 GHz. The resolution of the proposed mathematical model provides the optimal schedule for production and use of utilities in order to maximize the profit of the given production plant.

In order to study how this integrated methodology improves the profit, the problem was solved for different situations, considering:

(i) The production scheduling, without considering the use of utilities (situation 1).
(ii) The production scheduling, without taking into account neither water reuse nor heat integration (situation 2).
(iii) The simultaneous production scheduling and the water reuse (situation 3).
(iv) The simultaneous production scheduling and the heat integration (situation 4).
(v) The simultaneous production scheduling, water reuse and heat integration (situation 5).

The proposed formulation has allowed the integration of all resources involved in the production process. Particularly, the obtained results shows how the simultaneous management of production, use of water and energy consumption (Table 6.8) allows to:

- Improve the objective function, in particular, the profit of the production plant.
- Reduce the freshwater consumption and the generation of wastewater.
- Reduce the energy consumption.

Table 6.8. Comparison of the obtained results through the different solution approaches.

Key performance indicator	Only scheduling	No water reuse and no heat integration	Water reuse	Heat integration	Simultaneous water reuse and heat integration
Profit [m.u.]	-	1,803.7	1,846.8	1,811.7	1,854.2
Improvement rate [%]	-	-	+2.4%	+0.4%	+2.8%
Traditional scheduling profit [m.u.]	3,045.2	3,038.2	3038.2	3,025.7	3025.7
Water cost [m.u.]	-	539.2	465.2	539.2	465.2
Energy cost [m.u.]	-	695.6	695.6	674.8	674.8
Freshwater consumption [L]	-	431.4	396.9	431.4	396.9
Reused water [L]		0.0	54.5	0.0	54.5
Heating energy consumption [MJ]	-	32.6	32.6	31.4	31.4

Hence, Table 6.8 compares different solutions approaches associated to the same case study. In the first situation, the objective is to optimize the profit but considering only eq. (6.1) to eq. (6.5), without considering use of utilities nor demand management constraints. Other proposed situations consider the use of utilities as well as the demand management. The traditional scheduling profit (which takes into account incomes associated to sales and costs related to raw material purchases, storage and unsatisfied demand) decreases when constraints associated to the use of water and energy are introduced in the mathematical formulation, because the feasible domain where the constraints are satisfied is reduced in comparison with the traditional problem. However, the profit increases if water and energy management is considered, because this consideration reduces the use of this two sources, improving the value of the objective function.

Moreover, the impact of flexibility in the demand has been analysed. The possibility to postpone the shipment of final products introduces an extra degree of freedom, which allows to adapt the production to a better management and availability of resources. Particularly, in the simultaneous management of resources and production without demand side management situation (Table 6.8), the value of the objective function decreases, since without the consideration of flexibility in the demand side management, purchases of final products cannot take place in the pre-established duedates. In this case, the production is not carried out, since the final production will not be sold. This involves the reduction in the production rate, reducing the sales as well as the overall profit.

The optimal schedule without taking into account water and energy costs is shown in Figure 6.2, whereas Figure 6.3a determines this optimal schedule considering water and energy costs too. Moreover, Figure 6.3b shows the optimal schedule for the simultaneous management of production and water reuse. The water reuse can be carried out when a cleaning operation has been finished, and immediately, another cleaning operation starts. However, according to the explained constraints, the input contaminant concentration is delimited by a maximum, which can avoid the water reuse or which can require to mix reused water with freshwater, in order to reduce the contaminant concentration to satisfy the maximum inlet concentration. This explains why in time intervals 10 and 20, the water reuse must be mixed with freshwater, in order to satisfy this set of constraints.

Also, the heat integration is produced when a heating operation and a cooling operations run simultaneously. The optimal schedule for the simultaneous management of production and heat integration is observed in Figure 6.3c. In comparison with Figure 6.2, reaction 1 in reactor 1 has been advanced, in order to take profit of the heat exchange and save energy. Finally, Figure 6.4 shows the optimal schedule for the simultaneous management of production, water reuse and heat integration. This schedule allows the water reuse, as in situation 3, and the same heat integration obtained in situation 4.

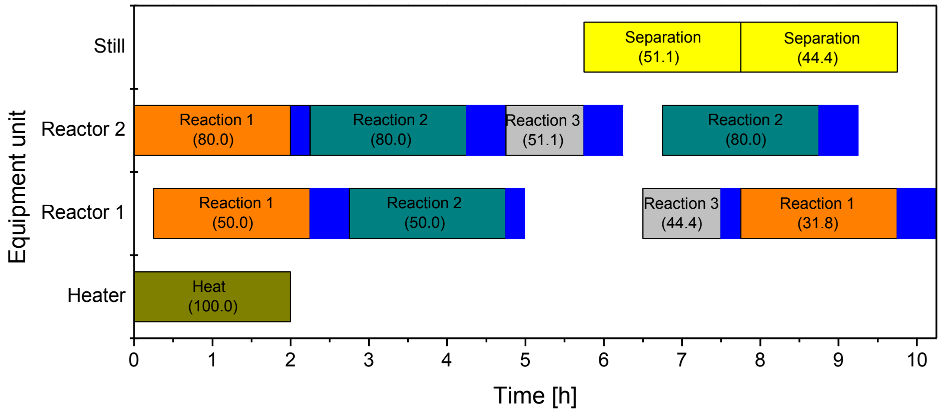

Figure 6.2. Optimal schedule for the production without considering neither water nor energy costs.

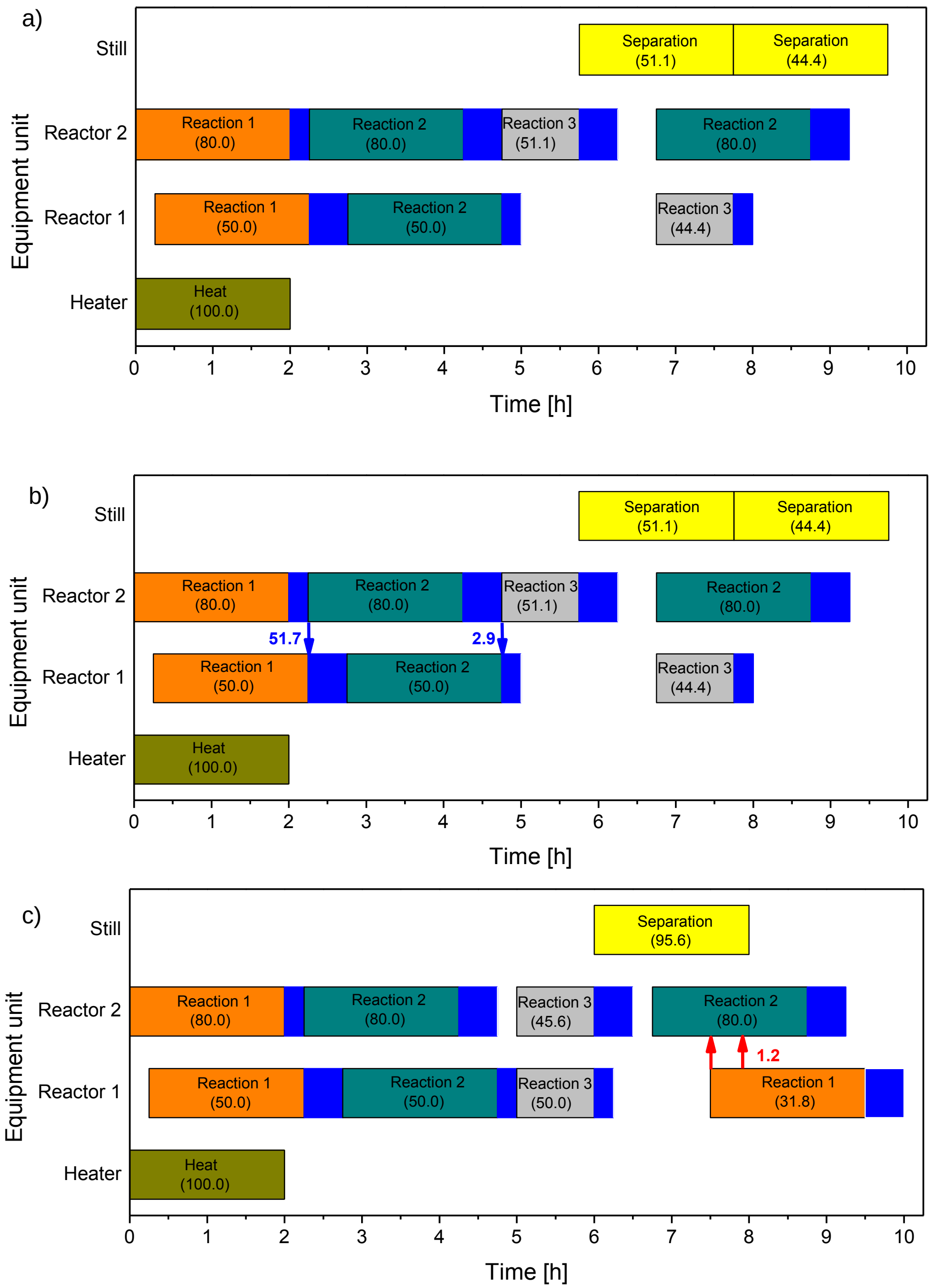

Figure 6.3. Optimal schedule for the production
a) taking into account water and energy costs, b) considering the water reuse and c) considering the heat integration.

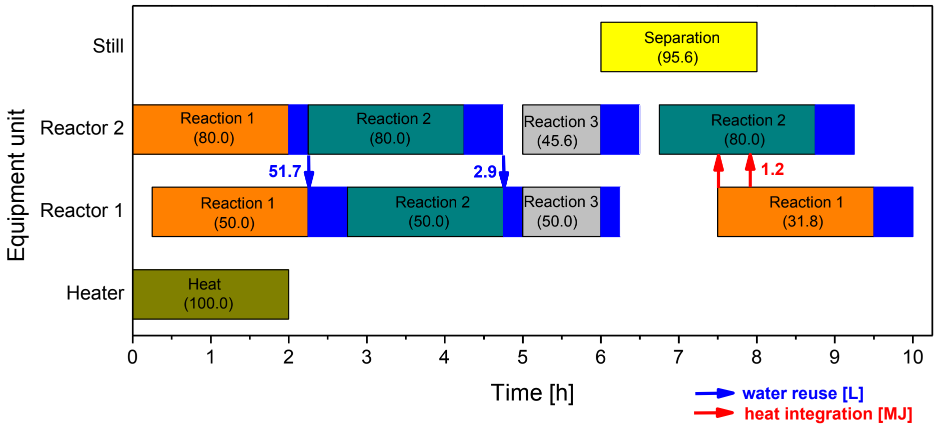

Figure 6.4. Optimal schedule for the simultaneous production scheduling, water reuse and heat integration.

So, this proposed mathematical formulation has allowed the integration of the management of resources within the production process, which has been used for the coordinated organisation of all procedures involved in the process. In contrast with previous formulations, this paper has presented a generalized procedure for this integrated management. However, the presence of non-linearities in the model constraints its size, due to the required computational time to obtain the optimal solution. If the size of the problem is huge, different techniques can be applied to relax the non-linearities (i.e., piecewise linearization).

This proposed approach requires more equations and more binary variables in comparison with the approaches in which the simultaneous management of production, water and energy is not taken into account (Table 6.9). This extra complexity in the model involves more computational effort to solve the problem.

Furthermore, this proves has been solved by using GloMIQO as optimizer, because this solver can be used to resolve mixed integer quadratic problems, which is the proposed case. This solver is a global optimizer, able to find the optimal solution. Moreover, other solvers were used to solve this mathematical formulation (i.e., BARON). However, the optimization procedure was not able to give the optimal solution in less than 3600 CPU s.

Table 6.9. Model statistics.

Key performance indicator	Only scheduling	No water reuse and no heat integration	Water reuse	Heat integration	Simultaneous water reuse and heat integration
Number of equations	5,205	10,012	15,047	18,607	23,617
Number of continuous variables	2,845	7,241	10,121	12,681	15,561
Number of binary variables	320	495	1,935	3,016	4,456
Solver	CPLEX	GloMIQO	GloMIQO	GloMIQO	GloMIQO
Computational time, CPU [s]	1.373	15.848	299.082	35.102	920.199
Gap	0.0 %	< 0.1 %	< 0.1 %	< 0.1 %	< 0.1 %

6.6. Concluding remarks

This chapter has developed a short-term scheduling of a production plant for the management of production and utilities. This is achieved by maximizing the profit of a given production plant. This objective function includes penalties for the delayed fulfilment of the product demand. The proposed formulation integrates all resource usage models and scheduling production models within a new generalized mathematical formulation, which manage all resources in a coordinated way, by integrating production and the use of resources.

