Proactive management of uncertainty to improve scheduling robustness in process industries

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Sow a thought, and you reap an act;
Sow an act, and you reap a habit;
Sow a habit, and you reap a character;
Sow a character, and you reap a destiny.

Charles Reade (1814 - 1884)

Summary

Dynamism, responsiveness, and flexibility are essential features in the development of the current society. Globalization trends and fast advances in communication and information technologies make all evolve in a highly dynamic and uncertain environment. Popular and modern things one day, become easily obsolete the day after. In addition, unexpected and sudden situations due to for example rush orders, delays, traffic jams, or weather conditions, are commonly encountered in our daily activities and prevent or modify the expected realization of a plan. Within such an environment, is planning reliable? What happens if expectations cannot be met, if changes cannot be faced immediately?

A parallelism can be established between these day to day situations and the planning of operations in a process system. Will raw materials be delivered on time and according to specifications? Will the required resources be available during production? Will customer orders be satisfied? Because of the dynamic and uncertain operation conditions, plans rarely developed as predicted.

The uncertainty involved in a real process system becomes a critical problem in decision making, as well as a recognized challenge in the area of Process Systems Engineering (PSE). In practice, effort is expended either searching for safety mechanisms, such as inventory and lead times, or reacting to the consequences of the uncertainty. Boards, colored cards, and marker pens initially used for scheduling have been progressively replaced by computer-aided decision-support systems. Models developed up to this point, as well as commercial advanced planning and scheduling (APS) systems, provide reactive scheduling capabilities and *what if* scenario analysis, but rely generally on estimated input information, implicitly assuming that a schedule will be executed without deviations. Rescheduling, though simple, is required at execution time to deal with disturbances arising as a consequence of the uncertainty, but it is not always effective or even possible. A promising alternative is to address the uncertainty *proactively* at the time of reasoning, though so far relatively few research work has been reported that exploits the knowledge available in the modeling procedure itself.

In view of this situation, the following questions arise: *what do we understand for uncertainty? How can uncertainty be considered within scheduling modeling systems? What is understood for schedule robustness and flexibility? How can schedule robustness be improved? What are the benefits?* This thesis gives an answer to all these questions in the context of operational analysis in PSE. Uncertainty is managed not from the traditional reactive viewpoint, but proactively, and decision-support systems are developed to identify robust schedules that serve as a useful guidance for the lower control level in the plant, as well as for dependent entities in a supply chain

environment.

The first contribution aims at formalizing the concept of *schedule robustness*, which is commonly understood as the ability of a schedule to deal with uncertain events at execution time while maintaining an acceptable performance, but a general formalism is missing. Proactive approaches are then developed based on stochastic and robust optimization methodologies, and using an statistical representation of the uncertainty. Both mathematical and procedure-oriented algorithms, coupling simulation and optimization capabilities, are assessed and compared. Particularly, research studies are conducted in three main directions:

I. Robust scheduling focused on operational uncertainties.

The main uncertainties in short-term production scheduling are first considered (variable operation times and equipment breakdowns). The problem is initially modeled using stochastic programming, and a simulation-based optimization framework is finally developed, which captures the multiple sources of uncertainty, as well as rescheduling strategies proactively, that is, in the reasoning stage.

II. Transport scheduling.

The coordination of production and transport activities, considered so far mainly in strategic and tactical levels of analysis, is assessed, thus providing a broader operational perspective. The procedure-oriented system developed in the context of production scheduling is extended to involve transport scheduling in multi-site systems with uncertain travel times.

III. Robust scheduling focused on tactical uncertainties.

The final research point focuses on the effect of product demands uncertainty in short-term scheduling decisions. The problem is analyzed from a risk management viewpoint, and *financial risk*, *downside risk* and *worst-case* are assessed as alternative measures to control the performance of the system in the uncertain environment.

Overall, this research work reveals the advantages of recognizing and modeling uncertainty, with the identification of more robust schedules able to adapt to a wide range of possible situations, rather than optimal schedules for an hypothetical scenario. Besides, the management of uncertainty proposed from an operational perspective can be considered as a first step towards its extension to tactical and strategic levels of analysis, as well as towards the integration of hierarchical decision-support systems. In general, the proactive perspective of the problem results in a more realistic view of the operation of a process system, and it is a promising way to reduce the gap between theory and industrial practices. It provides valuable insight on the process, visibility for future activities, as well as it improves the efficiency of reactive techniques and of the overall system, all highly desirable features to remain alive in the current global, competitive, and dynamic process environment.

Resum

Dinamisme, capacitat de resposta i flexibilitat són característiques essencials en el desenvolupament de la societat actual. Davant les noves tendències de globalització i els avenços en tecnologies de la informació i comunicació s'evoluciona en un entorn altament dinàmic i incert. Fets que un dia són populars i moderns, esdevenen fàcilment obsolets el dia següent. Alhora, en tota activitat diària poden presentar-se situacions inesperades degut a presses, retards, condicions meteorològiques, etc., que impedeixen o modifiquen el seguiment esperat d'un pla. En un entorn així, és possible confiar en la planificació? Què passa si no s'aconsegueixen les expectatives, si no es pot fer front als canvis de forma immediata?

Existeix un paral·lelisme entre aquestes situacions quotidianes i la planificació de les operacions en un sistema de procés. Les matèries primeres arribaran a temps i segons les especificacions? Els recursos necessaris estaran disponibles durant tot el procés de producció? Es satisfaran les demandes? Degut a les condicions de treball dinàmiques i incertes, els plans difícilment es desenvoluparan segons les previsions.

La incertesa present en tot procés real esdevé un factor crític a l'hora de prendre decisions, així com un repte altament reconegut en l'àrea d'Enginyeria de Sistemes de Procés. A la pràctica s'utilitzen tant mecanismes de seguretat (producció d'inventari, temps morts, etc.), com mètodes de programació d'operacions reactiva per fer front als efectes de la incertesa. L'ús inicial de pissarres, targetes de color i marcadors per programar les operacions ha estat substituït progressivament per sistemes de suport a la decisió assistits per ordinador. Els models proposats fins ara, així com també software comercial de planificació i programació d'operacions avançada, presenten capacitats de reacció i anàlisi d'escenaris *i si*, però es basen generalment en dades estimades, assumint implícitament que el programa d'operacions s'executarà sense desviacions. La programació reactiva de les operacions, tot i simple, sol ésser necessària en temps d'execució d'un pla per tal de fer front a pertorbacions que tenen lloc com a conseqüència de la incertesa, però no sempre resulta efectiva o factible. Una alternativa prometedora és considerar la incertesa de forma *proactiva*, és a dir, en el moment de prendre decisions; no obstant, relativament poques contribucions s'han presentat fins ara que explotin el coneixement disponible en la pròpia modelització del sistema.

Davant aquesta situació es plantegen les següents preguntes: *què s'entén per incertesa? Com es pot considerar la incertesa en un problema de programació d'operacions? Què s'entén per robustesa i flexibilitat d'un programa d'operacions? Com es pot millorar aquesta robustesa, i quins beneficis comporta?* Aquesta tesi dóna resposta a totes aquestes preguntes en el marc d'anàlisis a nivell d'operació en l'àrea de PSE. La incertesa es considera de forma proactiva enlloc de l'enfocament reactiu tradicional, i es desenvolupen sistemes de suport a la decisió per tal d'identificar

programes d'operació robustos que serveixin com a referència pel nivell inferior de control de planta, així com també per altres centres en un entorn de cadenes de subministrament.

La primera contribució d'aquest treball de recerca pretén formalitzar el concepte de *robustesa d'un programa d'operacions*, el qual es defineix generalment com la capacitat que presenta un programa d'operacions per fer front a les desviacions que puguin ocórrer en temps d'execució mantenint un rendiment acceptable, però no existeix encara una forma sistemàtica de formalitzar el concepte. A continuació es desenvolupen mètodes proactius en base a tècniques de modelització estocàstica i robusta, i utilitzant una representació estadística de la incertesa. S'avaluen i es comparen algoritmes tant matemàtics com heurístics, combinant sistemes de simulació i optimització. Concretament, la recerca es realitza en tres eixos principals:

I. Programació d'operacions robusta centrada en incerteses operacionals.

En primer lloc es consideren les principals fonts d'incertesa presents a nivell de programació de la producció (temps d'operació i ruptures d'equips). El problema es modelitza inicialment mitjançant programació estocàstica, desenvolupant-se finalment un entorn d'optimització basat en simulació que captura de forma proactiva les múltiples fonts d'incertesa, així com també estratègies de programació d'operacions reactiva.

II. Programació d'operacions de transport.

Amb una perspectiva més àmplia del nivell d'operació, s'estudia la coordinació d'activitats de producció i transport, analitzada fins ara des d'un punt de vista estratègic o tàctic. La metodologia desenvolupada en el context de programació de la producció s'estén per incloure la programació de les operacions de transport en sistemes de múltiples entitats i incertesa en els temps de transport.

III. Programació d'operacions robusta centrada en incerteses tàctiques.

L'estudi final considera l'efecte de la incertesa en la demanda dels productes en les decisions de programació de la producció a curt termini. El problema és analitzat des del punt de vista de gestió del risc, i s'avaluen diferents mesures alternatives per controlar l'eficiència del sistema en un entorn incert.

En general, la tesi posa de manifest els avantatges en reconèixer i modelitzar la incertesa, identificant programes d'operació robustos capaços d'adaptar-se a un ampli rang de situacions possibles, més que no pas programes d'operació òptims per un escenari hipotètic. Alhora, la metodologia proposada des d'un punt de vista operacional es pot considerar com un pas inicial per estendre's a nivells estratègics i tàctics, així com a la integració de sistemes jeràrquics de suport a la decisió. La visió proactiva del problema de la incertesa permet visualitzar l'operació d'un sistema de procés de forma més realista, i resulta prometedora per tal de reduir el buit existent entre la teoria i la pràctica industrial. S'obté un major coneixement del procés, visibilitat per planificar activitats futures, així com també una millora en l'efectivitat de les tècniques reactives i de tot el sistema en general, característiques altament desitjables per mantenir-se actiu davant la globalitat, competitivitat i dinàmica que envolten un procés.

Acknowledgments

It seems quite long ago when I finished my degree in chemical engineering and I had the opportunity to start a new period as a doctoral candidate in the CEPIMA group of the chemical engineering department in the Universitat Politècnica de Catalunya. It has been a very fruitful stage not only from an educational perspective, but also personally. Being at the end, I cannot feel anything else but fortunate. It has been worth extending the educational period for all I have learned, developed, and experienced, as well as the enriching and exceptional relationships I have established.

This thesis is just the reference document of the essential technical research work I have been doing during this period. It is the result of not only the effort and hope I have posed on it, but also of discussions, collaborations, ideas, and guidance deliberately received from my colleagues. These and other invaluable knowledge and contributions remain hide behind the dissertation, difficult to be translated into words.

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Contents

1. Introduction

It is not in the stars to hold our destiny but in ourselves; we are underlings.

W. Shakespeare (1564 - 1616)

The chemical process industry (CPI) is facing an ever-changing environment in an attempt to meet the current market needs. Operations are developed within dynamic and competitive markets with shorter product life-cycles, and pressures exist to improve safety, sustainability, as well as environmental and social impacts, thus claiming for efficiency and responsiveness. Besides, higher customer expectations, collaboration between organizations, and progress in information and communication technology, lead to new e-commerce markets and enhanced business-to-business communication over the Internet. The information revolution and globalization trends emerged during the last few years have significantly increased competitiveness and posed new challenges within the Process Systems Engineering (PSE) community (Grossmann, 2005).

The area of PSE emerged in the 1961 focused on the understanding and development of improved and systematic decision-making procedures for the design and operation of the process system itself. Lately, its interests have been extended covering from chemistry at the molecular level, to wider aspects of engineering concerned with the management of multi-site operations eventually considering the whole supply chain (SC) (Grossmann and Westerberg, 2000).

Because of the wider scope of research, the interests of process systems engineers have also been extended to a wider range of techniques and initiatives closely related with disciplines of computer science, operations research, applied mathematics, materials, and life sciences.

Within this highly complex environment, uncertainty and variability become inherent characteristics of process systems. As stated by Bogle (2000), "unsteady-state operations are becoming the norm, rather than the exception" and the traditional strategy of operating a plant independently from its environment is not appropriate any more. Rather, flexibility and responsiveness of production processes are important features to be considered and exploited to deal with the eventual effects of the uncertainty quickly and effectively.

The systematic treatment of the uncertainty is widely recognized as a real problem, and one of the main challenges in the area of process systems (Shah, 1998; Reklaitis, 2000; Grossmann, 2004; Sahinidis, 2004; Shapiro, 2004; Floudas, 2005; Sargent, 2005; Shah, 2005). The need to consider the uncertainty is also reflected in the following statement of George Dantzig, *"I am working on planning under uncertainty; that's the big field as far as I'm concerned. That's the future."* (Horner, 1999).

This chapter starts with a general perspective of the main problems addressed in the area of PSE to introduce the concepts and focus the context of the thesis. Being the basis of the research work conducted, the general scheduling problem is described, and a comprehensive example is next presented to illustrate some points that motivate the development of this research. An outline of the thesis is given in the final section.

1.1 Hierarchical decision making

The interests of PSE span from a molecular level to enterprise management, being the design and planning problems a central issue in this domain. Focusing on the planning area, a process system involves multiple and interrelated activities performed over single or multiple sites, with different time extents and degrees of uncertainty. Generally, the information flows from the marketing to the manufacturing department, where the production schedule meeting the required sales strategies is to be determined. The joint marketing and manufacturing plan is then passed to logistics for the development of appropriate transport, warehousing, and inventory strategies. The decisions made are finally executed, which involves the study of the operation conditions.

One common and practical view of the different temporal activities distinguishes between strategic, tactical and operational planning horizons (refer for example to Shapiro (2000)). Strategic planning involves decisions to be made over long-term planning horizons (generally 1 - 2 years); tactical planning implies decisions made over medium-term horizons (3 - 6 months); whereas operational planning covers decisions involved in the short-term execution of activities (the time horizon generally spans from days to one or several weeks). Each time horizon implies a different level of detail in the data describing the process system.

PSE provides the means to systematically transform all the information into decisions in a goal-oriented fashion. As outlined by Pekny (2002), this formalization and generation of knowledge involves the definition and assessment of the main features of the problem, the generation of a representative model capturing the constraints and the desired goals, the development of efficient algorithms to solve the model, and the validation and implementation of the results obtained. Pekny (2002) also discussed the features and relationships of several PSE applications, as well as algorithm architectures for their resolution.

First attempts to the development of computer-aided systems aimed at the use of monolithic models comprising all levels of decision. These models presented limited visibility of decisions made in different areas, frequent data inconsistencies, and they were only applicable to simple settings because of the large computational requirements (Shobrys and White, 2002). The need to support the decision making and improve operations over all levels of planning has lead to the development of several and hierarchical modeling systems, which have been beneficiated with the advances in information technology (IT).

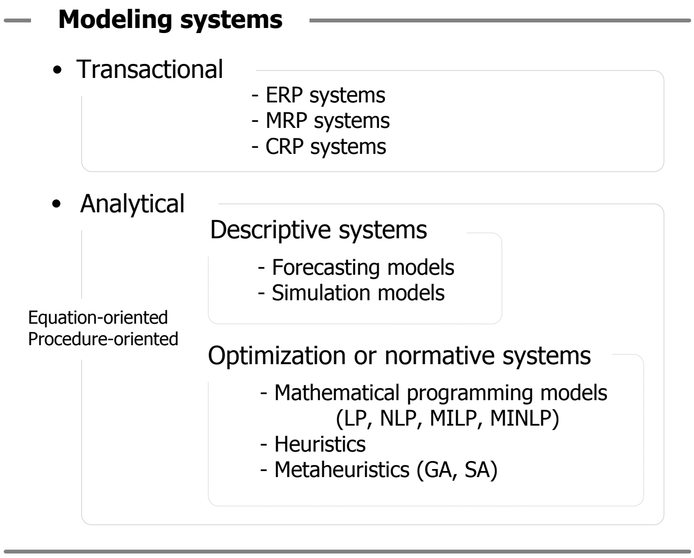


Figure 1.1: Taxonomy of modeling systems.

1.1.1 Modeling systems

A model formalizes the relationship between various flows of information and can adopt different forms, from spreadsheets to mathematical programs, neural networks and expert systems. Modeling systems can be categorized from different perspectives. A general taxonomy distinguishes between transactional and analytical modeling approaches (Figure 1.1).

Transactional systems are concerned with the acquisition, processing, and communication of data over the enterprise. *Analytical* techniques introduce some reasoning to evaluate the problems, and are further classified into descriptive and optimization models. Descriptive models can be used to analyze a system, but not to improve it, and provide a better understanding of internal and external functional relationships in the enterprise (included are forecasting models, cost relationships, resource utilization relationships, and simulation models). On the other hand, optimization or normative models are developed as decision-support systems to assist managers in the identification of efficient and improved decisions.

In general, descriptive and optimization algorithms can be broadly classified into equation-oriented or procedure-oriented approaches. Equation-oriented approaches involve rigorous mathematical programs, either deterministic or stochastic, constraint programming, and graph theory. Procedure-oriented approaches comprise rule-based techniques, heuristics, and meta-heuristics such as simulated annealing (SA), genetic algorithms (GA), or tabu search, which are based on generic principles and schemes; they attempt to improve a given solution effectively, but the optimality and convergence are difficult to assess; there is no systematic procedure for obtaining good bounds on the attainable optimum values of the objective function (Pekny and Reklaitis, 1998).

Figure 1.2 represents a hierarchy of particular modeling systems that can be dis-

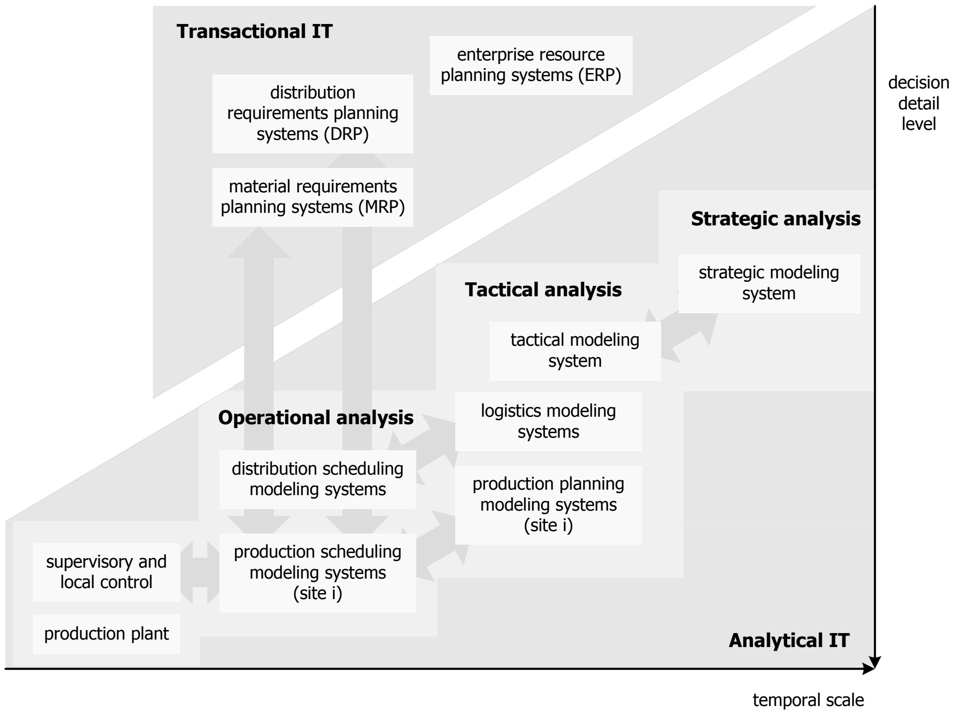


Figure 1.2: Hierarchy of modeling systems in the area of PSE.

tinguished in the broad area of PSE based on the temporal scale and the level of decision. The need to integrate the different modeling approaches in a hierarchical decision-support system makes necessary the use of consistent terminology and concepts to improve the communication and collaboration tasks over the entire system.

1.1.2 Integration standards

The integration of modeling systems for different levels of decision in an enterprise aims at providing visibility and avoiding data inconsistencies, thus leading to an efficient use of resources, as well as to improved response times and customer services. Financial incentives for better integration have been reported by companies, with a reduction of working capital up to 50 % (Shobrys and White, 2002).

Integration standards emerged to facilitate interoperability between disparate systems of different vendors by separating process application functions from transport and communication functions, and by providing models and a formal definition of the scope, terms and concepts.

Numerous integration standards have been defined from various industries and government groups. The standards ANSI/ISA S95 (International Soc. for Measurement and Control, 2000) and ANSI/ISA S88 (International Soc. for Measurement and Control, 1995, 2001) are specially important in the area of PSE for manufacturing and enterprise planning integration, and for batch process control, respectively. The

ANSI/ISA S95 international standard organizes the enterprise into four levels of decision: levels 1 and 2 focus on automation control of the plant facilities; levels 3 and 4 deal with the plant operations and the enterprise, respectively. This specification provides the models and terminology to define the interfaces and interactions between business systems at the enterprise level and manufacturing control systems at the plant floor level. Within the lower levels, the **ANSI/ISA S88** international standard provides models and terminology to develop operational modeling systems for batch manufacturing plants and batch control.

Other notable enterprise integration standards are OLE, from OPC Foundation[1] for process control, UML (Unified Modeling Language) for object-oriented program design, and XML (eXtensible Markup Language) for structured documents on the web. The most important standards can be found in the Purdue Enterprise Reference Architecture web site[2].

1.1.3 Operational analysis

A detailed discussion of software and hardware developments for all the modeling systems in the field of planning and scheduling is out of the scope of this thesis. Rather, the research focuses on the lower operational level of decision.

Operational analysis refers to short-term decision problems concerned with the detailed execution of activities within a single or contiguous sites of a SC. The physical configuration of the system is usually given (strategic decisions), and the aim is to support managers on operating decisions such as timing and sequencing.

Within this detailed level of analysis, modeling systems for production and logistics scheduling can be distinguished. Production systems analyze each plant individually, whereas distribution systems address logistic operations across the organization's network. In general, modeling approaches for operational planning require far more customization to the characteristics of the production environment than those for tactical and strategic planning.

Operational analysis maintains a close relationship with the lower control level by providing the production schedule to the process coordinator, which uses it as a guidance to set-up activities and manage the execution of control actions in the plant. On the other hand, operating results are also required by transactional systems of materials and distribution requirements planning (MRP and DRP). An MRP system is a tool used for establishing the needs of dependent components such as raw materials, parts, subassemblies, or modules; it provides a detailed bill of materials indicating the types and quantity of resources that need to be purchased from outside, the products to be manufactured internally, and the time to place the orders. This information is used by enterprise resource planning systems (ERPs) to integrate sales, finance, manufacturing and distribution activities, and provide an optimum enterprise efficiency (Waller, 2003).

However, MRP systems tend to aggregate resources into groups, assume infinite capacity, and are not able to determine feasible schedules with an improved management of resources and capacities. Therefore, operational analysis is required to identify schedules with the appropriate resource levels and allocations, to guarantee schedule feasibility, and to provide transactional systems with more accurate information.

[1] OPC Foundation, <www.opcfoundation.org>, [18 Apr. 2006]
[2] Purdue Enterprise Reference Architecture, <www.pera.net/Ind_stds.html> [18 Apr. 2006]

1.2 The scheduling problem

Effective production is very important in today's global competitive environment. Multiproduct and multipurpose plants operating mainly in batch mode, but also continuous or semicontinuous processes, manufacture a variety of products through a sequence of operations that share the available resources, intermediate products, and raw materials.

The scheduling of production facilities can be generally defined as a decision-making process that gives answer to the questions *how*, *where*, and *when* to produce. *How* refers to the plant resources required (processing units, steam, electricity, raw materials, manpower, etc.); the question *where* is answered by allocating every operation to a specific unit; finally, *when* consists of predicting the start and end times for each operation (Pekny and Reklaitis, 1998).