The proposed mathematical model has been applied to solve simultaneously the management of production and use of resources, in order to obtain the optimal scheduling that maximizes the overall profit and manages different utilities working under different usage policies. The need to introduce terms related to both quality and quantity of the production resources has led to the development of a MINLP model. A global non-linear solver has been used to solve this non-linear problem, which has allowed to solve this management problem simultaneously, instead of in a sequential way or partially. Also, this formulation can be applied to reduce the generation of wastewater reduction and the heat integration in the scheduling framework. The obtained results reveal how the simultaneous management of production and resources will lead to enhancements in the efficiency of the production plant.

However, the obtained results shows that this formulation can be used to solve future industrial problems with higher complexity. Moreover, the current and further work is focused on the introduction of uncertainty in the model (i.e., the presence of variability in the product demand) by using the stochastic programming, as well as the consideration of multi criteria decision making, in order to involve multiple considerations (i.e., economy, sustainability), through the use of multi-objective optimization techniques. Furthermore, this mathematical formulation can be extended in order to incorporate the recycle of the utilities.

6.7. Nomenclature

Indices, sets and subsets

$c \in C$	*Set of quality parameters*
$i \in I$	*Set of production operations*
$j \in J$	*Set of equipment units*
$k \in K$	*Set of resources*
$m \in M$	*Set of states*
$t \in T$	*Set of time intervals*
$i \in II_m$	*Subset of operations* i *requiring material from state* m
$i \in IO_m$	*Subset of operations* i *producing material from state* m
$i \in JI_j$	*Subset of operations* i *that can be assigned in equipment unit* j
$k \in CU_k$	*Subset of resources* k *used in continuous (or semi-continuous) operations*
$k \in DU_k$	*Subset of resources* k *used in discontinuous operations*
$m \in F_m$	*Subset of states* m *corresponding to final products*
$m \in R_m$	*Subset of states* m *corresponding to raw materials*

Parameters

B_i^{min}	*Minimum batch size of operation* i
B_i^{max}	*Maximum batch size of operation* i
$Ci_{c,k,i}^{min}$	*Minimum value for the inlet quality parameter* c *of resource* k *in operation* i
$Ci_{c,k,i}^{max}$	*Maximum value for the inlet quality parameter* c *of resource* k *in operation* i
$CL_{c,k,i}$	*Variation of quality parameter* c *of resource* k *in operation* i
$Co_{c,k,i}^{min}$	*Minimum outlet quality parameter* c *of resource* k *in operation* i
$Co_{c,k,i}^{max}$	*Maximum outlet quality parameter* c *of resource* k *in operation* i
Cp_i	*Characteristic parameter of operation* i
cu_k	*Resource cost*
D_i	*Period of time defined as deviation from the starting time of operation* i
$Dem_{m,t}$	*Demand of material state* m *at time interval* t
fd_i	*Fixed duration of operation* i
pnc_m	*Penalty cost for unsatisfied demand of material state* m
$prm_{m,t}$	*Price of material state* m *at time interval* t
$rmc_{m,t}$	*Raw material cost of material state* m *at time interval* t
S_m^{min}	*Minimum amount of stored material of all states* m
S_m^{max}	*Maximum amount of stored material of all states* m
$S0_m$	*Initial amount of stored material of all states* m
$stc_{m,t}$	*Storage cost of material state* m *at time interval* t
Ti_i	*Inlet characteristic of a process variable of operation* i

To_i	*Outlet characteristic of a process variable of operation i*
$Ui_{k,i}^{min}$	*Minimum amount of resource k in operation i*
$Ui_{k,i}^{max}$	*Maximum amount of resource k in operation i*
$Ur_{k,i',i}^{min}$	*Minimum reuse of resource k from operation i' to operation i*
$Ur_{k,i',i}^{max}$	*Maximum reuse of resource k from operation i' to operation i*
UT_i	*Time of use resource in operation i*
$\rho_{i,m}$	*Stoichiometry of material m to perform operation i*

Continuous and positive variables

$B_{i,t}$	*Batch size of operation i at time interval t*
$Ci_{c,k,i,t}$	*Inlet value for the quality parameter c of resource k in operation i at time interval t*
$Co_{c,k,i,t}$	*Outlet quality parameter of resource k in operation i at time interval t*
$P_{m,t}$	*Amount of raw material purchases of all states m at time interval t*
$S_{m,t}$	*Amount of stored material of all states m at time interval t*
$SS_{m,t}$	*Amount of sold material of all states m at time interval t*
$TDem_{m,t}$	*Total product demand of material state m at time interval t*
$Tr_{i,t}$	*Characteristic value of a process variable operation i at the beginning of time interval t*
$UDem_{m,t}$	*Unsatisfied product demand of material state m at time interval t*
$U_{k,i,t}$	*Amount/flow of fresh resource k in operation i at time interval t*
$Ue_{k,i,t}$	*Amount/flow of effluent resource k from operation i at time interval t*
$Ug_{k,i,t}$	*Amount/flow of produced/generated resource k in operation i at time interval t*
$Ui_{k,i,t}$	*Amount/flow of inlet resource k in operation i at time interval t*
$Un_{k,i,t}$	*Necessity of amount/flow of resource k in operation i at time interval t*
$Uo_{k,i,t}$	*Amount/flow of outlet resource k in operation i at time interval t*
$Ur_{k,i,i',t}$	*Amount/flow of resource k from unit operation i to unit i' at time interval t*

Continuous variables

$Profit$	*Overall profit*

Binary variables

$X_{i,t}$	*= 1, if task i is produced at time interval t*
$We_{k,i,i',t}$	*= 1, if resource k can be used from operation i' to operation i at time interval t*
$Wi_{k,i,t}$	*= 1, if resource k is used in operation i at time interval t*
$Wr_{k,i,i',t}$	*= 1, if resource k is reused after operation i to operation i' at time interval t*

Part III – Integrated Supply Chain Optimization

Chapter 7. Integration of different levels in the decision making hierarchy

Chapters 4, 5 and 6 were focused on the simultaneous management of production and resources in the short-term planning. This chapter analyses the integration of different time scales within the decision making process. Particularly, this chapter is focused on the integration of synthesis, planning and scheduling of a supply chain under uncertain conditions. The simultaneous consideration of integrated formulations provides flexibility to the production processes and plants. The typical state task network has been extended to consider the synthesis problem, in which both synthesis and process recipe information have been merged, evolving into a synthesis state task network representation. Thus, a MILP formulation has been developed. Plant and process operations have been described considering the characteristics of synthesis, planning and scheduling problems. The results show the flexibility introduced when considering design decisions while solving the scheduling problem and state/highlight the impact of future operating conditions (demand fluctuations, market trends, etc.) in today's decision. The model provides decision makers with tools to re-optimize existing plants, design new plants and include operating issues into design problems.

7.1. Introduction

Process recipe is the basic information required to be managed to run process (batch or continuous). The representation of such information is usually based on the flowsheet view of the plant as a basic schema to describe the process itself (units, operations, etc.). In the context of supply chain management Kondili et al. (1993) defined the state task network (STN) representation as a way to organize the information. This representation consists of a direct graph which includes two nodes: the state node and the task node. The STN is based on the identification of the process as a set of operations leading to different states, defining the links among them on the basis of the precedence rules and recipe information. Moreover, different details can be incorporated to such networks, in order to adapt the resulting information structure to the specific objectives of the analysis to be performed. This representation can be extended to represent all operations throughout the overall SC.

Hence, an extended version of the STN representation is proposed, in order to introduce information related to the synthesis problem. The resulting representation, Synthesis State Task Network (SSTN) extends the states and tasks nodes information (materials and resources, as well as operations within the SC), in such a way that the states are now also connected to synthesis blocks incorporating the information associated to the synthesis problem. Each synthesis block includes complementary information related to:

(i) The equipment costs (i.e., fixed, operational and installation costs),
(ii) The equipment unit performance (i.e., conversion rates, processing time).

Figure 7.1 summarizes the evolution of such network representations. Particularly, Figure 7.1a shows the flowsheet-based network representation (simple tasks and flows information). The STN representation (Figure 7.1b) introduces state nodes representing the flows, and tasks representing the process operations, which transform the material (input flow) to one or more output flows (state and task nodes are denoted by circles and rectangles, respectively). The proposed SSTN (Figure 7.1c) incorporates information related to the synthesis problem (i.e., equipment units' flexibility to be installed in different configurations, SC structure, process recipe), obtaining a superstructure which contemplates all configurations taken into account within the scheduling problem. Particularly, the solution obtained in the proposed case study considers different equipment options to solve the same process recipe. Hence, the information is extended by including different costs (fixed and variable) and conversion rates for each equipment unit.

This chapter address the integration of strategic, tactical and operational levels, through the coordination of the design of the production plant taking into account the short-term planning of the production plant and the overall SC. Tactical information is represented through market demands and the plant must be designed in order to satisfy the demand forecast. Once, the demand forecast is obtained, it is considered as an uncertain parameter with several scenarios to be considered. The corresponding formulation is implemented as a two stage stochastic programming model, considering the demand in each scenario and the possibility that this scenario will take place.

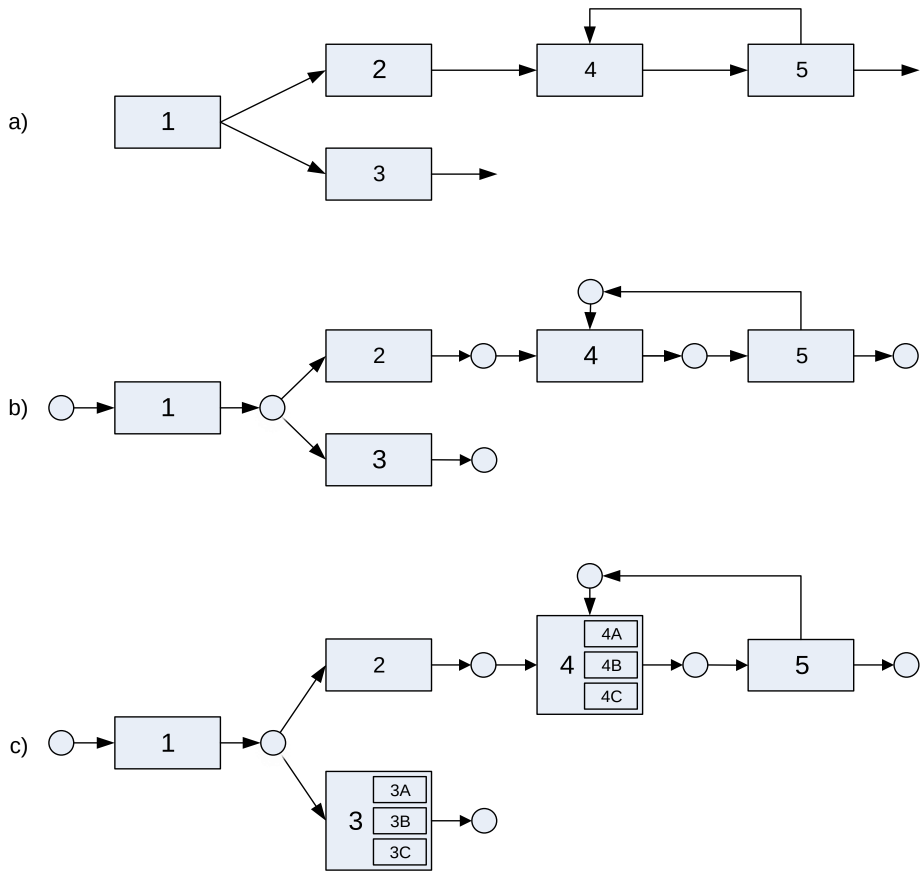

Figure 7.1. Evolution of network representations.

7.2. Problem statement

The new two-stage stochastic programming (TSSP) approach is presented as a MILP (Kondili et al., 1993), based on a discrete time representation. The goal is to obtain the optimal plant design (i.e., equipment unit installation) and the proposed working plan (i.e., allocation, storage levels, and the batch size) under uncertainty in order to maximize the profit of the SC. The proposed formulation incorporates the integration of operational decisions (scheduling) with process synthesis (design). The synthesis problem relates different equipment unit technologies available to be installed with their own characteristics, such as conversion rates, fixed cost, variable cost and installation cost.