In its most general form, the scheduling problem requires information related to the configuration of the plant (set of available equipment units and resources), the product recipes (set of processing tasks and resources required to manufacture a given product), precedence relationships between materials, and final product requirements (demands and related due dates). Given this data, the scheduling problem involves making decisions on the assignment of resources to tasks (*where*), the production sequence of tasks allocated to the same resource (*how*), and the detailed schedule of operations expressed as start and end times of each task, the distribution of inventory levels over time, and the resources profiles (*when*). Decisions such as *what* to produce and lot sizing are generally considered part of larger production planning or tactical decisions.

The scheduling problem is generally solved to optimize a given criterion. Typical performance criteria include the makespan (time required to complete all tasks), plant throughput, some measure of customer satisfaction, economic functions of production costs or profit, and the number of tasks completed after their committed due dates (Reklaitis, 1996). Several objective functions could be used simultaneously for determining the best schedule in a multi-objective basis.

Scheduling problems can be classified from different points of view. For example, problems can be *static* or *dynamic* based on the way the arrival time of the orders is managed. On the other hand, the problem is referred to as flow shop, or *multiproduct* scheduling, and job shop, or *multipurpose* scheduling, depending on the layout of the plant. Another categorization can be established based on the type of order being processed: *make-to-stock* facilities plan the production for inventory; instead, production is based on requested orders in *make-to-order* facilities. Finally, a distinction is made between *deterministic* and *stochastic* scheduling problems depending on the consideration of the uncertainty: deterministic problems rely on estimated values for the input parameters, whereas uncertain parameters are modeled as random variables in stochastic scheduling.

1.2.1 Modeling systems for scheduling

Scheduling plays a key role in most industries whenever there is a competition among activities for limited resources available over a finite time period. The need to coordinate and integrate all resources and manufacturing functions to exploit flexibility and drive profitability has given rise to an accelerating interest in planning and scheduling technology, especially from the early 1990s.

With the developments in IT, the traditional use of white boards, marker pens, or colored cards becomes out of date. Instead, computer-based modeling systems for scheduling, usually referred to as Advanced Planning and Scheduling systems (APS), provide the support to solve the problem effectively, allowing easy and frequent schedule generation, as well as the integration with other decision-making applications used in the enterprise. As described in Section 1.1.3, operational systems provide scheduling information to upper MRP systems, and serve also as a guidance for lower control levels.

Scheduling in the CPI implies the consideration of specific characteristics and constraints resulting from features such as shared resources, tightly integrated equipment, limited connectivity, precedence relationships, simultaneous transfer operations, unstable intermediate products, limited storage time or capacity, limited recover abilities, changeover and maintenance procedures, recycling streams, and scalable batch sizes. Special features of planning and scheduling problems in the CPI are discussed in Reklaitis (2000), and Kallrath (2002).

Because of the variety of problems and properties involved, it is difficult to define a general modeling system for scheduling. Numerous approaches, either rigorous or heuristic-based, have been reported in the literature. Detailed reviews of scheduling methodologies in the CPI can be found in Shah (1998); Pekny and Reklaitis (1998); Floudas and Lin (2004), as well as in the references cited therein. For a categorization of the scheduling problem and a detailed and uniform description of mathematical programming approaches refer to the recent contribution by Méndez et al. (2006b).

The necessity of single-site scheduling

While most of the work related to the scheduling problem focuses on single production sites, the scope of interest has been recently extended in the spatial dimension to manage of a whole SC. This view implies taking into account the stock and capacity of suppliers and customers when placing the orders, the coordination of multiple facilities, and the shipment of materials through an associated transport network.

However, and as stated by Shah (2005), the performance of a process industry SC is strongly affected by the flexibility and responsiveness of each production site involved. Therefore, when considering the static scheduling problem for a given time horizon, the identification of a reliable and flexible schedule in each entity of a multi-site system is of utmost importance for an efficient overall performance. The schedule not only serves as a basis for planning and coordinating external activities with customers and suppliers, thus ensuring the materials are ordered and served in time, but it is also useful for the identification of conflicts, bottlenecks, periods with extra or low capacity requirements, preventive maintenance periods, as well as for cash projections, thus providing a good insight on the performance of the site and visibility for future actions (Leon et al., 1994; Mehta and Uzsoy, 1998).

1.2.2 Scheduling under uncertainty

The scheduling problem has usually been seen as a function of known and reliable information. Modeling approaches developed are mainly deterministic, that is, they are based on nominal or estimated values for all the parameters, thus implicitly assuming that a *predictive schedule*[3] will be executed exactly as planned. However, this assumption is somehow utopian since most plants operate in an unstable and dynamic environment, where unexpected events continually occur. Scheduling problems involve data coming from different sources, and which varies rapidly over time as customer orders, resource availabilities and/or processes undergo changes. Data may be ambiguous, outdated or inaccurately predicted before the problem is solved.

Because of the dynamic and uncertain conditions of a real process system, the schedule executed in the plant will probably differ from the predicted one. The effects of the uncertainty may impact on the system's efficiency, eventually leading either to an infeasible situation, or to the generation of opportunities that improve its performance. These situations may become even more significant with the new trends towards managing the whole SC. As stated by Aytug et al. (2005), internet technology enables companies within a SC to share their production schedules. In this environment, changes to the production schedule at a downstream node of the SC can cause significant disruptions in upstream operations. These variations can be amplified causing what is known as the *bullwhip effect* (Lee et al., 1997).

The consideration of the uncertainty when modeling the problem is essential for the development of reliable and effective decision-support systems.

1.3 Motivating example

Consider as a comprehensive example the five-product three-stage flow shop plant illustrated in Figure 1.3, and detailed in Appendix B.1. The effects of variable operation times and uncertain product demands are next analyzed from an operation viewpoint.

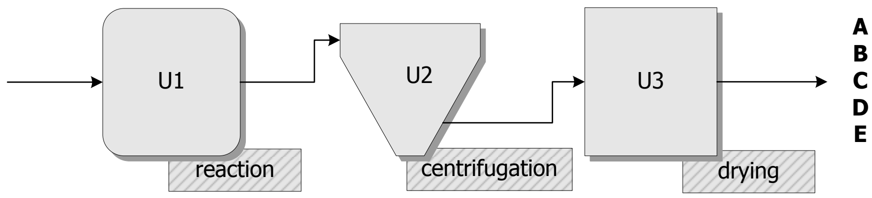


Figure 1.3: Flow shop plant scheme.

Operation times uncertainty

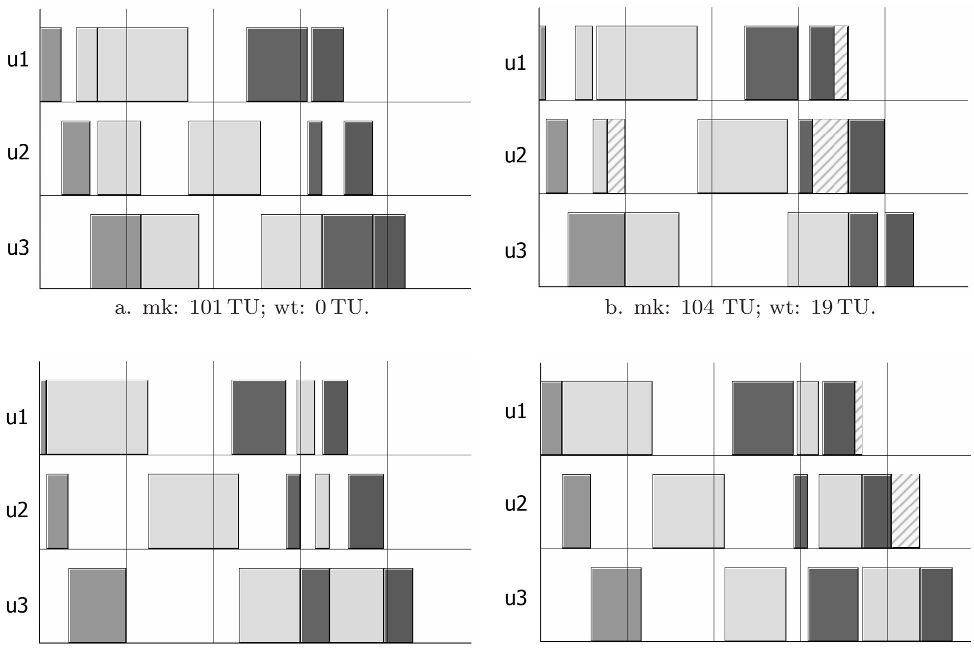
The predictive schedule with minimum makespan, determined using a deterministic model of the problem, is represented as a Gantt chart in Figure 1.4 (a). The optimal sequence for the schedule is A-B-D-E-C, and the makespan value is 101 TU. However, the actual processing times occurring at execution time can significantly differ from the estimated ones, leading to eventual inconsistencies, and/or wait times.

[3]The term *predictive schedule* is used throughout the dissertation to denote the schedule resulting from decision variables determined a priori using scheduling systems, before the schedule is executed and the uncertainty is revealed.

Assume that the actual operation times are as those reported in Appendix B.1 (Table B.7), where a random deviation from the nominal values has been introduced in each operation. Using as a guidance the predictive schedule identified assuming mean processing times (Figure 1.4 (a)), the actual schedule that would result after execution time in this random scenario is represented in Figure 1.4 (b). The makespan value increases up to 104 TU, and wait times appear between stages waiting for the availability of the next processing unit (19 TU). Notice, for example, that the second batch starts at the predicted time, but the intermediate product can not be transferred immediately after the second operation since its processing lasts shorter than expected, and the third equipment unit is still executing the last operation of the first batch. A similar situation occurs in the last two batches.

Is the predictive schedule determined assuming mean operation times (Figure 1.4 (a)) the optimal one to be implemented if the random scenario actually occurs? Could other decisions be made to improve the performance of the schedule?

These questions can easily be answered with the resolution of the deterministic scheduling model for this new (randomly generated) scenario. Proceeding in this way, an optimal predictive schedule is determined (Figure 1.4 (c)) with a slightly different production sequence (A-D-E-B-C), a makespan value of 103 TU, and no expected wait time. Instead, 19 TU of wait times are generated in a makespan of 104 TU if the predictive schedule identified using the nominal operation times is executed (Figure 1.4 (b)).



a. mk: 101 TU; wt: 0 TU.

b. mk: 104 TU; wt: 19 TU.

c. mk: 103 TU; wt: 0 TU.

d. mk: 114 TU; wt: 14 TU.

Figure 1.4: Gantt charts of the: a) optimal predictive schedule for the nominal scenario; b) schedule (a) executed in the random scenario (Table B.7); c) optimal predictive schedule for the random scenario; d) schedule (c) executed in the nominal scenario.

On the other hand, if the optimal predictive schedule in the random scenario is used as a guidance when the nominal conditions are actually realized, the execution takes 114 TU, and 14 TU of wait time are generated. The Gantt chart of this executed schedule is depicted in Figure 1.4 (d).

These results suggest that any deterministic modeling may yield suboptimal solutions in the face of uncertainty.

Product demands uncertainty

Assume now that the objective is to maximize the profit value (PV) taking into account production and inventory costs for each product i (c_i^P, c_i^I), costs for product changeovers ($c_{ii'}^c$), and a penalty for underproduction (c^U) as expressed in equation 1.1. Problem data is reported in Appendix B.1 (for the nomenclature refer to page 153).

$$\begin{aligned} \max PV = \sum_i \big[\big(\gamma_i \cdot Q_i^S - c_i^P \cdot Q_i^P - c^U \cdot (\gamma_i - c_i^P) \cdot Q_{ik}^U\big) - \\ - c_i^I \cdot Q_i^I - \sum_{b,i,i'} c_{ii'}^c \cdot XM_{bii'} \big] \end{aligned} \tag{1.1}$$

Using a deterministic modeling of the problem, considering the nominal demand values given in Table B.2, the predictive schedule depicted in Figure 1.5 (a) is identified, with an optimum profit value of 3546 MU. Table 1.1 details the results for each product related to the number of batches performed (n_i), amount produced (Q_i^P), quantity sold (Q_i^S), inventory (Q_i^I), and amount of product not satisfied (Q_i^U).

Can the optimality of this schedule be guaranteed if the product demands to be received are uncertain?

Table 1.1: Optimal results for the nominal predictive schedule.

	A	B	C	D	E
n_i	2	1	3	1	1
Q_i^P	200	100	300	100	100
Q_i^S	200	100	300	100	100
Q_i^I	0	0	0	0	0
Q_i^U	0	0	0	0	0
PV	3546				

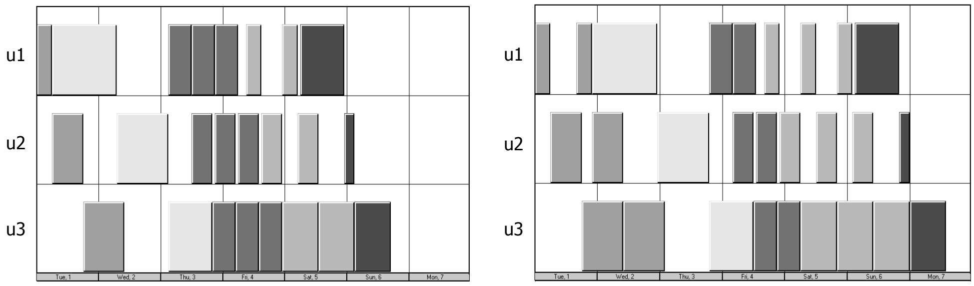
Consider a particular scenario with the demands detailed in Table B.6, which imply a deviation around 30 % from the nominal values. If the predictive schedule identified with the nominal conditions (Figure 1.5 (a)) is implemented when the scenario with these random demands occurs, orders for products A and B can not be completely satisfied due to production shortfalls, whereas overproduction occurs for products C and E. This situation is summarized in Table 1.2. Notice that the expected profit decreases from 3546 MU to 1790 MU.

The solution of the deterministic model considering the demands of this random scenario results in a new schedule (Figure 1.5 (b)), with an optimum profit value of 2723 MU as detailed in Table 1.3. This profit is about 35 % higher that the expected

Table 1.2: Results for the nominal predictive schedule executed in the random scenario.

	A	B	C	D	E
n_i	2	1	3	1	1
Q_i^P	200	100	300	100	100
Q_i^S	200	100	200	100	80
Q_i^I	0	0	100	0	20
Q_i^U	50	30	0	0	0
PV	1790				

one when using the predictive schedule optimal for the nominal product demands (1790 MU). Analyzing the performance of the optimal predictive schedule for the random scenario (Figure 1.5 (b)) in the nominal conditions, the situation detailed in Table 1.4 is expected. Notice that a profit value about 53 % lower is obtained (1286 vs. 3546 MU).



a. PV: 3546 MU.

b. PV: 2723 MU.

Figure 1.5: Gantt charts of optimal predictive schedules: a) for the nominal demand scenario; b) for the random demand scenario.

It is then obvious that the executed schedule can differ significantly from the predictive one based on a deterministic model with some estimated conditions that can not be foreseen with certainty. The presence of this uncertainty may result in a serious reduction of the process efficiency, as well as in opportunity losses.

Table 1.3: Optimal results for the random predictive schedule.

	A	B	C	D	E
n_i	3	2	2	1	1
Q_i^P	300	200	200	100	100
Q_i^S	250	130	200	100	80
Q_i^I	50	70	0	0	20
Q_i^U	0	0	0	0	0
PV	2723				

Table 1.4: Results for the random predictive schedule executed in the nominal scenario.

	A	B	C	D	E
n_i	3	2	2	1	1
Q^P	300	200	200	100	100
Q^S	200	100	200	100	100
Q^I	100	100	0	0	0
Q^U	0	0	100	0	0
PV	1286				

This simple example clearly suggests that the analysis of the uncertainty becomes essential for an effective and realistic scheduling. Then, the following questions arise: how can the uncertainty be addressed? Can the different sources of uncertainty be generalized and categorized? Is there a general scheduling methodology to deal with the uncertainty? Is it desirable or rewarding? All these points pose recognized challenges in the area of process operations, and motivate the development of this research work.

1.4 Management of the uncertainty

In an operational level of activities, two stages of action can be generally abstracted. On the one hand, there is an *off-line* stage based on deciding *how*, *where*, and *when* to produce or deliver a set of products in order to determine a predictive schedule. On the other hand, there is an *on-line* stage with the execution of actions based either on a predictive schedule determined off-line, or on decisions taken dynamically and for the immediate future using real-time dispatching procedures. The latter resembles a process control application in that it implies a rolling horizon perspective.

The *management of the uncertainty in scheduling* can be considered as the ability to achieve high quality or robust schedule execution despite the occurrence of unforeseen events. The need to analyze the uncertainty in modeling systems is minimum when using dispatching-based scheduling procedures, since they provide only guidance for the immediate activities, with very little visibility into the future. Instead, it becomes essential for static scheduling.

Assuming the use of a predictive schedule, and in line with the above stages, two general strategies can be distinguished to deal with uncertainties in operational analysis: on the one hand, the uncertainty can be faced proactively in the off-line stage, prior to its realization at execution time; on the other hand, uncertainty can be dealt with on-line by reacting to the consequences of its realization occurring at execution time (Figure 1.6).

1.4.1 Proactive approaches

Conventional proactive approaches are based on the introduction of safety measures such as buffers in time, capacity or inventory, to avoid the consequences of unexpected events. These methods are often expensive or inefficient due to additional costs for inventory handling and plant under-utilization. In addition, if materials leaving a

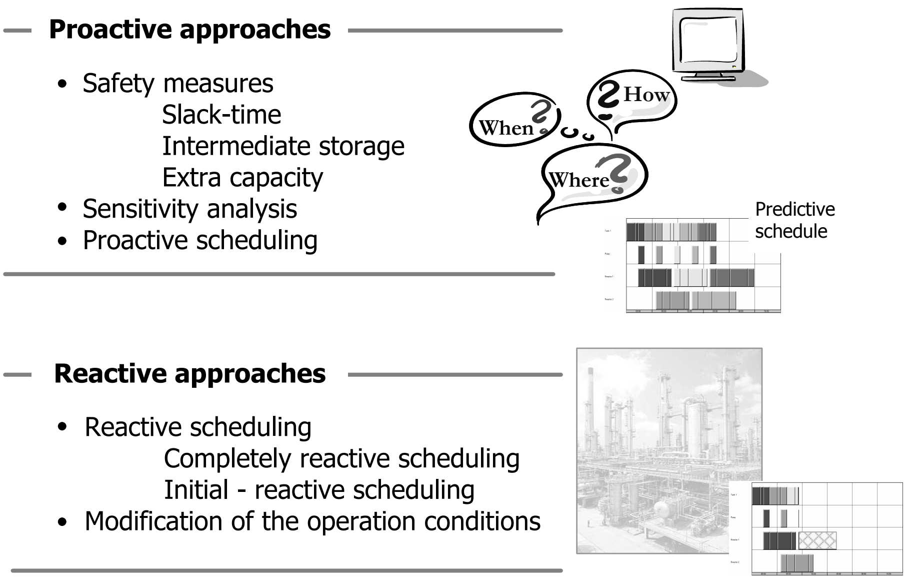


Figure 1.6: Classification of scheduling approaches to manage uncertainty.

processing unit are unstable, and therefore consecutive operations must be performed under a zero wait transfer policy, intermediate storage is not a viable solution. These techniques attempt to reduce the impact of the uncertainty, but they lack of insight on the process, and limit the possibility to improve its efficiency.

Sensitivity analysis is commonly used to assess the robustness of a proposed schedule to perturbations in the model's specifications or input data. It determines, on individual parameters of the model, the range in which the solution remains optimal provided all other parameters are fixed at their given values. Although valuable knowledge can be obtained, sensitivity analysis is usually considered as a post-optimization approach that does not provide any mechanism to control and improve the robustness of a given schedule (Mulvey et al., 1995).

Information of the uncertainty can be exploited within the decision process itself. This is the goal of *proactive scheduling* approaches, which explicitly incorporate some knowledge of the uncertainty in the decision-making stage with the aim to generate predictive schedules that are in some sense robust or insensitive to a priori supposed uncertainties. These approaches depend to some extent on whether the uncertainty can be somehow characterized.

Proactive methods, and mainly proactive scheduling approaches, can be viewed as sub-optimization strategies that provide visibility for future actions to achieve a greater system's performance. If the uncertainty occurs as predicted, the loss of opportunities and reschedule requirements are reduced, whereas the full force of the perturbation affect the expected results if the uncertainty is neglected (Aytug et al., 2005).

Engell et al. (2001) pointed out that proactive approaches disregard the ability to react to new information in the future, thus reducing the optimization capabilities. In contrast, these methods allow to fully exploit the flexibility of the process and, consequently, to fulfill the production goals to a higher degree. As stated by Gupta and Maranas (2003a), underestimating uncertainty and its impact can lead to decisions that neither safeguard a company against the threats, nor take advantage of the opportunities that higher levels of uncertainty may provide. For instance, not taking into account demand fluctuations could either lead to customer dissatisfaction, with the consequent loss of market share, or to excessively high inventory holding costs, undesirable situations in the current market trends. The former scenario does not recognize an opportunity to capture additional market share, whereas the later translates into an ineffective management of the risk exposure of the company.

The challenge of introducing some flexibility into the scheduling model in order to increase robustness without sacrificing efficiency was emphasized in Honkomp et al. (2000).

1.4.2 Reactive approaches

Most of the attempts for reaction rely on the implementation of reactive scheduling algorithms accounting for the occurrence of a disturbance. Two main categories can be distinguished within this field: completely reactive approaches, which make decisions dynamically when some event occurs; and reactive approaches based on the modification of a predictive schedule to update the decisions according to the actual situation.

Another approach consists of the modification of the process operating conditions to adjust the processing times so as to return to the original requirements. The major drawback of this procedure is that there may be little flexibility for the modification of these conditions to guarantee the quality of the products.

In general, reactive methods may be more appropriate for high degrees of uncertainty, or when information about the uncertainty is not available.

1.5 Thesis outline

As introduced so far, with the new globalization trends and the progress on IT the attention of the PSE community has focused on the area of enterprise management, with the development of modeling systems to manage a whole SC network. An important step in this line is the improvement of the strategies used for the operation and flexible adaptation of individual sites to the dynamic and uncertain environment.

In practice, significant effort is expended either searching for safety mechanisms to protect against disruptions, or reacting to the consequences of the uncertainty. Commonly, orders are expedited, order status is checked at frequent intervals, inventory is deployed just-in-case, and lead times are increased. All these activities are costly and directly result from the uncertainty caused by a lack of visibility and communication among the entities involved in the process system (Geary et al., 2002).

The future is obviously uncertain. Therefore, deviations from a predictive schedule can always occur at execution time, and reactive approaches cannot be excluded. However, reactive scheduling is not always effective or even possible to deal with the uncertainty. Particularly, the ability to recover is usually limited in CPIs, and reconfigurations may be prohibitively costly. Instead, the knowledge of the uncertainty can be usefully exploited proactively at the time of scheduling, before disruptions occur, with the use of more practical models that improve scheduling robustness.

In this sense, this thesis attempts to contribute in the area of operational analysis with the development of proactive scheduling approaches as decision-support systems that exploit the flexibility of processes to come up with efficient and robust predictive schedules coping with the risk of poor performances, and taking advantage of the opportunities that some levels of uncertainty may provide.

With a general perspective of this research, the following questions can be formulated:

(1) What do we understand for uncertainty?

This question leads to the definition of the concept in the context of PSE, and to the analysis and characterization of the main sources of uncertainty that can be encountered in the field, as well as the way they can be formally represented. These points are examined in Chapter 2.

(2) How can uncertainty be considered within scheduling modeling systems?

Proactive and reactive scheduling approaches to deal with the uncertainty have been distinguished. It is clear that some reasoning, though simple, will have to be done at execution time, but the identification of robust predictive schedules is also required so as to serve as a useful guidance not only for the control level in the plant, but also for dependent entities in the SC. General descriptive and optimization modeling systems developed in the area of decision-making under uncertainty are also reviewed in Chapter 2, along with related applications reported in the literature.

(3) What is understood for schedule robustness and flexibility? Is there any formalism established for these concepts?

Although robustness and flexibility are usually used with a same purpose, there is a slight distinction between them. The formalization of these concepts is addressed throughout the state-of-the-art surveyed in Chapter 2, and further discussed in Chapter 3.

(4) Is the problem well solved or deficiencies can be identified?