Consequently, the problem under study is described in the following terms:

(i) A scheduling horizon which is divided into a set of time intervals $t \in T$.
(ii) A set of operations $i \in I$.
(iii) A set of equipment units $j \in J$ to perform the involved operations i.
(iv) A set of production plants $p \in P$.
(v) A set of distribution centres $d \in D$.
(vi) A set of markets $k \in K$.
(vii) A set of scenarios $n \in N$.
(viii) A set of material states, including raw material, and intermediate and final products $m \in M$.
(ix) The investment cost of each equipment unit j.
(x) The capacity of production plants p and distribution centres d.
(xi) The demand of final products.
(xii) The dimension of a given production plant, which constraints the number of equipment units j to be install.
(xiii) The initial amount of each material.
(xiv) The production recipe (stoichiometric data).
(xv) The process unit configuration.
(xvi) The operation processing times.
(xvii) The costs and prices of raw materials, intermediate products and final products.

The proposed approach is implemented as a two-stage stochastic formulation (see Chapter 3.5.4). The TSSP problem is divided into first and second stage variables. First-stage variables consist on variables that must be decided before the uncertainty has been revealed (also known here-and-now variables), which does not depend on the scenario. Otherwise, second-stage variables are considered as the recourse actions in the feasibility problem and they are scenario dependent variables. Thus, the expected profit is then obtained after the realization of all the scenarios, both first and second stage variables are described below:

(i) First stage variables (does not depend on the scenario):
  a. The equipment technology to install in each production plant p, $y_{j,p}$.
(ii) Second stage variables (depends on the scenario):
  a. The equipment unit j to be used to perform operation i in scenario n at time t, $W_{i,j,p,n,t}$.
  b. The amount of material $B_{i,j,p,n,t}$ processed according to operation i at equipment unit j in each scenario n at time t.
  c. The amount of material $S_{m,p,n,t}$ stored at state m in scenario n at time t.

d. The amount of raw material m acquired in scenario n at time t, $Rm_{m,p,n,t}$.

The uncertain sources in the developed mathematical model are:

(i) Product demand uncertainty.
(ii) Initial storage level uncertainty.

The following assumptions have been considered:

(i) Each material is stored the production plant.
(ii) Intermediate materials can be stored in finite capacity with unlimited waiting time.
(iii) Product delivery to the customer can be delayed according to a penalty cost.
(iv) Transfer times between process units within the production plant p are considered negligible.

The proposed mathematical formulation can be extended by introducing the management of resources in the production process (i.e., water and energy), which incorporates non-linearities in the model, leading to a MINLP model. This fact introduces more complexity in the optimization procedure. Moreover, the consideration of uncertainty through the stochastic programming involves more computational time to obtain the optimal solution in comparison with deterministic conditions. Both factors simultaneously involves that the computational effort to solve the problem is unaffordable. Thus, the management of resources is not going to be taken into account, because the objective of this chapter is to integrate different hierarchical levels under uncertain conditions, and high degree of details associated to the production process can be considered posteriorly in the short-term planning.

This model is based on a discrete time formulation, since the simultaneous introduction of hybrid and continuous time representation and uncertainty may increase the computational time to solve it, making unaffordable its resolution.

7.3. Mathematical formulation

The MILP-based mathematical model integrates operational, tactical and strategic decisions. The mathematical formulation takes into account the production plant synthesis (Grossmann and Daichendt, 1996), the production plant schedule and the management of the SC.

The scheduling constraints takes into account allocation constraints, capacity constraints and material balances. Eq. (7.1) forces that, at most, one operation can start at equipment unit j at any time t, which avoids any overlap in the production plant p in any equipment unit in each scenario n. Eq. (7.2) determines the allocation of equipment units j along the scheduling horizon in production plant p for each scenario n, taking into account residence time of the operations in the equipment unit j. The amount of material $B_{i,j,p,n,t}$ processed at equipment unit j at time t in production plant p is limited in eq. (7.3) by the consideration of maximum and minimum capacity of the equipment units. Also, eq. (7.4) constraints the amount of material stored $S_{m,p,n,t}$ of all states in each scenario n in each period of time t, by maximum and minimum storage limits of the states. Furthermore, the material balances in production plant p along the processing network are controlled through Eq. (7.5) where, given an initial storage, the storage at the state m at time t is computed adding the input of material that arrives from the previous operations and subtracting the material that feeds the following operations, as well as shipments to distribution centres. This balance is given by the stoichiometry and the conversion degree of the chemical process as well as sales of final products and purchases of raw material, the possibility of receiving quantities of raw materials $Rm_{m,n,t}$ at feed states m at any time t during the schedule, rather than having all the required feedstock stored locally at the start of processing. Notice that the initial amount of stored material m depends on the scenario n. This is because this parameter is defined as uncertain, since the initial storage of each short-term planning problem may depend on each scenario.

$$\sum_{i \epsilon JI_j} X_{i,j,p,n,t} \leq 1 \qquad \forall j,p,n,t \qquad (7.1)$$

$$\sum_{\substack{t \leq t' \epsilon T \\ t' < t + fd_{i,j} - 1}} \sum_{i' \in JI_j} X_{i',j,p,n,t'} - 1 \leq M \cdot \left(1 - X_{i,j,p,n,t}\right) \qquad \forall i,j,p,n,t \qquad (7.2)$$

$$X_{i,j,p,n,t} \cdot B_{i,j}^{min} \leq B_{i,j,p,n,t} \leq X_{i,j,p,n,t} \cdot B_{i,j}^{max} \qquad \forall i \in JI_j, j,p,n,t \qquad (7.3)$$

$$S_{m,p}^{min} \leq S_{m,p,n,t} \leq S_{m,p}^{max} \qquad \forall m,p,n,t \qquad (7.4)$$

$$\begin{aligned} S_{m,p,n,t} = {} & S0_{m,p,n}\big|_{t=1} + S_{m,p,n,t-1}\big|_{t>1} + \sum_{i \epsilon IO_m} \sum_{j} \rho_{i,m} \cdot \alpha_j \cdot B_{i,j,p,n,t-fd_{i,j}} \\ & - \sum_{i \epsilon II_m} \sum_{j} \rho_{i,m} \cdot B_{i,j,p,n,t} + Rm_{m,p,n,t} \\ & - \sum_{d \epsilon D} STD_{m,p,d,n,t-Tr1_{p,d}} \end{aligned} \qquad \forall m,p,n,t \qquad (7.5)$$

Regarding the specific synthesis decisions, the binary variable $y_{j,p}$ in eq. (7.6) establishes the equipment technologies to be installed in each production plant p. If this binary variable takes value 1, this means that the optimal solution is to install this equipment unit in the corresponding production plant p. If the equipment unit j to perform operation i in production plant p and in scenario n is used at any time t, then y_j will take value 1. In addition, the equipment installation is constrained in eq. (7.7) by a maximum number of equipment units in each production plant p, which cannot be exceeded.

$$X_{i,j,p,n,t} \leq y_{j,p} \qquad \forall i,j,p,n,t \qquad (7.6)$$

$$\sum_{j \in J} y_{j,p} \leq \overline{Y_p} \qquad \forall p \qquad (7.7)$$

The following equations are focused on the management of the supply chain. The tactical-synthesis integration has been done through the transportation of the products to the distribution centres and the final markets, the demand satisfaction and the backlogged demand (time window). Eq. (7.8) constraints the amount of final products m to be transported from each production plant p to each distribution centre d by a minimum and maximum value. Also, eq. (7.9) establishes the material balance in each distribution centre, considering the storage level in the previous period of time and shipments from production plants p and to markets k. Notice that the initial amount of stored final product m in each distribution centre d depends on the scenario n. This is because this parameter is defined as uncertain, since the initial storage of each short-term planning problem may depend on each scenario. Moreover, eq. (7.10) constraints the storage level of distribution centre d, delimited by a minimum a maximum level for each product. Eq. (7.11) restricts the amount of final products m to be transported from each distribution centre d to each market k by a minimum and maximum value. Furthermore, eq. (7.12) determines that the overall amount of shipments corresponds to the sales of products m to markets k.

$$STD_{m,p,d,n,t}^{min} \leq STD_{m,p,d,n,t} \leq STD_{m,p,d,n,t}^{max} \qquad \forall m \in F,p,d,n,t \qquad (7.8)$$

$$SSD_{m,d,n,t} = SS0_{m,d,n}\big|_{t=1} + SSD_{m,d,n,t-1}\big|_{t>1} + \sum_{p \epsilon P} STD_{m,p,d,n,t} - \sum_{k \epsilon K} STM_{m,d,k,n,t} \qquad \forall m \in F,d,n,t \qquad (7.9)$$

$$SSD_{m,d,n}^{min} \leq SSD_{m,d,n,t} \leq SSD_{m,d,n}^{max} \qquad \forall m \in F,d,n,t \qquad (7.10)$$

$$STM_{m,d,k,n,t}^{min} \leq STM_{m,d,k,n,t} \leq STM_{m,d,k,n,t}^{max} \qquad \forall m \in F,d,k,n,t \qquad (7.11)$$

$$\sum_{d \in D} STM_{m,d,k,n,t} = SS_{m,k,n,t+Tr2_{d,k}} \qquad \forall m \in F, k, n, t \qquad (7.12)$$

The proposed approach may also consider the exploitation of the eventual flexibility in the demand duedates, which might be delayed from their initial targets, but at a cost associated to a penalty term in case of not satisfying a given demand. Flexible demand is useful to alleviate any mismatch between production capacity and demand. Eq. (7.13) establishes that sales of final products are limited by the total demand, and eq. (7.14) determines that the unsatisfied demand is given by the difference between the demand and the product sales.

$$SS_{m,k,n,t} \leq Dem_{m,k,n,t} \qquad \forall m \in F, k, n, t \qquad (7.13)$$

$$UDem_{m,k,n,t} = Dem_{m,k,n,t} - SS_{m,k,n,t} \qquad \forall m \in F, k, n, t \qquad (7.14)$$

The economic analysis of different alternatives associated to this problem has been taken into account. The overall installation cost for the overall horizon is given by Eq. (7.15) which considers the acquisition cost associated to each equipment unit j of each technology. Next equations are focused on the daily costs. Eq. (7.16) determines the variable cost, given by the start-up cost of each equipment unit j at period time t and the batch size $B_{i,j,p,n,t}$. Eq. (7.17) calculates the raw material cost through the required purchases to perform the production process. Additionally, a penalty cost in case of deviation between the initial quantity demanded and the production reached has been determined in Eq. (7.18). Also, eq. (7.19) determines the storage cost in distribution centres, considering the amount of stored products and its individual inventory cost. Transport costs are calculated throughout eq. (7.20), taking into account the amount of transported products, the distance between different elements within the supply chain and the individual shipment cost of each product. Total operational costs for the overall horizon are calculated through the summation of previous costs in Eq. (7.21), taking into account the number of operating days. Incomes are determined in Eq. (7.22), considering production sales and its selling price. Finally, the goal is to maximize the expected profit, given by Eq. (7.23) as the difference between incomes and costs, taking into account the probability in which scenario n can occur.

$$IC = \sum_{j \in J} \sum_{p \in P} Cins_j \cdot y_{j,p} \qquad (7.15)$$

$$VC_n = \sum_{i \in I} \sum_{j \in J} \sum_{p \in P} \sum_{t \in T} Csup_j \cdot X_{i,j,p,n,t} + \sum_{i \in I} \sum_{j \in J} \sum_{p \in P} \sum_{t \in T} Cvar_{i,j} \cdot B_{i,j,p,n,t} \qquad \forall n \qquad (7.16)$$

$$RMC_n = \sum_{m \in R_m} \sum_{p \in P} \sum_{t \in T} Crm_{m,t} \cdot Rm_{m,p,n,t} \qquad \forall n \qquad (7.17)$$

$$PC_n = \sum_{m \in F_m} \sum_{k \in K} \sum_{t \in T} Cpen_{m,k} \cdot UDem_{m,k,n,t} \qquad \forall n \qquad (7.18)$$

$$SC_n = \sum_{m \in F_m} \sum_{d \in D} \sum_{t \in T} Csto_{m,d,t} \cdot SSD_{m,d,n,t} \qquad \forall n \qquad (7.19)$$

$$TC_n = \sum_{m \in F_m} Ctra_m \cdot \left(\sum_{p \in P} \sum_{d \in D} \sum_{t \in T} STD_{m,p,d,n,t} \cdot d1_{p,d} + \sum_{d \in D} \sum_{k \in K} \sum_{t \in T} STM_{m,d,k,n,t} \cdot d2_{d,k} \right) \qquad \forall n \qquad (7.20)$$

$$Cost_n = ND \cdot (FC_n + VC_n + RMC_n + UC_n + PC_n + SC_n + TC_n) \qquad \forall n \qquad (7.21)$$

$$Incomes_n = ND \cdot \sum_{m \in F_m} \sum_{k \in K} \sum_{t \in T} prm_{m,k} \cdot SS_{m,k,n,t} \qquad \forall n \qquad (7.22)$$

$$Profit = IC + \sum_{n \epsilon N} pr_n \cdot (Incomes_n - Cost_n) \qquad (7.23)$$

The proposed model takes the advantage of the flexibility of the process definition, by considering several alternatives to be installed determining the plant superstructure. Also states that the design decision making is very important at the operational level. In addition, the model allows to the decision makers to reformulate the plant and process superstructure, by re-optimizing the existing plant and/or design the plant.