From the contributions reviewed in Chapter 2, limitations and open issues to be further considered are identified in Chapter 3, thus leading to the definition of the detailed objectives and overview of this research.

(5) How can schedule robustness be improved? What are the benefits?

These last questions are directly related to the underlying research, and are addressed throughout Chapters 4 to 7. The use of both equation-based and procedure-oriented approaches is examined to analyze different issues of the problem and capture novel features in the modeling systems.

General conclusions and future research directions are finally drawn in Chapter 8.

A representation of the contents of the thesis is outlined in Figure 1.7.

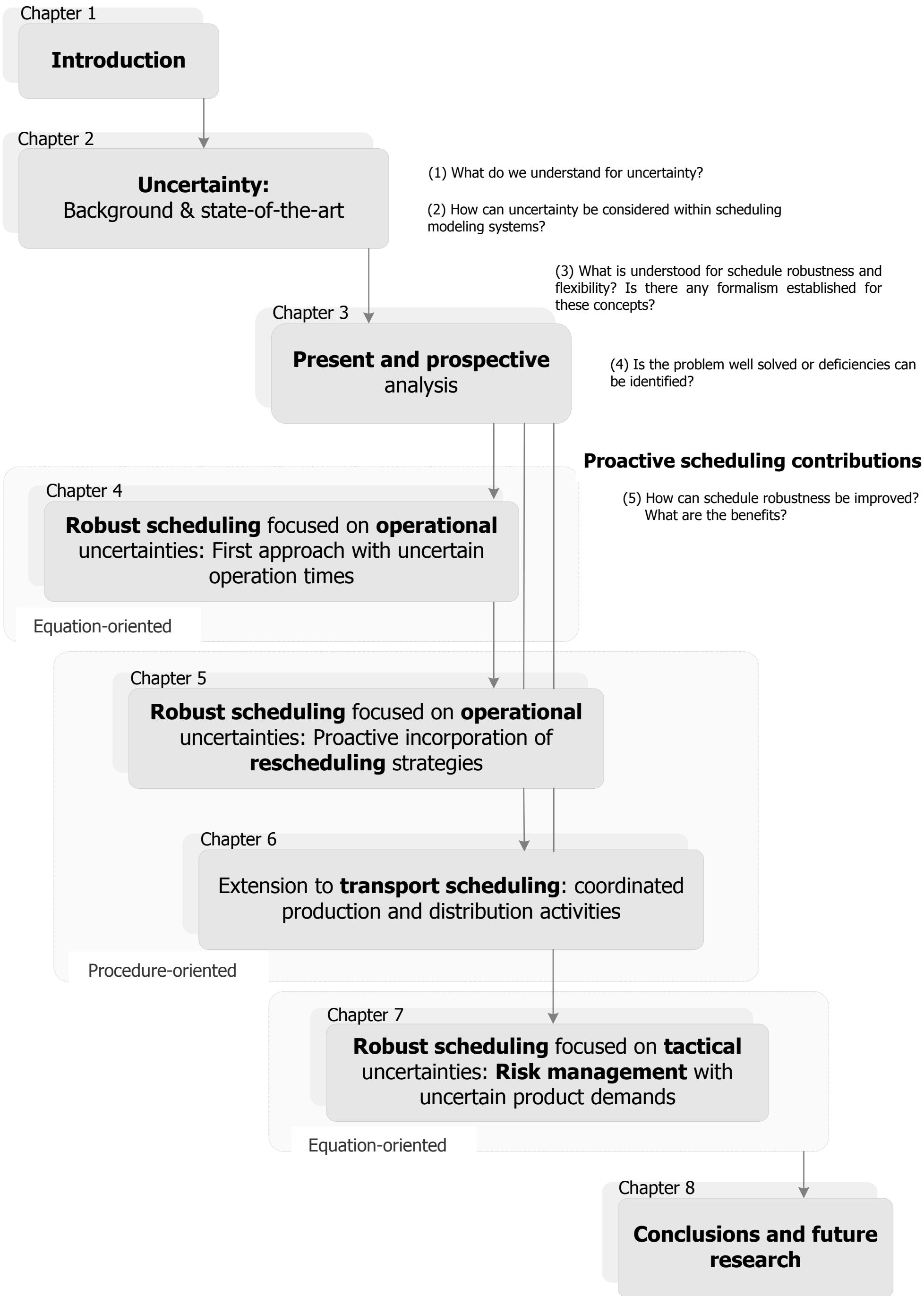


Figure 1.7: Schematic representation of the contents of the thesis.

2.

Uncertainty: Background & State-of-the-Art

He conocido lo que ignoran los griegos:
la incertidumbre.

La loteria en Babilonia, J.L. Borges (1899 - 1986)

The notion of uncertainty is quite ambiguous, subjective, and context dependent. Uncertainties may be different in nature, and caused by imprecise, outdated or incomplete information, inability to accurately model the impact of possible or unexpected events, imprecision in judgment, or lack of effective control actions. They propagate through the system usually leading to inefficient processing and non-value added activities. It is then difficult to give a proper and unique definition of the uncertainty, as well as to establish a general modeling methodology.

This thesis focuses on uncertainty caused by unexpected events as well as ambiguous or incomplete data in the context of Process Systems Engineering (PSE), rather than errors of numerical methods, rounding off, and human errors. From this perspective, this chapter provides a survey of uncertainty issues and a state-of-the-art in the field. Specifically, different sources of uncertainty are first categorized. Methodologies for the representation and assessment of the uncertainty and its effects in the context of decision making are next reviewed, along with modeling approaches and remarkable contributions proposed so far. The role of the uncertainty in current industrial practices, as well as its concern in commercial software packages, are finally discussed.

2.1 Sources of uncertainty

An attempt to provide a general categorization of the uncertainty causes, types of information, and modeling methods was made by Zimmermann (2000) from an application point of view. He identified the lack of information, complexity of information, conflicting evidence, ambiguity, and measurement errors as general sources of uncertainty; the difficult, if not impossible, generalization of the concept and its context dependency was emphasized.

In a more detailed level, process systems are subject to a large range of uncertainties, which have increased significantly with the new globalization trends. Common unexpected events are unplanned machine breakdowns, sales and demand deviations from forecasts, variable operation times, and raw materials or components out of specification. What will customers order? How many products should remain in stock? Will the required resources be always available during the production time? Will the supplier deliver the requested materials on time and according to the specifications? These and other questions are commonly formulated and express uncertain situations around.

Various criteria have been used so far to categorize the sources of uncertainty. Based on the time scope over which the uncertainties may alter the system, Subrahmanyam et al. (1994) distinguished between *short-term* and *long-term* uncertainties. *Short-term* uncertainties alter the system in a short period of time, and include day-to-day processing variations such as canceled or rushed orders, operation times variabilities, and equipment breakdowns. Instead, *long-term* uncertainties occur over longer time horizons, and involve technology changes and variable market trends such as unit price fluctuations, demand variations, and production rate changes.

A more definite classification was posed by Pistikopoulos (1995), who differentiated between *model*, *process*, *external* and *discrete* uncertainties. *Model* uncertainties include parameters obtained usually from experimental and pilot-plant data such as kinetic constants, physical properties and transfer coefficients. *Process* uncertainties involve data obtained from measurements such as processing times or rates, product yields, stream quality, flowrates and temperatures. *External* uncertainties are caused by environmental conditions, technology changes, and variable market trends such as canceled or rush orders, and fluctuating product demands, prices, specifications, and raw material availabilities. Finally, *discrete* uncertainties describe random discrete events like the equipment availability.

Though originally suggested in a more financial context, another classification was proposed by Bräutigam et al. (2003) in the two extreme categories of *endogenous* and *exogenous* uncertainties. *Endogenous* or technical uncertainties refer to enterprise-specific uncertainties that can be modified; uncertainties concerning time and complexity belong to this category, as well as financial uncertainty in terms of cost and liquidity, and the variable quality and properties of products. On the other hand, *exogenous* or market-related uncertainties involve uncertainties coming from the outside; market uncertainties in terms of competition, price and quantity are considered within this group, along with region-specific uncertainties covering potential risks such as armed conflicts, regulatory, taxation and legal issues, natural phenomena, infrastructure uncertainty, and social risks.

Within the context of a supply chain (SC), Geary et al. (2002) typified the uncertainty in *process*, *supply*, *demand*, and *control*. *Process* uncertainties focus on each entity of the SC, and include variations primarily related with process yield ratios and lead time estimates for operations; this source of uncertainty affects the organization's internal ability to meet a production delivery target. *Supply* uncertainties result from the lack of suppliers to fulfil the requirements. Instead, *demand* uncertainties come from the difference between the end market demand and the orders placed in the enterprise by its customers. Finally, *control* uncertainties concern the entire network, and involve disturbances in the information flows, the procedures used to transform customer orders into production targets, and supplier raw material requests (inflexible capacities, wrong decision rules, information delays, and misjudgement by a decision maker).

With the aim to match the sources of process systems uncertainty in a simple and useful classification, without attempting to underestimate the alternative categories previously established, a taxonomy based on the strategic, tactical, and operational levels of modeling introduced in the previous chapter (see Section 1.1) is abstracted, and will be referred to throughout the document:

- *Strategic* uncertainties concern those sources of uncertainty with a main effect on decisions made over long-term planning horizons. Included are, therefore, external or exogenous uncertainties coming from environmental conditions, technology changes, competitors, and governmental regulations among others.

- *Tactical* uncertainties cover several sources of uncertainty that may alter decisions over medium-term planning horizons such as market parameters, and disturbances in information and material flows.

- *Operational* uncertainties comprise uncertainties primarily affecting detailed short-term decisions such as variable processing times, yield ratios, operators absenteeism, and equipment availability.

This taxonomy of uncertainty sources is illustrated in Figure 2.1. It is important to note that most sources of uncertainty do not fit totally within one of these categories, but the boundaries are somehow diffuse. Besides, because of the interactions between the different levels of decision making, uncertainties from one level may affect decisions made in other levels. Variable demands, for example, not only alter tactical planning decisions, but also the production process itself, as it is analyzed later in Chapter 7.

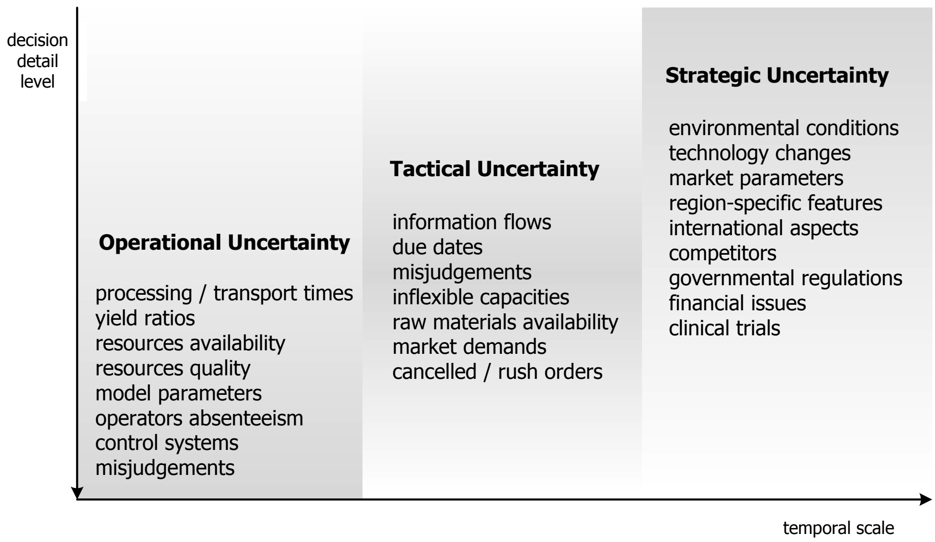


Figure 2.1: Taxonomy of uncertainty sources.

2.2 Decision making under uncertainty

"*Uncertainty refers to decision-making situations in which the decision maker does not know definitely what to decide as he is indistinct about the outcomes*". This definition was given by Van der Vorst and Beulens (2002) referred to a SC, though it is as well applicable to the broad PSE area.

The development of proactive scheduling systems to deal with the uncertainty involves the research direction of decision making under uncertainty. A decision must be made before the actual parameter values and the outcome become known. Decision making under uncertainty has its basics in the area of *decision theory*, which focuses mainly on the study of systematic methods for decision making (Lapin and Whisler, 2002; Waller, 2003).

A decision is usually made from a combination of quantitative analysis and subjective reasoning based on the experience. Under certain conditions it is relatively straightforward to make a decision, since the performance of the system can be known in advance. Therefore, the decision to be made is the one which results in the best desired performance. However, when there is an element of uncertainty, the final performance is unknown at decision time, since it depends on the realization of the uncertainty once made the decision. Common deterministic optimization techniques are based on the use of nominal or estimated parameter values for optimal decision making. They fail to recognize the presence of probable situations other than the most likely one. In hindsight, that is after the realization of the uncertainty, optimal decisions made for the nominal conditions may turn out to be infeasible or perform poorer than other decisions if some different situation occurs.

As it is noticed in Kouvelis and Yu (1997), the best way to cope with the uncertainty is to accept it, make an effort to understand and characterize it, and finally, involve it in the decision-making stage.

Then, how can uncertainty be involved in the reasoning procedure?

Basic approaches considering the uncertainty rely either on the resolution of a deterministic optimization problem for each of different parameter scenarios and the assessment of each outcome in terms of a preferred criterion, or on the application of *parametric programming* or *sensitivity analysis* techniques (see for example the contribution by Acevedo and Pistikopoulos (1997)).

According to Wallace (2000), approaches based on sensitivity or parametric analysis provide a systematic way to analyze the effect of parameter changes on the optimal solution of a model, but are not appropriate for decision making under uncertainty. Sensitivity analysis is a deterministic approach used mainly for deterministic decision problems to forecast what will happen when making a decision under certainty, rather than used for making decisions in the face of uncertainty.

Besides, studies have been published which define criteria to assess the effects of particular sources of uncertainty on predictive schedules. Insight is obtained on the actual performance of the proposed solutions. However, the knowledge of the uncertainty is not explicitly modeled within the decision procedure. Some related contributions can be found in Mignon et al. (1995); Basset et al. (1997); Lawrence and Sewell (1997); and Jia and Ierapetritou (2004).

Reasoning under uncertainty implies the reformulation of deterministic models, either descriptive or optimization systems, to include the uncertainty into the input data. The need for including uncertainty into the modeling systems arose early in the history of mathematical programming, and has experienced rapid development in both theory and algorithms. A key difficulty is the management of large-scale optimization models derived from a huge uncertainty space, and from the presence of integer decision variables used to model logical and other discrete decisions in a multi-period or multi-stage environment (Sahinidis, 2004). Dantzig (Horner, 1999) considered planning under uncertainty as one of the most important open problems in optimization.

Several methodologies for simulation and optimization under uncertainty have been developed based on different criteria, modeling philosophies, and for a wide variety of application areas. The first main step in this direction is the characterization of the uncertainty. Once the uncertainty is described, some formal measure can be defined to assess the robustness or flexibility of a decision in the context of the uncertainty, to eventually implement an optimization algorithm that improves the decision to be made in terms of the robustness criterion established.

2.2.1 Representation of the uncertainty

Statistical forecasting techniques relying on the analysis of historical data and/or market indicators are commonly used in combination with human judgement for the representation of the uncertainty. Besides, Zimmermann (2000) also identified linguistic information, provided in a natural language rather than a formal language, and symbolic information. No single methodology exists to model all kinds of uncertainty (Zimmermann, 2000), but it depends on the context and the information available. The main approaches considered in PSE for a formal representation of the uncertainty associated to model parameters and constraints involve *probabilistic methods* and *fuzzy numbers*.

The characterization of the uncertainty in any process system is a critical technical challenge, and deserves an own and complete study which remains out of the scope of this research. The knowledge of the uncertainty will be assumed an input to the system.

Statistical or probabilistic representation

The probabilistic description of the uncertainty is based on probability theory or stationary random processes, and constitutes the most widely used method for this purpose. Within this approach, scenario-based and distribution-based representations are differentiated.

The *scenario-based* representation of the uncertainty provides a straightforward way to incorporate the uncertainty into a model using a finite number of discrete instances that capture how the uncertainty may evolve in the future; a *scenario* is defined as a particular realization of all the uncertain parameters, and it has associated a probability level representing the expectation of its occurrence.

On the other hand, instead of defining a finite set of possible realizations of the uncertainty, the *distribution-based* approach associates a probability distribution function to the uncertain data. The normal form is largely assumed to describe uncertain parameters, and it is justified on the basis of the central limit theorem considering that the parameters are affected by a large number of stochastic events (Petkov and Maranas, 1997).

Forecasting techniques, evidence from the past, or subjective probability are generally used to approximate the probability distribution functions or the range of possible scenarios. Despite being the most used method, the analysis and manipulation of the uncertainty statistically represented may be difficult, and require considerable computational effort.

Fuzzy numbers

Fuzzy set theory, developed as a generalization of classical set theory, is applied to represent uncertain parameters by means of *fuzzy numbers*. Fuzzy sets have to be defined for each uncertain variable, based generally on subjective judgement and managerial experience. Each element of the set has associated a degree of membership between 0 (not at all in the set) and 1 (completely in the set). Fuzzy approaches provide a simple representation of the uncertainty, which is specially useful when little information is available. The main drawbacks are the definition of the membership function and the computational complexity.

2.2.2 Assessment of the uncertainty effects

The deviations from a predictive schedule occurred at execution time as a consequence of the uncertainty are more or less critical depending on the robustness and flexibility features implied by the decisions made. The effects of the uncertainty can then be assessed by means of some quantifiable measure that indicates how robust or flexible a predictive schedule is. This criterion can also be regarded as a measure of the performance of a process system in an uncertain environment, or of the ability to handle the uncertainties.

Most of the measures proposed when using a probabilistic-based representation of the uncertainty rely on the assessment of the set of outcomes arising from various scenarios of the input data, and from different decisions. Some of these metrics are defined in general terms as *maximin*, *minimax*, *equally likely*, *minimax regret*, *maximum likelihood*, and *Bayes decision* criteria.

- *Maximin criterion* implies the selection of the decision with the best of the worst possible outcome from the different scenarios, completely neglecting their probabilities. It is considered a conservative and pessimistic measure that guarantees a minimum performance level assuming the given data is correct, though the actual situation may not be as bad as supposed. The use of this measure is also known as *worst-case analysis*.

- *Maximax criterion* is an optimistic measure based on the selection of the alternative with the highest of the best outcome from the set of scenarios.

- *Equally likely criterion*, also known as insufficient reason, assigns equal probability values to each scenario assessed, and selects the decision with the highest expected outcome.

- *Minimax regret criterion* makes use of the regret resulting from making a non-optimal decision. The regret is defined for each scenario as the difference between the performance of the decision made, and the performance of the best decision that could have been made if the scenario had been known at decision time.

- *Maximum likelihood criterion* focuses on the most likely scenario, with the exclusion of all others, even if its performance results poorer that the others.

- *Bayes decision rule* implies the selection of the decision with a better expected performance. The expected value is merely a quantitative theoretical value used for decision making, rather than the actual performance because of the mutual exclusivity of the scenarios. The main drawback of this criterion occurs when decisions involve different attitudes towards risk, since it assumes that the decision maker is risk-neutral. This aspect is further discussed in Section 2.4.

Focusing on specific formalisms, a measure of flexibility was proposed by Grossmann et al. (1983) in order to quantify the ability of a chemical process to deal with uncertainty. The notion of *stochastic flexibility* was later introduced in Straub and Grossmann (1993) as a measure of the probability of feasible operation, and methods were presented for the evaluation and optimization of this metric in non-linear design models of chemical processes accounting for uncertainties. Reviews of the literature on flexibility in process design and operations can be found in Straub and Grossmann (1993); Pistikopoulos (1995); and Georgiadis and Pistikopoulos (1999).

Alternatively, the concept of robustness has been used to evaluate the ability of a predictive schedule to recover from unexpected events resulting mainly from operational uncertainties. Some robustness measures have been defined to manage the incorporation of slack time into the schedule, which are based on a linear combination of expected makespan and expected delay (Leon et al., 1994), on expected job completion time deviations (Mehta and Uzsoy, 1998; O'Donovan et al., 1999; Davenport et al., 2001), or on deviations of predicted start times (Herroelen and Leus, 2004a; Van de Vonder et al., 2005).

Robustness metrics based on the economical or temporal performance of a set of schedules located around a central schedule were defined by Jensen (2001). Other criteria have been proposed based on a *Taguchi loss function* (Bernardo et al., 2001), or on some reliability index (Sanmartí et al., 1996).

In general, no firm principles exist for preferring one criteria to another, but multiple formalisms are applied based on the context and the preferences of the decision maker.

2.2.3 Optimization under uncertainty

Several methodologies are available in PSE for optimization under uncertainty. They are categorized, in line with the method used to represent the uncertainty (see Section 2.2.1), as outlined in Figure 2.2. It is beyond the scope of this thesis to cover all the approaches in detail. Rather, the main ideas and contributions reported are summarized in the following sections, with a special emphasis on stochastic and robust optimization for being the basis of the modeling systems developed in this research. For illustration purposes, a schematic representation of a decision-making process in scheduling under uncertainty is presented in Figure 2.3.

Probabilistic data-based methods

Approaches based on a probabilistic representation of the uncertain data generally involve an iterative procedure that comprises, either explicitly or implicitly, an opti-

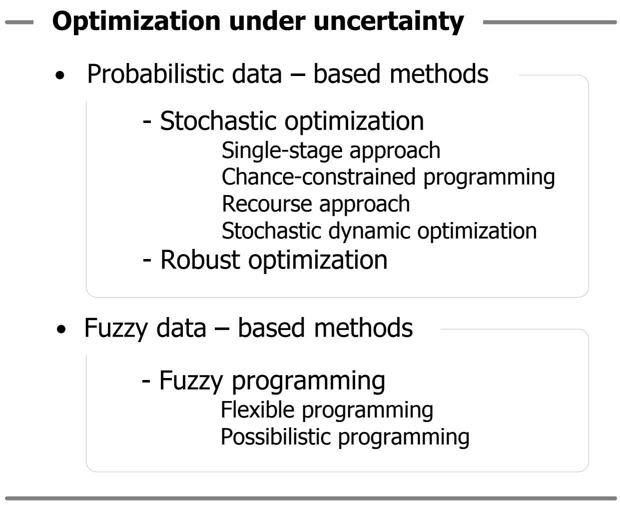


Figure 2.2: Optimization approaches under uncertainty.

mization loop controlling the search for those decisions that improve the desired probabilistic criterion, and an inner loop managing the stochastic features of the problem (Diwekar, 2002). Sampling techniques are usually embedded in the inner loop when a scenario or discrete distribution-based representation of the uncertainty is used; for continuous distribution functions, other analytical or numerical methods are applied. Generally, most of the algorithms rely on sampling techniques, and proceed according to the following main steps:

STEP 1. Specification of the uncertainties in the input parameters (see Section 2.2.1).

STEP 2. Sampling from the uncertain parameter domain in an iterative fashion.

STEP 3. Propagation of the effects of the uncertainties through the model, i.e., resolution of the model in each scenario sampled.

STEP 4. Application of statistical techniques to analyze the results.

Stochastic and robust optimization, either equation or procedure-oriented, are differentiated as approaches based on a probabilistic characterization of the uncertainty. The main ideas underlying these methods are outlined below in Sections 2.3 and 2.4.

A review of probabilistic techniques for scheduling with uncertainty, as well as contributions reported in the operations research literature, can be found in Davenport and Beck (2000); Herroelen and Leus (2004b); and Herroelen and Leus (2005).

Nikulin (2004) provided a survey of approaches based on a definition of robustness in terms of solutions with a *minimax regret* (minimum worst-case scenario) in the areas of combinatorial optimization, scheduling theory, and economics.