7.4. Case study

The proposed MILP formulation has been applied to a case study based on the widely used scheduling example initially proposed by Kondili et al. (1993). The problem to be solved involves 5 operations (heating, reaction 1, reaction 2, reaction 3 and separation), 9 states, which corresponds to three raw material (Feed A, Feed B, Feed C), four intermediate products (Hot A, Int AB, Int BC, Imp E) and two final products (Prod 1 and Prod 2). The production recipe of the two final products from feedstocks FeedA, FeedB and FeedC is given as follows:

- Heating: Raw material Feed A is heated for 1 hour, forming the intermediate product Hot A. This operation is performed in a heater.
- Reaction 1: A mixture of 50% Feed B and 50% Feed C reacts for 2 hours, forming the intermediate product Int BC. This reaction must take place in reactor.
- Reaction 2: A mixture of 40% Hot A and 60% Int BC reacts for 2 hours, forming Int AB (60%) and Prod 1 (40%). This reaction is performed in a reactor.
- Reaction 3: A mixture of 20% Feed C and 80% Int AB reacts for 1 hour in order to produce intermediate product Imp E. This operation is performed a reactor.
- Separation: Imp E is distil in order to separate Prod 2 (90%) and Int AB (10%), which is recycled, after 1 hour. The separation takes place in the distiller.

Seven potential equipment units have been considered for the production plant (heater 1, heater 2, reactor 1, reactor 2, reactor 3, reactor 4 and distiller). All reactions can take place in all considered reactors. All equipment units can be installed simultaneously. Table 7.1 presents the economic and production information of each equipment unit j.

Table 7.1. Equipment units, conversion degrees and costs.

Equipment	Conversion degree α_j	Variable cost $Cvar_{i,j}$	Fixed cost $Cfix_j$	Investment cost $Cins_j$
Heater 1	-	0.4	800	125,000
Heater 2	-	0.6	500	115,000
Reactor 1	1.00	1.5	1,500	500,000
Reactor 2	1.00	1.0	1,000	150,000
Reactor 3	0.90	0.9	800	125,000
Reactor 4	0.90	0.8	750	112,500
Distiller	-	0.5	1,000	250,000

Figure 7.2a represents the typical synthesis problem that considers different equipment units able to perform the same operation in the process flowsheet. Moreover, Figure 7.2b shows the STN representation for the scheduling problem that considers the recipe of the process, including states, equipment units and operations. Finally, Figure 7.2c shows the proposed SSTN representation introducing the synthesis considerations into the STN. Additional aggregated data to be considered include, for example, the different conversions which can be achieved when using different reactors or the equipment costs (fixed and variable costs).

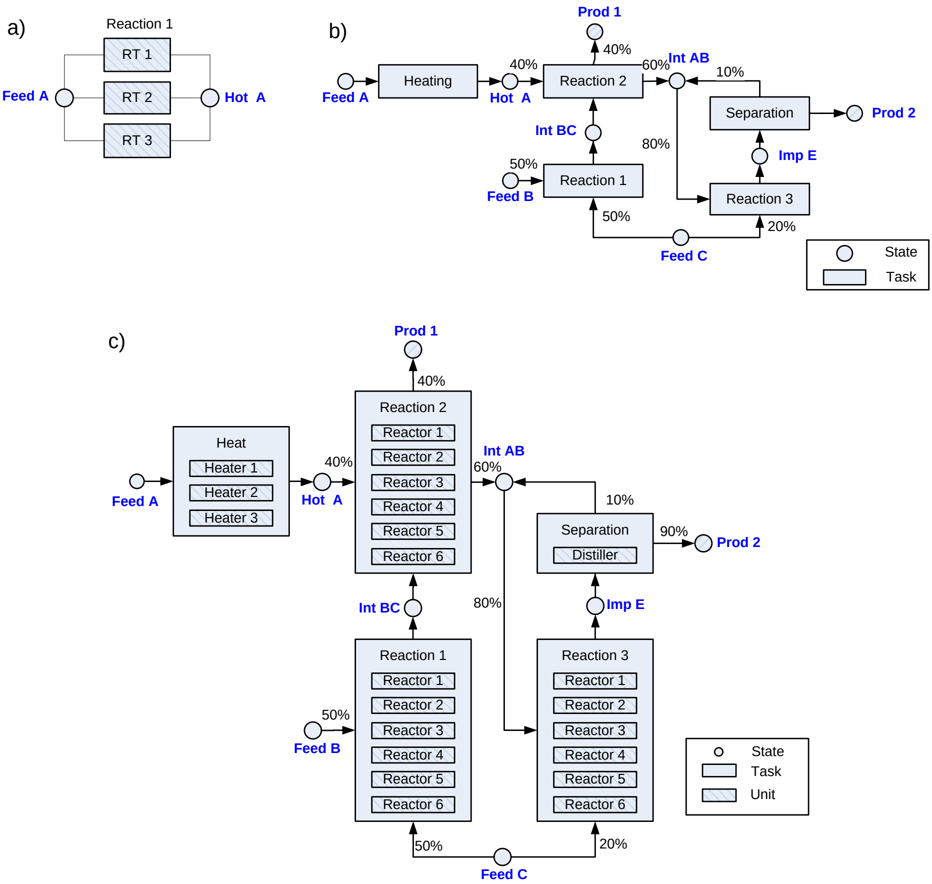

Figure 7.2. Description of the Synthesis State Task Network.

The model has been discretized in equal time intervals for the scheduling problem considering 15 time periods per day and considering 250 working days in one year as the overall time horizon. Table 7.2 shows information related to process units as well as to processing times of all operations. Also, Table 7.3 contains data related to the initial, minimum and maximum storage.

Table 7.2. Production data.

Operation i	Unit j	Minimum batch size, $B_{i,j}^{min}$	Maximum batch size, $B_{i,j}^{max}$	Processing time, $fd_{i,j}$
Heating	Heater 1	10	100	1.00
	Heater 2	10	100	1.00
Reaction 1	Reactor 1	10	100	2.00
	Reactor 2	10	80	2.00
	Reactor 3	10	60	2.00
	Reactor 4	10	20	2.00
Reaction 2	Reactor 1	10	100	2.00
	Reactor 2	10	80	2.00
	Reactor 3	10	60	2.00
	Reactor 4	10	20	2.00
Reaction 3	Reactor 1	10	100	1.00
	Reactor 2	10	80	1.00
	Reactor 3	10	60	1.00
	Reactor 4	10	20	1.00
Separation	Distiller	40	200	2.00

Table 7.3. Scheduling data.

Material state m	Initial inventory, $S0_{m,p,n}$ [kg]	Minimum storage, $S_{m,p}^{min}$ [kg]	Maximum storage, $S_{m,p}^{max}$ [kg]
Feed A	0	0	500
Feed B	0	0	1000
Feed C	0	0	500
Hot A	0	0	0
Int AB	0	0	200
Int BC	0	0	150
Imp E	0	0	100
Prod 1	0	0	500
Prod 2	0	0	500

The supply chain consists on a set of suppliers that provide raw materials to one production plant, which produce two products that can be stored in two distribution centres, and finally the products are delivered to three markets. Figure 7.3 represents the supply chain under study.

The production plant remains opened during 10 time intervals each day. Also, the demand is referred to the last time interval of each day.

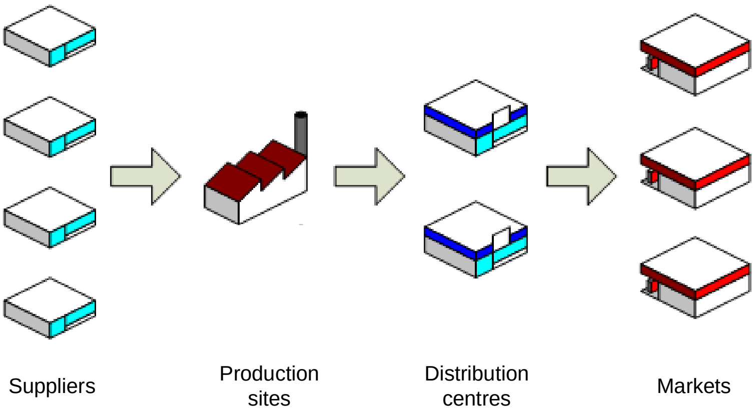

Figure 7.3. Supply chain case study.

Table 7.4 shows the demand of final products in each market and scenario. Notice that the demand may include the unsatisfied demand of previous periods of time (i.e., previous day). Note that this value corresponds to the demand at the end of the scheduling horizon.

Table 7.4. Demand.

Scenario	Product 1			Product 2		
n	Market 1	Market 2	Market 3	Market 1	Market 2	Market 3
1	27.0	27.0	45.0	58.5	45.0	49.5
2	27.0	27.0	45.0	58.5	45.0	49.5
3	27.0	27.0	45.0	58.5	45.0	49.5
4	27.0	27.0	45.0	65.0	50.0	55.0
5	27.0	27.0	45.0	65.0	50.0	55.0
6	27.0	27.0	45.0	65.0	50.0	55.0
7	27.0	27.0	45.0	71.5	55.0	60.5
8	27.0	27.0	45.0	71.5	55.0	60.5
9	27.0	27.0	45.0	71.5	55.0	60.5
10	30.0	30.0	50.0	58.5	45.0	49.5
11	30.0	30.0	50.0	58.5	45.0	49.5
12	30.0	30.0	50.0	58.5	45.0	49.5
13	30.0	30.0	50.0	65.0	50.0	55.0
14	30.0	30.0	50.0	65.0	50.0	55.0
15	30.0	30.0	50.0	65.0	50.0	55.0
16	30.0	30.0	50.0	71.5	55.0	60.5
17	30.0	30.0	50.0	71.5	55.0	60.5
18	30.0	30.0	50.0	71.5	55.0	60.5
19	33.0	33.0	55.0	58.5	45.0	49.5
20	33.0	33.0	55.0	58.5	45.0	49.5
21	33.0	33.0	55.0	58.5	45.0	49.5
22	33.0	33.0	55.0	65.0	50.0	55.0
23	33.0	33.0	55.0	65.0	50.0	55.0
24	33.0	33.0	55.0	65.0	50.0	55.0
25	33.0	33.0	55.0	71.5	55.0	60.5
26	33.0	33.0	55.0	71.5	55.0	60.5
27	33.0	33.0	55.0	71.5	55.0	60.5

Table 7.5 contains the initial storage level of final products in each distribution centre. Since the initial storage level is considered as uncertain, this value depends on the scenario. This fact allows to solve the problem once, instead of solving it again if this value changes.

Table 7.5. Initial storage level in distribution centres.

Scenario n	Product 1		Product 2	
	Distribution centre 1	Distribution centre 2	Distribution centre 1	Distribution centre 2
1	24	24	24	24
2	30	30	30	30
3	33	33	33	33
4	24	24	24	24
5	30	30	30	30
6	33	33	33	33
7	24	24	24	24
8	30	30	30	30
9	33	33	33	33
10	24	24	24	24
11	30	30	30	30
12	33	33	33	33
13	24	24	24	24
14	30	30	30	30
15	33	33	33	33
16	24	24	24	24
17	30	30	30	30
18	33	33	33	33
19	24	24	24	24
20	30	30	30	30
21	33	33	33	33
22	24	24	24	24
23	30	30	30	30
24	33	33	33	33
25	24	24	24	24
26	30	30	30	30
27	33	33	33	33

Table 7.6 and Table 7.7 shows, respectively, the distances and the transportation times between the production site, distribution centres and markets. Moreover, Table 7.8 and Table 7.9 include the transportation capacities (i.e., minimum and maximum transport levels) between production site, distribution centres and markets. Also, Table 7.10 establishes the minimum and maximum storage levels in each distribution centre.

Table 7.6. Distances [km].

$d1_{p,d}$ or $d2_{d,k}$	Distribution centre 1	Distribution centre 2	Market 1	Market 2	Market 3
Production site	20	25			
Distribution centre 1			100	250	150
Distribution centre 2			70	200	180

Table 7.7. Transport time [h].

$Tr1_{p,d}$ or $Tr2_{d,k}$	Distribution centre 1	Distribution centre 2	Market 1	Market 2	Market 3
Production site	1	1			
Distribution centre 1			1	2	1
Distribution centre 2			1	2	2

Table 7.8. Transport capacity constraints between production sites and distribution centres.

Final product m	Production site p	$STD_{m,p,d,n,t}^{min}$	$STD_{m,p,d,n,t}^{max}$	
			Distribution centre 1	Distribution centre 2
Prod 1	Production site 1	0	100	100
Prod 2	Production site 1	0	100	100

Table 7.9. Transport capacity constraints between distribution centres and markets.

Final product m	Distribution centre d	$STM^{min}_{m,d,k,n,t}$	$STM^{max}_{m,d,k,n,t}$		
			Market 1	Market 2	Market 3
Prod 1	Distribution centre 1	0	30	20	20
Prod 1	Distribution centre 2	0	30	20	20
Prod 2	Distribution centre 1	0	40	40	40
Prod 2	Distribution centre 2	0	40	40	40

Table 7.10. Storage capacity constraints distribution centres.

Final product m	$SSD^{min}_{m,d,n}$	$SSD^{max}_{m,d,n}$	
		Distribution centre 1	Distribution centre 2
Prod 1	0	40	60
Prod 2	0	80	100

Table 7.11 contains data related to the price of final products, and costs associated to raw material purchases, storage cost in the distribution centres, transport cost between the production site, distribution centres and markets, and penalty cost in case of deviation from the established demand.

Table 7.11. Revenues and costs [m.u.].

Material state m	Price, $prm_{m,k}$	Raw material cost, $Crm_{m,t}$	Storage cost, $Csto_{m,d,t}$	Transport cost, $Ctra_{m}$	Penalty cost $Cpen_{m,k}$
Feed A		80			
Feed B		80			
Feed C		80			
Prod 1	137.5		1.2	0.01375	15
Prod 2	112.5		1.1	0.01250	15

Furthermore, Table 7.12 includes the probability of each scenario occurs.

Table 7.12. Probability of scenario n.

Scenario n	Probability
1	0.003
2	0.005
3	0.004
4	0.010
5	0.040
6	0.010
7	0.004
8	0.005
9	0.003
10	0.030
11	0.040
12	0.050
13	0.100
14	0.400
15	0.100
16	0.050
17	0.040
18	0.030
19	0.001
20	0.005
21	0.002
22	0.010
23	0.040
24	0.010
25	0.002
26	0.005
27	0.001

7.5. Results

The resolution of the model provides the daily optimal schedule of the supply chain, as well as the decision associated to the equipment unit installation. Given the problem definition and parameters the optimal solution is not expected, since only 3 equipment units have been installed, which are:

- Heater 2
- Reactor 2
- Distiller

Figure 7.4 shows the optimal scheduling of the production plant for a scenario, particularly for scenario number 14, where the demand of both products are in a medium level. Moreover, the production level in each operation and in each equipment unit can be found in Table 7.13:

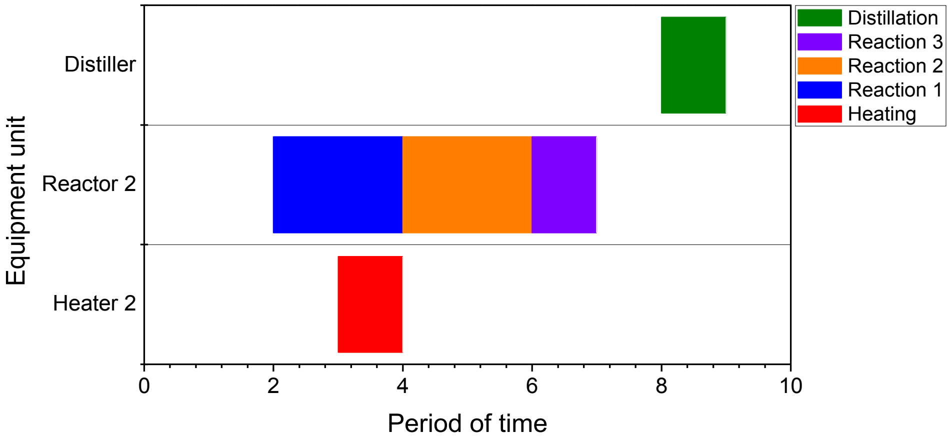

Figure 7.4. Production plant scheduling for scenario 14.

Table 7.13. Batch size.

Operation i	Unit j	Batch size, $B_{i,j,p=1,n=14,t}$
Heating	Heater 2	32
Reaction 1	Reactor 2	48
Reaction 2	Reactor 2	80
Reaction 3	Reactor 2	60
Separation	Distiller	60

As expected, one of the selected equipment units is the distiller, since it is essential to complete the overall process. In the same way, another of the selected equipment units is one of the heaters, particularly the heater number 2. Although its variable cost is higher in comparison with the other two heaters, its investment cost and its fixed cost is lower than the mentioned heaters, and with the production level, the installation and use of heater 2 is more economic that the installation and use of heater 1. Furthermore, reactor number 2 is selected to be installed. This reactor is selected due to its capacity, which allows to reach the product demand, as well as its investment cost. Although reactor 1 has more production capacity than reactor 2, its investment cost makes unaffordable its installation. The investment cost of reactors 3 and 4 is quite similar to the reactor 2, however they offer less production capacity. Only one reactor is installed, since the range of the production demand can be satisfied by installing reactor 2.

The main results of this case study can be found in Table 7.14. Moreover, in order to study the influence of the number of equipment units installed in the production plant, different situations have been considered:

- Situation 1: installation of 3 equipment units.
- Situation 2: installation of 4 equipment units.
- Situation 3: installation of 5 equipment units.
- Situation 4: installation of 6 equipment units.
- Situation 5: installation of 7 equipment units.

According to the results of Table 7.14, the profit of the supply chain decreases as the number of equipment installed increases. This is because the installation of one heater, one reactor and one distiller can reach the product demand. Although more equipment units may alleviate any eventual increase in demand, their investment cost involves a significant reduction in the expected profit.

The integration of different hierarchical levels in the same mathematical model allows to obtain a global optimum. On another hand, the procedure where the decisions are taken sequentially in each decision level may lead to a suboptimal solution, or may involve that the obtain solution in one hierarchical level becomes unfeasible when this solution is applied to another hierarchical level.

Table 7.14. Results.

Key Performance Indicator	Situation 1	Situation 2	Situation 3	Situation 4	Situation 5
Expected profit (m.u./year)	1,014,307.7	965,842.9	921,967.9	873,217.9	679,208.1
Number of required equipment installation	3	4	5	6	7
Equipment installed	Heater 2 Reactor 2 Still	Heater 2 Reactor 2,3 Still	Heater 2 Reactor 2,3,4 Still	Heater 1,2 Reactor 2,3,4 Still	Heater 1,2 Reactor 1,2,3,4 Still
Expected incomes (m.u./year)	8,442,731.3	8,442,731.3	8,442,731.3	8,442,731.3	8,468,184.4
Expected overall cost (m.u./year)	5,841,942.3	5,966,211.0	6,078,711.0	6,203,711.0	6,726,625.3
Installation cost (m.u.)	512,500.0	637,500.0	750.000.0	875,000.0	1,375,000.0
Expected raw material acquisition cost (m.u./year)	1,721,836.5	1,726,002.8	1,726,002.8	1,726,002.8	1,739,064.5
Expected fixed cost (m.u./year)	2,128,500.0	2,123,600.0	2,123,600.0	2,123,600.0	2,131,100.0
Expected variable cost (m.u./year)	55,483.4	55,486.7	55,486.7	55,486.7	56,278.7
Expected penalty cost (m.u./year)	90,525.0	90,525.0	90,525.0	90,525.0	87,356.3
Expected storage cost (m.u./year)	394,072.8	394,072.8	394,072.8	394,072.8	394,072.8
Expected transport cost (m.u./year)	939,024.6	939,023.7	939,023.7	939,023.7	943,753.0

The resulting MILP model has been implemented in GAMS 24.1 and solved using CPLEX 12 in a Pentium Intel® Core™ i7 CPU 2600 @ 3.40 GHz. The statistics associated to the resolution of this mathematical model can be found in Table 7.15. The implementation of the stochastic programming involves a high increase in the computational to reach the optimal solution.

Table 7.15. Model statistics.

Key Performance Indicator	Value
Equations	61,160
Continuous variables	38,351
Binary variables	9,396
Generation time (CPU, s)	0.422
Resource time (CPU, s)	1,544.969
Memory required (Mb)	19
Relative gap (%)	< 3
Requirements	GAMS 24.1 / CPLEX 12 Pentium Intel® Core™ i7 CPU 2600 @ 3.40 GHz

7.6. Concluding remarks

This chapter addresses the integration of different hierarchical decision levels, determining the optimal equipment allocation (task assignment and timing), tactical decisions (i.e., distribution tasks, storage levels) and strategic decisions (i.e., installation of equipment units). Plant and process flexibility has been improved by considering elements typically distributed in different hierarchical decision making levels. The resulting combined problem has been modelled using a MILP-based approach, obtaining improved solutions in strategic, planning and scheduling problems.

The integration of different hierarchical decision levels (i.e., strategic, tactical and operational decisions) has been addressed. The proposed two-stage stochastic MILP formulation has allowed to design new production facilities, taking into account different production scenarios and the overall supply chain planning. One challenge of this integration was to combine the consideration of multiple scenarios and the high degree of detail in the production process and in the planning of the supply chain.

The proposed approach may be also used as the basis for solving problems with higher complexity, such as industrial cases. The time representation can be improved by the introduction of a continuous time formulation. However, the current techniques to solve this formulation may be unaffordable in terms of computational effort. The proposed formulation can be extended to consider the use and management of internal and external resources. Moreover, this mathematical model can be reformulated to consider more entities in the supply chain, such as the management of several suppliers. Another challenge of this problem is to reduce the computational time to achieve the optimal solution, since the consideration of multiple scenarios increases the computational burden. This fact is linked with the final challenge, which is the consideration of multiple sources of uncertainty (i.e., prices, availability of sources, production times).