Another methodology to find robust solutions for LP problems with uncertain linear coefficients was introduced by Ben-Tal and Nemirovski (2000). The methodology

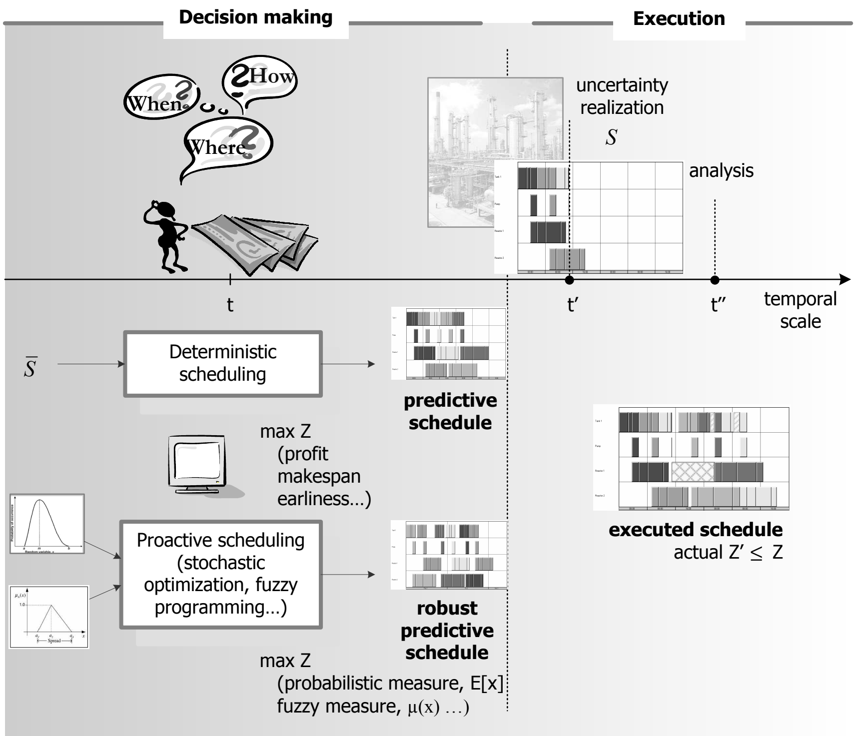


Figure 2.3: Decision-making procedure in scheduling under uncertainty.

was extended to mixed-integer linear programming (MILP) problems by Lin et al. (2004), and further applied to address the short-term scheduling problem with uncertain processing times, market demands, and/or prices of products and raw materials; two types of statistical uncertainty representation were considered: bounded uncertainty, and bounded and symmetric uncertainty. A robust schedule was obtained in the sense that it was feasible within the specified uncertainty level and infeasibility tolerance, though an explicit robustness measure was not defined.

Finally, probabilistic procedure-oriented approaches have also been applied in multi-site systems. For example, Blackhurst et al. (2004) proposed a network-based methodology to model and analyze the operation of a SC as an abstracted network, with uncertainty in variables such as requirements, capacity, material delivery times, manufacturing times, costs, due dates and priorities. For a *simulation-optimization framework* for supply chain management (SCM) based on a multi-agent approach, as well as a detailed review in the field, refer to Mele (2006).

Fuzzy data-based methods

Fuzzy approaches address optimization problems under uncertainty based on a fuzzy description of the uncertain data (see Section 2.2.1), and differ from probabilistic-based methods in the formalism used to model the uncertainty. They are a useful approach in the sense that only information about the range of the uncertain parameters is required, although this limits its capacity to deal with a complex representation of the uncertainty.

The idea underlying fuzzy optimization is the representation of uncertain parameters by fuzzy numbers, and constraints by fuzzy sets. In addition, objective functions in fuzzy mathematical programming are treated as constraints, with lower and upper bounds defining the decision-maker expectations.

Two types of fuzzy programming approaches have been distinguished: *flexible programming* and *possibilistic programming* (Sahinidis, 2004). Both approaches use membership functions to represent the range of uncertainty of coefficients, the expectations of decision makers about the objective function level, and the degree of satisfaction of constraints, thus allowing some degree of violation. For a detailed description of fuzzy set theory refer to Zimmermann (1996).

Fuzzy programming models were compared with stochastic programming by Liu and Sahinidis (1996) considering the process planning problem under uncertainty in market demands and supplies; the study concluded that fuzzy techniques require fewer assumptions and computational effort, but stochastic approaches appear to be more rigorous and, what is more important, they explicitly address the feasibility of a solution over the entire range of random parameters. The study implies that stochastic approaches outperform fuzzy programming models even when the complete probability distributions of the uncertain parameters are unavailable.

Scheduling contributions based on fuzzy approaches generally address operational uncertainties in temporal data such as processing times and due dates. For example, Fortemps (1997) extended a disjunctive graph representation of the job shop scheduling problem to deal with uncertain time durations described by imprecise probability distributions defined as fuzzy numbers. Balasubramanian and Grossmann (2003) applied concepts from fuzzy set theory and interval arithmetic to address flow shop scheduling and new product development process scheduling with uncertain processing times.

Overviews of fuzzy scheduling can be found in the book by Slowinski and Hapke (2000), and the paper by Dubois et al. (2003). The latter contribution distinguishes fuzzy modeling approaches for scheduling under flexible constraints to introduce preference notions, from fuzzy approaches for scheduling with uncertain data due to incomplete or imprecise information.

Fuzzy-based applications have also been reported for strategic and/or tactical analysis in multi-site systems. For example, Sakawa et al. (2001) used fuzzy programming to address production and transport planning in a multi-site environment accounting for uncertain capacities and demands in the different sites. Petrovic (2001) presented a simulation tool (SCSIM) that coupled SC fuzzy analytical models and a SC simulation model to analyze the dynamic performance of a serial production SC with uncertain customer demands, external suppliers reliability, and/or lead times to the sites. Finally, Chen and Lee (2004) proposed a fuzzy multi-objective optimization approach to maximize the degree of satisfaction of multiple objectives in a SC with uncertain product demands and prices; the problem was formulated as a mixed-integer non-linear programming (MINLP) model, the scenario-based approach was considered to represent the demands uncertainty, and fuzzy sets were used to describe different preferences on product prices (note that fuzziness was used for multi-objective optimization, rather than for the representation of the uncertainty).

2.3 Stochastic optimization

Stochastic optimization is based on a probabilistic view of the problem. The underlying idea is to simultaneously consider multiple scenarios of an uncertain future, each with an associated probability of occurrence, and to optimize an objective function expressed in terms of some probabilistic measure (see Section 2.2.2).

The term stochastic optimization is sometimes used referred to meta-heuristics because of the probabilistic nature of these optimization methods. In general, and as differentiated by Fu (2001), stochastic optimization involves methods specially developed to address problems with uncertain data, whereas meta-heuristics use stochastic properties in their search. Although meta-heuristics were not originally formulated with that purpose, they can be adopted for stochastic optimization.

Stochastic optimization is used throughout the dissertation related to either rigorous or procedure oriented optimization techniques for models involving uncertain data. However, most of the contributions on stochastic optimization concern the *stochastic programming* paradigm, where programming implies that various parts of the problem can be mathematically modeled by linear programming (LP), non-linear programming (NLP), integer programming (IP), mixed-integer linear programming (MILP), or mixed-integer non-linear programming (MINLP) models.

Stochastic programming dates back to Beale (1955) and Dantzig (1955), and numerous studies have been conducted from then on to obtain efficient rigorous solution algorithms. The increasing interest on stochastic programming is well illustrated in Figure 2.4; there exists a large literature, with applications covering areas from production planning, scheduling and routing problems to capacity expansion, energy investment, as well as electricity production, environmental management and control, water management, design and optimization of chemical process systems, and finance.

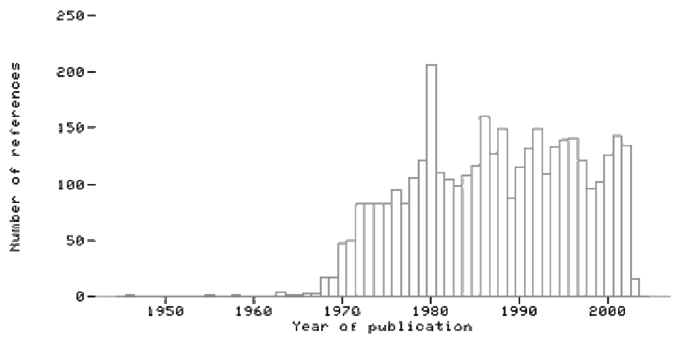


Figure 2.4: Stochastic Programming Bibliography. Maarten H. van der Vlerk. http://mally.eco.rug.nl/index.html?spbib.html, last updated on May 2003.

A survey of stochastic programming applications can be found in a recent contribution by Sahinidis (2004); for an extensive and detailed discussion refer to the standard books of Birge and Louveaux (1997); Kall and Walace (1994); as well as the Stochastic Programming Community Home Page (2004). Commercial packages for stochastic programming have recently emerged (IBM Stochastic Extensions, 2004), and a description of some available software can also be found in the same Stochastic Programming Community Home Page (2004).

Based on the characteristics of the model, the main stochastic optimization problems can be categorized in single-stage, chance-constrained programming, and recourse problems. Stochastic dynamic optimization can be also included within this classification.

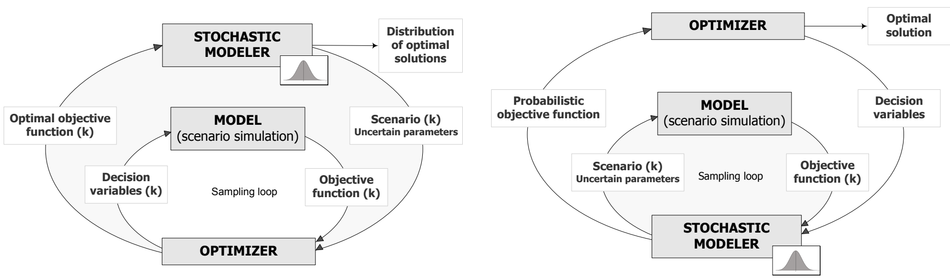
2.3.1 Single-stage approaches

Single-stage stochastic optimization problems are further classified into two categories or behavioral models of decision making under uncertainty referred to as *"wait-and-see"* and *"here-and-now"* (Diwekar, 2002).

The *wait-and-see* approach involves the resolution of a deterministic optimization problem for each scenario of uncertain parameters. A distribution of optimal decisions is finally obtained. However, and as underlined by Wallace (2000), the solution with the best expected performance can not be assured from the evaluation of different deterministic solutions, since part of the solution space is neglected.

On the other hand, *here-and-now* problems imply a probabilistic representation of the objective function and/or constraints, and generate a single optimal solution with a given level of performance.

Figure 2.5 depicts the stochastic optimization frameworks for the generalized solution of these single-stage problems. The difference between the solutions obtained from both strategies is known as the *expected value of perfect information* (EVPI). This concept has been used to analyze the importance of accounting for future information in the decision stage. It was examined in Pistikopoulos (1995). Later, Ierapetritou et al. (1996) focused on the planning problem under uncertainty, and developed a stochastic model explicitly incorporating the EVPI as a measure of the opportunity losses involved in high risk decisions; flexibility was also considered as a measure of the inherent future plan feasibility.



a. Wait-and-see.　　b. Here-and-now.

Figure 2.5: Single-stage stochastic optimization frameworks.

2.3.2 Chance-constrained programming

Chance-constrained programming, also known as *probabilistic approach*, considers the uncertainty by introducing a probabilistic level of constraint satisfaction. It can be considered as a particular category of single-stage *here-and-now* problems, where the uncertain parameters are enclosed in an inequality constraint subject to a probability or reliability level. A solution is pursued which ensures that a set of constraints will be satisfied with a certain probability when the uncertainty is realized. This method is useful to deal with inequality constraints the satisfaction of which is highly desirable, but not absolutely essential.

Relatively few work has been reported for operational analysis using the chance-constrained approach. Orçun et al. (1996) used chance constraints in scheduling batch processes with uncertain set-up and processing times to assess the risk of ending an operation before its processing was completed. Petkov and Maranas (1997) applied the chance-constrained approach to address a multiperiod planning and scheduling of multiproduct plants, and to impose explicit lower bounds on the probabilities of satisfying correlated uncertain product demands.

2.3.3 Recourse approaches

Recourse problems are staged problems that alternate decisions and realizations of stochastic data, and nowadays constitute the most common stochastic approach. They involve both *here-and-now* and *wait-and-see* problems, since they comprise decisions to be determined before the realization of the uncertainty (*here-and-now*), as well as recourse actions to be taken when information is disclosed (*wait-and-see*).