7.7. Nomenclature

Indices, sets and subsets

$d \in D$	*Set of distribution centres*
$i \in I$	*Set of operations*
$j \in J$	*Set of equipment units*
$k \in K$	*Set of markets*
$m \in M$	*Set of states*
$n \in N$	*Set of scenarios*
$p \in P$	*Set of production plants*
$t \in T$	*Set of time periods*
$i \in II_m$	*Subset of operations i requiring material from state m*
$i \in IO_m$	*Subset of operations i producing material from state m*
$i \in JI_j$	*Subset of operations i that can be assigned in equipment unit j*
$m \in F_m$	*Subset of states m corresponding to final products*
$m \in R_m$	*Subset of states m corresponding to raw materials*

Parameters

$B_{i,j}^{min}$	*Minimum equipment capacity for the operation i processed in equipment unit j*
$B_{i,j}^{max}$	*Maximum equipment capacity for the operation i processed in equipment unit j*
$Cins_j$	*Installation/investment cost of equipment unit j*
$Cpen_{m,k}$	*Penalty cost for unsatisfied demand of final product m in market k*
$Crm_{m,t}$	*Raw material cost of state m at time t*
$Csto_{m,d}$	*Storage cost of final product m in distribution centre d*
$Csup_j$	*Start-up cost of equipment unit j*
$Ctra_m$	*Transportation cost of final product m*
$Cvar_{i,j}$	*Variable cost of operation i produced in equipment unit j*
$d1_{p,d}$	*Distance between production plant p and distribution centre d*
$d2_{d,k}$	*Distance between distribution centre d and market k*
$Dem_{m,k,n,t}$	*Demand of the state m in scenario n at time t*
$fd_{i,j}$	*Fixed duration of operation i in equipment unit j*
ND	*Number of days*
pr_n	*Probability of scenario n*
prm_m	*Price of final product m*
$rmc_{m,t}$	*Raw material cost of material state m at time interval t*
$S_{m,p}^{min}$	*Minimum amount of stored material of all states m in production plant p*
$S_{m,p}^{max}$	*Maximum amount of stored material of all states m in production plant p*
$S0_{m,p,n}$	*Initial amount of stored material m in production plant p in scenario n*

$SSD_{m,d,n}^{min}$ *Minimum amount of stored final products m in distribution centre d in scenario n*

$SSD_{m,d,n}^{max}$ *Maximum amount of stored final products m in distribution centre d in scenario n*

$stc_{m,t}$ *Storage cost of material state m at time interval t*

$STD_{m,p,d,n,t}^{min}$ *Minimum amount of transported material m from production plant p to distribution centre d in scenario n at time t*

$STD_{m,p,d,n,t}^{min}$ *Maximum amount of transported material m from production plant p to distribution centre d in scenario n at time t*

$Tr1_{p,d}$ *Transportation time between production plant p and distribution centre d*

$Tr2_{d,k}$ *Transportation time between distribution centre d and market k*

$\overline{Y_p}$ *Maximum number of equipment units to be installed in production plant p*

α_j *Conversion degree of the chemical reaction performed in equipment unit j*

$\rho_{i,m}$ *Stoichiometry of material m to perform operation i*

Continuous and positive variables

$B_{i,j,p,n,t}$ *Amount of material processed according to operation i in equipment unit j in production plant p in scenario n at time t*

$Cost_n$ *Overall operational costs in scenario n*

IC *Installation cost*

$Incomes_n$ *Overall incomes in scenario n*

PC_n *Overall penalty cost in scenario n*

$Rm_{m,p,n,t}$ *Amount of raw material m in scenario n acquired in production plant p at time t*

RMC_n *Expected raw material cost in scenario n*

$S_{m,p,n,t}$ *Amount of material stored of state m in production plant p in scenario n at time t*

SC_n *Overall storage cost in scenario n*

$SS_{m,k,n,t}$ *Amount of sold material of all states m in market k in scenario n at time interval t*

$SSD_{m,d,n,t}$ *Amount of stored final products m in distribution centre d in scenario n at time interval t*

$STD_{m,p,d,n,t}$ *Amount of transported material m from production plant p to distribution centre d in scenario n at time t*

$STM_{m,d,k,n,t}$ *Amount of transported material m from distribution centre d to market k in scenario n at time t*

TC_n *Overall transportation cost in scenario n*

$UDem_{m,k,n,t}$ *Unsatisfied product demand of material state m in market k in scenario n at time interval t*

VC_n *Overall variable cost in scenario n*

Continuous variables

$Profit$ *Expected profit*

Binary variables

$X_{i,j,p,n,t}$ *= 1 if equipment unit j is being used and processing operation i in production plant p in scenario n at time t*

$y_{j,p}$ *= 1 if equipment unit j is installed in production plant p*

Chapter 8. Use of communication systems for the decision making

The integration of the different hierarchical decision making levels involved within a Chemical supply chain is essential for its adequate management in dynamic and competitive markets. Any approach encompassing design issues, planning, coordination and responses to customer demands, requires the consideration of huge amounts of data, which are a valuable source of information only if properly managed. But these data could also cause a lack of coordination if not stored and interpreted appropriately, so standardizing information structures and tools to improve the availability and communication of data information between different hierarchical decision levels is essential. Thus, this work addresses the problem of making the best use of the information systems associated to a supply chain, in order to improve the knowledge and the information comprehension capabilities in the area of Process Systems Engineering.

8.1. Introduction

In the current context of economic crisis, improving the efficiency of the industrial processes is essential to ensure the viability of the companies. Therefore, a holistic management of the different elements composing a SC and, in many cases, the relations among them, are necessary to improve resource use, minimize production costs and inventory, enhance economic benefits, increase customer satisfaction or improve process control, among other objectives usually associated to process profitability. The complexity of simultaneously considering the whole decision making process involved, lead to the traditional division of such process in different hierarchical levels (strategic, tactical and operational, as usually recognised even by the ISA standards). The process engineer is also frequently responsible for the continuous improvement of the production processes, the products and the associated techniques. Currently, tasks related to management, research and development involves the generation of huge amount of data that must be analysed, interpreted and stored throughout the decision making process, using computer simulation and computer control techniques. In chemical companies, these data are related to design issues, planning and production, coordination, cooperation and attention to customer demands, as well as constraints related to economy, environmental impacts, social policy, ethical topics, health, safety and sustainability (Noakes et al., 2011; Accreditation Board for Engineering and Technology, ABET, 2008).

Nowadays, factories often use industrial control systems in order to acquire data to supervise processes. The most common tools are classified in:

- Management information systems, including databases, Programmable Logic Controllers (PLC) or Supervisory Control And Data Acquisition (SCADA).
- Modelling systems able to explain and/or complement process information, based on the knowledge of the process, like plant/process simulators.
- Decision making systems (selection among alternatives), including procedural tools like Material Requirements Planning (MRP) systems, model based mathematical optimization, etc.

The implementation and use of this set of control systems involve a huge number of data to handle. For this reason, standardizing information structures and tools to improve the availability and communication of data is essential to integrate these data and use the previously mentioned tools efficiently for Chemical SCs management (Bessiris et al., 2011).

8.1.1. Open communication systems

In order to organize all the information available about the process, it has been proposed a system that consists of the following components: a data generator (real or virtual plants), an information repository, a customer interface and a diagnosis module, all of them following a basic model prescribed by ISA standards specification. Figure 8.1 shows a scheme of the proposed system.

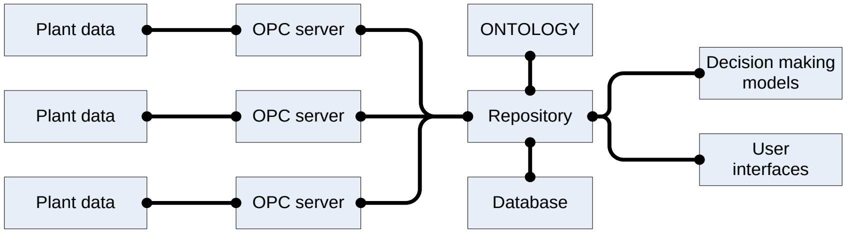

Figure 8.1. Proposed communication platform.

First of all, the system includes the acquisition of real-time data from industrial processes, in order to provide operational conditions to the system. All these data can be generated in real systems or through simulation techniques. The simulation system provides real-time information (simulated measurements) that is written and read through the different user interfaces, including all the variables required to describe the process. In case of simulation of real processes, through the use specific tools (i.e., ASPEN Hysys, Matlab, Simulink).

The Object Linking and Embedding for Process Control (OPC) standard is used to communicate and distribute the data generated by the simulators. This selection is based on current and commercial practice and tools, permitting the definition of a standard set of objects, interfaces and methods to be used in process control and automated manufacturing applications in order to facilitate interoperability (Soudani et al., 2002).

A platform for real-time management and decision making support at the different production levels has been also designed. This platform is based on an information repository, acts as a database of all information of the different processes and plays an important role by sending the appropriate information to the different information clients, where it will be filtered by the customer interface.

Furthermore, graphical user interfaces have been designed and run as Web applications to monitor, visualize and understand the evolution of the process and also to understand the decision making consequences, through the extensive use of the different Key Performance Indicators (KPIs) incorporated in the ontological model to assess not only the economic performance of the process (Figure 8.2) but also the performance of the information system (data availability and reliability) associated the different processes. This interface allows users to on-line supervise and diagnose of processes, taking corrective actions and evaluating the success of the given activity. Finally, decision making models have been developed to be applied in different scenarios.

This integrated information management system improves competences in the area of exploitation of on-line available data for decision making, as discussed in previously. This integration facilitates the storage and sharing of knowledge in a specific domain, and allows improve the effectiveness of decision support systems. Thus, it is important the training and the exploitation of an integrated framework to integrate all decision levels within a common structure, in order to reduce the gap between optimization approaches and task processing data. The implementation of this application is not only academic but also industrial, through the use of this open source software applied to real case studies.

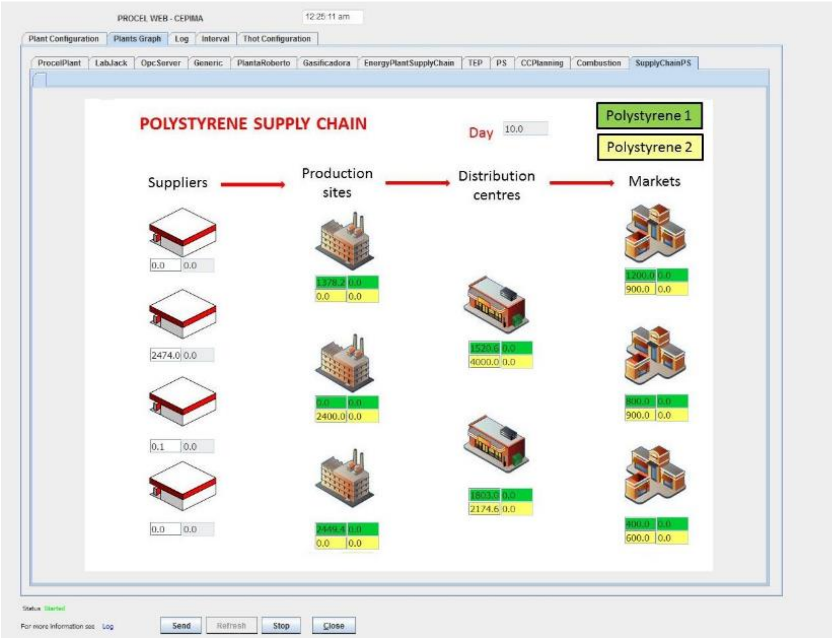

Figure 8.2. Example of user interface associated to the overall supply chain, where real time and target data related to raw material acquisition, production level, storage level and sales are visualized, in order to achieve the stipulated Key Performance Indicators.

One example of its application is the implementation of Operator Training Simulators (OTS), which are computer-based training techniques that use dynamic simulations of real processes, usually integrated with an emulator of the system under study. The OTS uses the dynamic simulation of the process to generate the appropriate data to feed the emulation of the process control and safety system (Feliu et al., 2015). The use of OTS systems allows the establishment of expertise and best practices among operators, enhancing process understanding. Some applications of the use of OTS are (Naranjo et al., 2013):

- Training of new operators and refresher training (including start-up, shutdown, and emergency procedures), which increase operator awareness and skills and reduce the risks of operational incidents and start-time times.
- Verify DCS.
- Verify SIS.
- Provide a test-bed system for scenario analysis.
- Validate and improve plant operating procedures such as detection of bottleneck units and processes.

- Reduce Environmental concerns.
- Development and test of new control strategies and production procedures.

In addition, this open information platform can be used for training in the overall SC decision making (Silvente et al., 2012b) as well as for the fault diagnosis (Silvente et al., 2012c).

8.1.2. Ontologies

Among the different types of knowledge-based systems which can be applied in complex scenarios to help decision making, ontologies provide structures for the coordination of information sources (Muñoz et al., 2010), and so, they can be used in the process engineering area to coordinate the development of new products, to identify new manufacturing recipes (Singh et al., 2010) and also to integrate different decision levels within a SC (Muñoz et al., 2011). This includes facilitating communication and knowledge, which allow the information exchange among the different modelling paradigms used for the enterprise-wide optimization, and also helps the acquisition, maintenance, access, reuse and sharing of information related to processes, with the aim of increasing the efficiency of cost, time and resources (Fensel, 2010). The use of such systems allows the establishment of common standards and enables the full exploitation of the stored relationships among all available data.

Ontologies (Figure 8.3) are considered a key semantic tool to reduce or eliminate conceptual and terminological confusion and come to a shared understanding of all available information, specifying the structure of a domain of knowledge in a generic way that can be read by a computer and presented in a human readable form. Moreover, ontologies incorporate knowledge of processes, incorporating the relationship between different processes into a logical structure. The main advantages of using ontologies are the communication in a shared framework among people and across application systems as well as the conceptualization that describes the semantics of all data in a standard way, using a common language.

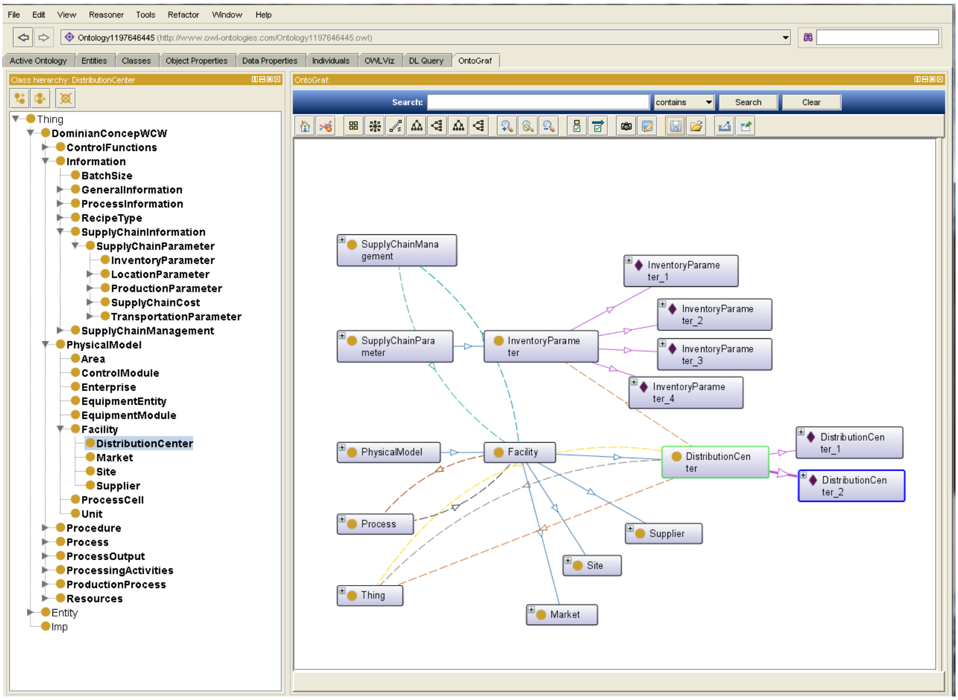

Figure 8.3. Ontology system, representing the relationship between different hierarchies within a SC.

8.2. Methodology

The main objective of this chapter is to coordinate all accessible and available data in an integrated information system to manage the decision making process in an overall and unique model, establishing common standards in the data structure, following ISA specifications, and linking the relationships between data in different hierarchical levels associated to a complete SC. Hence, a coordinated information system, which includes data generators, an information repository, a user interface and decision making models, has been integrated with an ontological framework in order to organize the decision making process. The use of this organized structure allows increasing the knowledge in Process Systems Engineering tools for modelling, simulation, planning, control and optimization of a variety of process under several constraints and objectives, with the purpose of applying this methodology in a realistic environment and integrating the individual knowledge of different modules in a coordinated way. This methodology provides new views of the Chemical Engineer management roles in real industrial environments.

Thus, this chapter proposes and describes the use of this integrated system to automatize the decision making process through a Chemical SC network (including several production plants, raw materials, final products, storage centres, markets) using the SCM techniques at tactical and operational decisions levels, by obtaining integrated information in real time, using dynamic simulation and optimization models and tools, including issues like objective function decisions, the different ways of introducing practical constraints and the way of using this support tools to face fluctuations in the demand.

Regarding the proposed methodology, all information related to different processes can be obtained through databases or on-line systems, from data sources available on-line. Hence, an information management system has been designed and implemented in order to integrate and organize all this available data to coordinate the decision making process through the three historical hierarchical levels in a SCM. This information flow system is integrated in an ontological framework, in order to organise all data in a common structure. This information system could be understood through Figure 8.4, which represents a SCM problem.

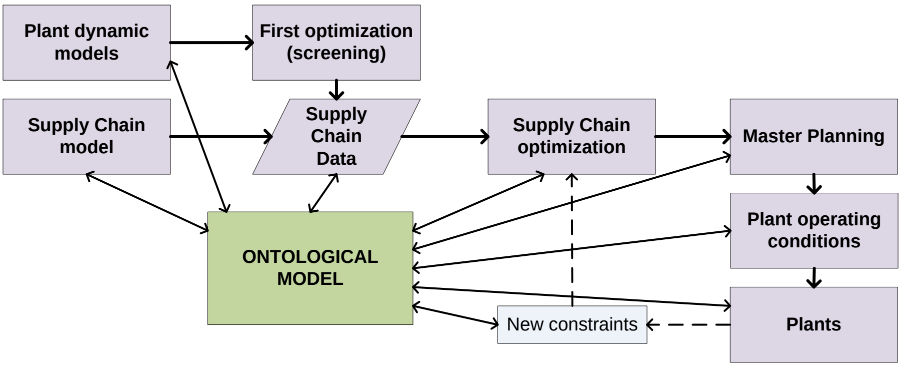

Figure 8.4. Information flow system related to a Supply Chain Management problem.

On the top of the decision making hierarchy, a SCM model should be incorporated in order to attain the optimization of the SC control decisions. Below it, plant dynamic models associated to the different processes in the different manufacturing centres will emulate, from their respective input and control information, all involved outputs, allowing the dynamic assessment of the different control decisions obtained from the SCM model optimization. This information may be also used to readjust the SCM model parameters and constraints, leading to a comprehensive view of both plant operating conditions at the detailed level, as well as the coordination of the production levels at the different elements of the SC in order to maintain the flow material through the SC while keeping adequate product inventories (master planning).

This proposed architecture and the use of standard modelling and information exchange protocols is compatible with the joint use of different simulation and optimization tools, like GAMS™ based models and optimization algorithms, MATLAB™ and Microsoft

Excel^{TM} based applications and many other. Depending on the characteristics of each problem, the models are implemented in order to develop decision making modules, develop simulations and model dynamic processes.

The incorporation of the ontology in this integrated information management system has the purpose of enforcing the use of common standards (i.e., terminology, communication, data management), maintaining the coherence among the different sources of information (and/or detect eventual inconsistencies), ensuring the consistency on the use of the available decision support systems and specially of helping users to obtain and understand data in a systematic way, using a common language.

8.3. Supply Chain Management application

In the area of process decision making and optimization, numerous applications can be used for decision making management and business productivity improvement. The application developed around the decisions associated to a SCM is described.

A SC related to the production and distribution of a polymer (i.e., polystyrene) has been proposed as a case study. This specific SC consists of suppliers, production sites, distribution centres and markets. The decision variables of this SC problem include raw material necessities, production level and distribution to warehouses, stock level and distribution to markets. This case study includes the dynamic simulation of the polymerization process at industrial level. The aim of these simulated plants is to generate data in order to obtain on-line information in real time, such as energy cost, conversion degree, reaction time and generation of pollutants. The purpose of this information management system is to conduct the optimization of a SC using SCM techniques by acquiring integrated information in real time, using dynamics optimization models and tools, including modelling issues like objective or multi-objective function decisions, the different ways of introducing practical constraints and also the manner of using this support tools to face uncertainty in the SC.

The proposed integrated communication platform allows its users to exploit the use of optimization and simulation tools to enhance the decision making problems, solving production planning problems (SC planning, which takes the decisions of the optimal production, stock and distribution levels, given production plants, warehouses, distribution centres and customers). In most cases, the resulting optimization problems can be considered as a hybrid optimizations because the solution approach should be solved as follows:

- First of all, the planning problem is to be solved, for a time horizon of months. This time horizon is too high compared with the simulation time, which is about hours, minutes or seconds, but this is the time indicated in the literature (Sung et al., 2007) to solve the problem of production planning (2-12 months).
- The optimal master recipe is introduced into the simulation. In other words, taking the decisions made in the previous problem, these data are introduced as set points for the simulation of the plant.
- In the simulation of a production plant, data from master recipe are introduced into the system, and the problem is optimized in the lowest level (scheduling level), controlling different variables of the plant to reach production levels proposed by the planning problem. This optimization is performed by adjusting the parameters of the dynamic model, optimizing different criteria (such as environmental impact and energetic costs). Figure 8.5 shows processing variables for the given production process.

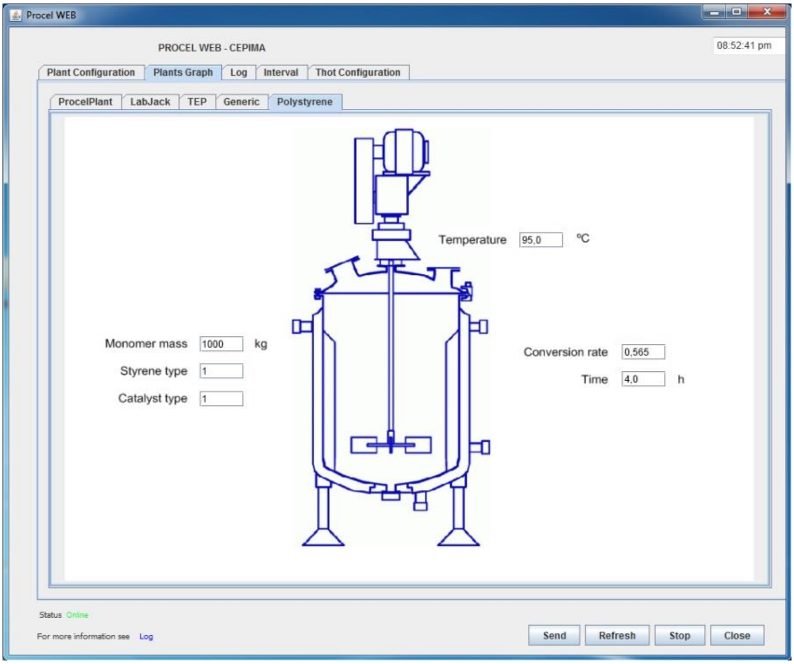

Figure 8.5. Example of graphical user interface associated to the production process.

- In addition, the system generates faults and external events that should be detected and solved. In some cases, these events should be propagated event to the master plan.

- With the availability to get data using the proposed methodology, the simulator will compile all available data to validate the optimization problem.

Figure 8.6 shows the connection between the master planning and the simulator block:

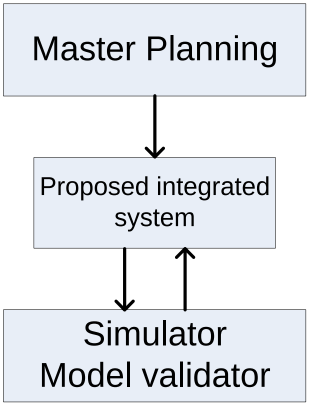

Figure 8.6. Connection between the master planning and the simulator.

The use of this and other case studies not only helps trainees to understand the operational conditions of the production plant, but also to understand the dynamics associated to external fluctuations. One of these fluctuations is associated to the changes in the expected, which determine, for example, the production and the acquisition of raw material and resources. Moreover, trainees will become familiar the presence of several supply chains in a competitive environment, understanding the market situation.

8.4. Results

The development and implementation of an ontological model allows the integration of all available data into a specific and unique information system/model, which allows improving the decision making process. Specific advantages of using ontologies are:

- To improve the information management, since all information related to a process is integrated in a generic platform, eliminating inconsistencies and ensuring completeness. Particularly:
  - ✓ To understand the global behaviour of the model, and to evaluate how a change impacts at different levels, due to the connection between all data.
  - ✓ To evaluate KPIs at different levels, related through ontology, which contains the global model.
  - ✓ To restrict a phenomenon known as the "bullwhip effect", which is the increase in fluctuation of demand upstream in the SC, due to a better data control.
- To reduce or eliminate conceptual and terminological confusion and come to a shared understanding, following the ISA standard specifications.
- To extract information in an uncomplicated way, allowing the development of global models using the mentioned above specifications, due to the fact that all information is integrated and the relationships between categories and hierarchies are stipulated.
- To increase the possibilities of determining the global optimum of the overall system, not just a local optimum, reducing the inefficiencies and improving the solution, because of data integration.

8.5. Concluding remarks

The use of an integrated information management system based on an ontological framework is introduced in order to facilitate the exploitation of on-line available data for decision making. The use of open communication systems, a platform for real-time management and a Web-based user interface with different view layers, allow monitoring the evolution of the process and facilitate the introduction of corrective actions using similar patterns in very different scenarios, and also standardizing the communication between different hierarchical levels.

This system may be also helpful for operator training, improving transversal competences in Process System Engineering techniques, including modelling, planning, simulation, optimization and process control in real-time. This system may be also helpful for operator training, throughout the implementation of Operator Training Systems. The use of this methodology will help trainees to understand and to integrate the concepts of production processes. Moreover, these tools are useful to understand current technology in process and planning operations, in order to contextualize trainees on his current/future work as Chemical Engineers, offering additional chances to improve their knowledge.

Part IV – Final remarks

Chapter 9. Final remarks

9.1. Conclusions

The objective of this thesis has been to establish mathematical programming techniques and approaches for the efficient solution of complex decision making problems. Specifically, different new mathematical formulations have been developed to tackle supply chain management problems in deterministic and uncertain conditions. Hence, several case studies has been addressed and solved by the new mathematical programming frameworks devised in this thesis.

According to the thesis outline, Part I introduces an overview related to the overall Supply Chain Management and describes the main Process Systems Engineering challenges in the area of optimization. Thus, Chapter 2 analyses the major open issues to be addressed through an extensive state of the art review. Although the decision making process within a supply chain has become the subject of intensive research, an attentive review reveals the areas where new contributions are needed for a major impact in real-world applications. From these areas, this thesis has been focused on the integration of hierarchical levels, the coordination of supply and demand and the consideration of different sources of uncertainty. The theory and concepts behind the most used methods, techniques and tools to solve the Supply Chain Management problems has been described in Chapter 3.

Part II addresses the **simultaneous management of production and demand**. This coordinated view, in comparison with the production side management, introduces an additional degree of freedom to the supply chain problem. Thus, delays in the nominal demands are allowed under associated penalty costs. This new potential flexibility enhances the management and the efficiency and autonomy of the supply chain and on the use of resources. The case study presented in Chapter 4 demonstrates that the profit of the supply chain increases when production and demand are considered in a simultaneous way.

Related to this simultaneous management, in this thesis it has been also studied the role of the **time representation** in a mathematical model, which affects the optimal solution of a problem. In particular, Chapter 4 compares two time representations, which are the discrete and hybrid time formulations, applied to the short-term daily scheduling problem of a supply chain. According to the obtained results, the hybrid time representation improves the results in comparison to the discrete time formulation, due to a better adjust of times using the hybrid time formulation. However, this formulation involves an increase in the required computational effort. Moreover, the length of the time interval in the discrete time formulation influences the optimal solution. As the length of the time interval decreases, the value of the objective function is improved and closes the gap from the hybrid time representation.

On another note, the consideration of **uncertainty** is essential to ensure the generation of good quality and practical interest management decisions. Thus, a rolling horizon approach has been presented to deal with continuous variations in input parameters, by solving iteratively the managerial problem once the mentioned parameters are updated or modified (see Chapter 5). This formulation has allowed to react to variations from the nominal schedule, adapting production and demand to update parameters. In this kind of formulations, the length of the prediction horizon affects the optimal solutions, since longer prediction horizons favour the generation of better solutions.

Other approaches to deal with the uncertainty are focused on the consideration of different scenarios, such as stochastic programming. In this line, Chapter 7 has presented a stochastic programming for the integration of strategic, tactical and operational levels. The consideration of multiple scenarios has allowed to improve the design specifications to better satisfy the potential necessities of the supply chain. The best methodology to deal with uncertainty will depend on the characteristics of the problem. For example, the high complexity related to estimate all scenarios with a high degree of precision may make unaffordable the consideration of all possible external scenarios.

Moreover, Chapter 6 has analysed **the integration of production and resources** within the decision making process in a production plant. A new mathematical model has been developed to embrace different resource usage models and scheduling production models within a coordinated model that integrates production and the use of all resources. The need to introduce terms related to both quality and quantity of the production resources may lead to the introduction of additional non-linearities, which requires more computational effort to obtain the optimal solution or may become unaffordable. The obtained results demonstrate how the simultaneous management of production and resources will lead to improvements in the efficiency of the production plant.

Part III deals with the integrated supply chain optimization. More specifically, the **integration of different hierarchical decision levels** (i.e., strategic, tactical and operational decisions) has been addressed (see Chapter 7), exploiting the process and the plant flexibility by integrating synthesis, planning and scheduling models. This mathematical formulation has allowed to design new production facilities, taking into account different production scenarios and the overall supply chain planning. One challenge of this integration was to combine the consideration of multiple scenarios (stochastic programming) and the high degree of detail in the production process and in the planning of the supply chain.

Finally, the use of an **integrated information management system** based on an ontological framework has been presented. This platform facilitates the exploitation of historical and on-line available data for decision making. This platform has allowed to monitor the evolution of processes and has facilitated the introduction of corrective actions using similar patterns in very different scenarios, and also standardizing the communication between different hierarchical levels. This system may be also helpful for operator training, through the implementation of Operator Training Systems.

9.2. Future work

A range of issues requiring further investigation has been revealed in the course of this work. Therefore, this section suggests some of the potential research lines.

Particularly, further study and improvement of the mathematical-based solution techniques. For instance, the results obtained through the case studies demonstrate that the proposed approach may be also used as the basis for solving problems with higher complexity, such as industrial cases. Furthermore, the formulations presented in Chapter 4, Chapter 5 and Chapter 6 can be prolonged by the simultaneous consideration of coordinated production and demand as well as different factors (i.e., environmental impact, social aspects) through the implementation of multi-objective optimization approaches. Moreover, the presented mathematical models can be reformulated to consider more entities in the supply chain, such as the management of several suppliers.

With regard to the time representation, the presented mathematical models in Chapter 4 were based on discrete and hybrid time representations. The formulation of a continuous time model represents a challenge, due to the high computational time to solve this kind of problems. Moreover, the integrated synthesis, planning and scheduling framework presented in Chapter 7 has been modelled using a discrete time representation. However, this proposed approach may be also used as the basis for solving problems with higher complexity and using more accurate time representations.

Regarding the uncertainty, Chapter 5 presents a rolling horizon approach to deal with variability. However, this formulation can be extended by combining reactive and proactive approaches (i.e., rolling horizon approach and stochastic programming) to take advantage of both techniques. The implementation of the rolling horizon approach may involve changes in the obtained schedule, since all parameters are updated in each iteration. Hence, rescheduling actions penalties could be included to the proposed optimization framework to avoid major changes in the initial schedule after the occurrence of an unexpected event. Regarding the integration of resources in the decision making system developed in Chapter 6, the further work can be focused on the introduction of uncertainty in the model. Furthermore, another challenge of this problem is to reduce the computational effort to achieve the optimal solution, since the consideration of multiple scenarios increases significantly this effort. Additionally, the presented mathematical formulations can be extended to consider multiple sources of uncertainty (i.e., prices, availability of sources, production times).

On another note, the mathematical formulation presented in Chapter 6 considers the reuse of resources. This formulation can be extended in order to incorporate the treatment and recycle of these resources. Also, the proposed formulation in Chapter 7 can be extended by considering the use and management of internal and external resources.

The integrated information management system can be improved by reducing the time to update available data as well as creating user interfaces in a friendly framework.

Appendixes

Publications

This is a list of the works carried out so far within the scope of interest of his thesis, in reversed chronological order. The list has been divided in manuscripts to international refereed journals and articles presented and published to different international specialized conferences. Moreover, the participation in research projects is included.

Scientific journals

Silvente, J., Zamarripa, M. & Espuña, A. (2016). An optimization model for the integration of hierarchical decision levels in a demand side framework. *Ready*.

Silvente, J. & Espuña, A. (2016). An optimization model for the integrated management of production resources in a demand side framework. *Ready*.

Zamarripa, M., Silvente, J. & Espuña, A. (2016). Integrated synthesis and scheduling decision making. *Ready*.

Silvente, J., Kopanos, G.M., Pistikopoulos, E.N. & Espuña, A. (2015). A rolling horizon optimization framework for the simultaneous energy supply and demand planning in microgrids. *Applied Energy*, 155, 485-501.

Silvente, J., Aguirre, A., Zamarripa, M., Méndez, C.A., Graells, M. & Espuña, A. (2015). Improved time representation model for the simultaneous energy supply and demand management in microgrids. *Energy*, 87, 615-627.

Zamarripa, M., Hjaila, K., Silvente, J. & Espuña, A. (2014). Tactical management for coordinated supply chains. *Computers & Chemical Engineering*, 66, 110-123.

Conference proceedings articles

Silvente, J., Kopanos, G.M. & Espuña, A. (2015). A rolling horizon stochastic programming framework for the energy supply and demand management in microgrids. *Computer-Aided Chemical Engineering*, 37, 2321-2326.
25th European Symposium on Computer Aided Process Engineering, Copenhagen, Denmark, 2015.

Medina, S., Shokry, A., Silvente, J., & Espuña, A. (2015). A meta-multiparametric framework: Application to the operation of bio-based energy supply chains. *Computer-Aided Chemical Engineering*, 37, 1955-1960.
25th European Symposium on Computer Aided Process Engineering, Copenhagen, Denmark, 2015.

Silvente, J., Kopanos, G.M., Pistikopoulos, E.N. & Espuña, A. (2014). A reactive scheduling for the coordination of energy supply and demand management in microgrids. *Computer-Aided Chemical Engineering*, 33, 493-498.
24th European Symposium on Computer Aided Process Engineering, Budapest, Hungary, 2014.

Silvente, J., Aguirre, A., Crexells, G., Zamarripa, M., Méndez, C.A., Graells, M. & Espuña, A. (2013). Hybrid time representation for the scheduling of energy supply and demand in smart grids. *Computer-Aided Chemical Engineering*, 32, 553-558.
23rd European Symposium on Computer Aided Process Engineering, Lappeenranta, Finland, 2013.

Zamarripa, M., Silvente, J., Hjaila, K. & Espuña, A. (2013). Simplified model for integrated Supply Chains Planning. *Computer-Aided Chemical Engineering*, 32, 547-552.
23rd European Symposium on Computer Aided Process Engineering, Lappeenranta, Finland, 2013.

Silvente, J., Zamarripa, M., Crexells, G., Muñoz, E. & Espuña, A. (2013). Use of ontological structures for integrated supply chain management. *Chemical Engineering Transactions*, 32, 1165-1170.
11th International Conference on Chemical & Process Engineering, Milan, Italy, 2013.

Zamarripa, M., Cóccola, M., Hjaila, K., Silvente, J., Méndez, C.A. & Espuña, A. (2013). Knowledge-based approach for the integration of the planning and scheduling decision making levels. *Chemical Engineering Transactions*, 32, 1139-1144.
11th International Conference on Chemical & Process Engineering, Milan, Italy, 2013.

Silvente, J., Zamarripa, M. & Espuña, A. (2012). Use of a distributed simulation environment for training in Supply Chain decision making. *Computer-Aided Chemical Engineering*, 30, 1402-1406.
22nd European Symposium on Computer Aided Process Engineering, London, United Kingdom, 2012.

Silvente, J., Monroy, I., Escudero, G., Espuña, A. & Graells, M. (2012). A promising OPC-based computer system applied to fault diagnosis. *Computer-Aided Chemical Engineering*, 30, 892-896.
22nd European Symposium on Computer Aided Process Engineering, London, United Kingdom, 2012.

Zamarripa, M., Silvente, J. & Espuña, A. (2012). Supply chain planning under uncertainty using genetic algorithms. *Computer-Aided Chemical Engineering*, 30, 457-461.

22nd European Symposium on Computer Aided Process Engineering, London, United Kingdom, 2012.

Silvente, J., Graells, M., Espuña, A. & Salas, P. (2012). An optimization model for the management of energy supply and demand in smart grids. *IEEE International Energy Conference and Exhibition*, 424-429.
IEEE Energycon, Firenze, Italy, 2012.

Other conferences

Silvente, J. & Espuña, A. Development of a multi-objective optimization model for the integrated management of internal and external production resources.
20th Conference of the International Federation of Operational Research, Barcelona, Spain, 2014.

Zamarripa, M., Silvente, J. & Espuña, A. Exploiting plant and process flexibility at the operational level.
22nd European Symposium on Computer Aided Process Engineering, London, United Kingdom, 2012.

Silvente, J., Monroy, I., Escudero, G., Espuña, A. & Graells, M. An open architecture for the fault diagnosis of chemical processes.
12th Mediterranean Congress of Chemical Engineering, Barcelona, Spain, 2011.

Participation in research projects

SIGERA Project, supported by the Spanish Economy and Competitiveness Ministry (Ministerio de Economía y Competitividad) and the European Regional Development Fund (DPI2012-37154-C02-01), 2014-present.

EHMAN Project (Expanding the Horizons of Manufacturing, Solving the Integration Paradox), supported by the Spanish Economy and Competitiveness Ministry (Ministerio de Economía y Competitividad) and the European Regional Development Fund (DPI2009-09386), 2010-2013.

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