The main class of stochastic problems with recourse involves two stages of decision. The first stage implies those decisions that need to be made *here-and-now*, prior to the realization of the uncertainty. The second-stage or recourse variables correspond to those *wait-and-see* decisions made after the uncertainty is unveiled and subject to the restrictions given by a second-stage problem. Recourse variables can be interpreted as corrective actions taken to deal with disturbances arising as a consequence of the uncertainty. Different second-stage decisions exist for each scenario realization of the uncertainty. Therefore, the objective function is somehow uncertain at the first-stage, and is generally defined as the sum of the first-stage performance measure and the expected second-stage performance.

Similarly, *multi-stage stochastic optimization* deals with problems that involve a sequence of decisions to be made over time. At each stage, decisions are made based on past realizations of the uncertainty, and prior to the occurrence of future events.

Many applications of recourse techniques in the area of PSE focus on strategic and tactical analysis for process design and production planning in single-site systems, and for optimally configuring and managing a SC according to some economic objective. As reviewed by Shah (1998), research is primarily based on recourse approaches with two stages in which product demands are assumed to be uncertain. Some examples for single-site facilities can be found in the papers by Subrahmanyam et al. (1994); Liu and Sahinidis (1996); Ierapetritou and Pistikopoulos (1996); Petkov and Maranas (1998); Cheng et al. (2003); as well as in the references cited therein.

For multi-site systems, stochastic mathematical models with recourse were reported by Tsiakis et al. (2001), and Gupta and Maranas (2003a). For a recent survey in this field refer to Guillén (2006).

Related to the operational level, two-stage stochastic programming models considering product demand uncertainties have also been presented. See, for example, the papers by Vin and Ierapetritou (2001); Sand et al. (2000); Engell et al. (2001); and Engell et al. (2002). Besides, the scheduling problem of multiproduct batch plants under demand uncertainty was addressed applying multi-stage stochastic programming models by Sand and Engell (2004) and Balasubramanian and Grossmann (2004).

A review of application areas, problem formulations, and solution strategies for multi-objective multi-stage decision processes under uncertainty was presented in a recent contribution by Cheng et al. (2005).

2.3.4 Stochastic dynamic programming

Dynamic programming is usually categorized within the literature of stochastic optimization since the uncertainty is identified as an integral part of a dynamic environment (refer to Kall and Walace (1994), and Birge and Louveaux (1997)).

Dynamic programming allows the solution of multi-stage or *sequential decision processes* in which decisions are made periodically, based on policies and state information available at decision time. A dynamic programming algorithm decomposes the problem into a sequence of single-period subproblems that are solved recursively backward in time (Bellman, 1957). It is the basis for designing stochastic optimal control algorithms, also known as Markov decision processes.

Stochastic optimal controlstochastic optimal control algorithms and multi-stage stochastic programming were compared in Cheng et al. (2004a) for solving multi-objective decision processes involving sequential decision making under uncertainty. Both approaches appear to be equivalent, but stochastic programming methods search for an optimal decision tree that hedges against the tree of scenarios representing the uncertainty, whereas optimal control focuses mainly on optimal policies that match each state with the optimal action. It was recognized that both approaches suffer numerically from the curse of dimensionality due to the large state space in optimal control, and large sample space in stochastic programming; it was also emphasized that different solution strategies should be selected and tailored, based on the specific problem considered.

Applications of multi-objective Markov decision processes in strategic and tactical analysis with uncertain demands and technology developments can be found in a series of contributions by Cheng (Cheng et al., 2003, 2004a,b).

2.3.5 Evaluation of expectations

Extensions of deterministic models to stochastic models are very appealing. However, technical challenges mainly related to the statistical representation of the uncertainty and the evaluation of expected functions appear when attempting to design and implement a stochastic model. Using a *scenario-based* representation of the uncertainty or *discrete probability* distributions, the expectation functions are written as finite sums, and stage variables and constraints are explicitly defined for each scenario. This leads to large-scale formulations, usually referred to as *deterministic equivalent problems*. Applications of the scenario-based approach were reported by Subrahmanyam et al. (1994) and Tsiakis et al. (2001) to account for uncertain product demands in the design of batch plants and the design of multiproduct multiechelon SCs, respectively.

When the uncertainty is described with *continuous probability* distributions the problem becomes computationally intractable because of the multivariate numerical integration. To overcome this drawback, the multivariate probability integrals can be approximated by the explicit or implicit discretization of the distribution functions using *sampling techniques* or *Gaussian quadrature integration*. Such discretization methods are relatively insensitive to the form of the distribution of the uncertain parameters. However, Gaussian quadrature integration requires the incorporation of extra variables into the model in order to account for the quadrature points, which are selected within the optimization process; in addition, the number of points required increases exponentially with the number of uncertain parameters. On the other hand, using sampling methods the number of samples required does not necessarily increase with the integral dimension, but multiple function evaluations are needed to estimate the objective function constraints and their gradients at every iteration of the optimization algorithm (Petkov and Maranas, 1997).

Focusing on sampling techniques, *Monte Carlo sampling* is one of the most widely used methodologies. Its main advantage lies in the fact that the results obtained from Monte Carlo simulation can be treated using classical statistical methods because of the randomness and independence of the generated samples. Other techniques such as *Importance sampling*, *Stratified sampling*, and *Latin Hypercube sampling* have been designed to reduce the variance of Monte Carlo estimates (Diwekar, 2003).

Quasi-Monte Carlo methods, also known as low discrepancy sequences, have also been developed to cover the integration region with a set of uniformly distributed points. It is established that these methods provide faster convergence rates because of the better uniformity properties of the sampling design, as compared to Monte Carlo sampling, although their efficiency and precision diminishes with the increase of dimensionality (Kocis and Whiten, 1997). Some well-known constructions for quasi-Monte Carlo sequences are the ones due to Halton, Hammersley, Sobol, Faure, Korobov, and Niederreiter (Diwekar, 2003). A sampling technique based on the Hammersley sequence was introduced by Diwekar and Kalagnanam (1997).

The use of discretization methods has extensively been examined in the areas of process planning and design to estimate the expectation of an objective function. The use of Monte Carlo sampling was considered by Liu and Sahinidis (1996). Applications and comparative studies of different integration techniques, ranging from alternative Gaussian quadrature formula and cubature methods to Monte Carlo integration and Hammersley sequence sampling, have been reported by Pistilopoulos and coworkers (Ierapetritou and Pistikopoulos, 1996; Acevedo and Pistikopoulos, 1998; Bernardo et al., 1999, 2001).

In general, multivariate continuous distributions need to be mapped into a finite number of scenarios to avoid the high-dimensional numerical integration, the size of the problems increases exponentially with the number of uncertain parameters when dealing with discrete scenarios, and the probabilities of occurrence associated with each scenario may be difficult to estimate. The generation of scenarios to approximate the expectations requires the forecasting of a representative set of possible realizations of the uncertain parameters, and it is a research subject itself as also recognized by Cheng et al. (2004a).

An alternative methodology to avoid the discretization of the probability space and to reduce the computational limitations is based on the resolution of the inner recourse problem analytically for the second-stage variables in terms of the first-stage variables, followed by analytical integration for expectation evaluation. This strategy was used by Petkov and Maranas (1998) to solve the design of multiproduct batch plants operating in single-product campaign mode under normally distributed uncertain product demands. Later, Gupta and Maranas (2003a) applied the same methodology to address the medium-term planning problem of multi-site SCs.

Focused on the scheduling problem of zero wait and unlimited intermediate storage flow shop plants, Balasubramanian and Grossmann (2002) developed an stochastic MILP model based on an analytical expression for the expected makespan to deal with uncertain operation times modeled using discrete probability distributions; the extension of the model to the case of continuous distribution functions was also examined using a discretization scheme to approximate the expected makespan of a given sequence.

2.4 Robust optimization

The notion of *robust optimization* was introduced by Mulvey et al. (1995) to explicitly deal with the uncertainty and make decisions less sensitive to variations of the input data. Within this approach, a solution is termed to be robust if the performance of the actual scenario remains close to the optimal expected performance in the uncertain space.

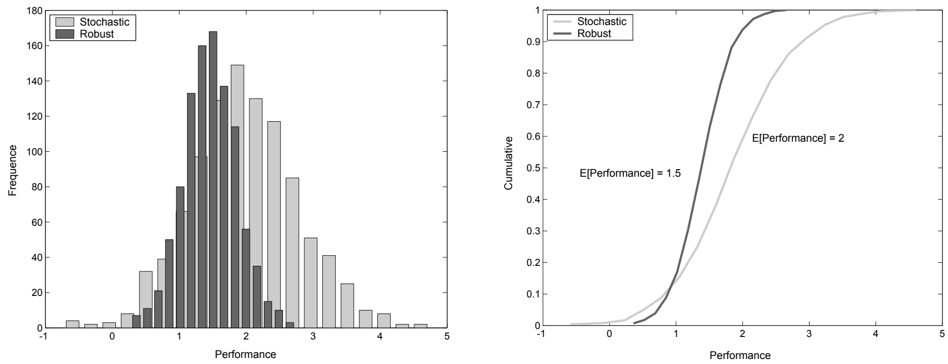
In general, stochastic optimization accounts for the uncertainty by optimizing an expected value, without controlling the variability of solutions that can be attained depending on the scenario eventually realized. Although the decisions can be considered more robust than those obtained from an optimization based on nominal parameter values, by taking a purely expected criterion the model ignores the whole distribution of the objective function values, and assumes that the decision maker is risk-neutral or indifferent to variability. Therefore, there is no guarantee that the process will perform at a certain level over all the uncertain parameters space. The only guarantee is that average is optimized (Samsatli et al., 1998; Suh and Lee, 2001). This limitation of *pure* stochastic optimization approaches is well recognized in management applications (Mulvey et al., 1995).

Some decision makers might prefer a solution with a high expected performance, even if this implies a considerable risk. Others might be interested in solutions with low risk of poor system performance, despite obtaining relatively lower efficiency. An extremely risk-averse decision maker might even prefer the solution with the best worst-case performance, independently of its expected outcome (Sevaux and Sörensen, 2004). The performance of a decision in all potentially realizable scenarios is then important.

In this line, robust optimization extends stochastic optimization by incorporating a measure of variability or risk into the objective function. An additional distinction of robust optimization is the explicit consideration of feasibility issues; penalty terms are usually incorporated in the objective function to determine a solution with a minimum violation of constraints. Instead, stochastic optimization generally assumes complete recourse, that is, every scenario is supposed to be feasible.

Therefore, robust optimization involves the disciplines of stochastic and *multi-objective optimization* to systematically search for efficient frontiers describing the trade offs between expected efficiency and variability. Generally, it integrates goal programming formulations with a scenario-based description of problem data (Mulvey et al., 1995), though other methodologies could be considered (refer to Steuer (1986) for a review of multi-objective optimization). Limitations of robust optimization approaches come mainly from the need to specify effective procedures for selecting the representative scenarios (as in stochastic optimization), as well as the way to prioritize or select among the multiple objectives (e.g., use of weights).

The histograms and cumulative curves depicted in Figure 2.6 for two generic solutions illustrate the differences between stochastic and robustness notions. The stochastic solution shows a higher expected performance, though it is also riskier since losses occur for several scenarios. Instead, the robust solution performs with reduced variability of possible outcomes, and relatively good performances are expected in all the scenarios. A risk-averse decision maker would prefer the later solution for giving almost the same expected level of efficiency, with lower risk of poor performance. These preferences cannot be captured using a pure stochastic model, since information about the distribution of outcomes is not considered at all.



a. Histograms.

b. Cumulative distribution functions.

Figure 2.6: Illustration of stochastic and robust optimization concepts.

The *variance* is probably the most commonly used measure of variability. However, variance-based measures are symmetric, and may turn unsuitable in many cases and overcompensate for the uncertainty. Other criteria have been proposed in the literature providing one-sided properties; for a review of these measures refer to Ahmed and Sahinidis (1998), and Samsatli et al. (1998).

Applications of the robust optimization approach defined by Mulvey et al. (1995) as an extension of the objective beyond simple expectations have recently been reported in the area of process design and long-term planning. For example, Ahmed and Sahinidis (1998) applied this method to address the capacity expansion problem in chemical process industries with uncertain product demands and availabilities; a two-stage stochastic formulation was extended incorporating the *upper partial mean* as an asymmetric measure of variability. Suh and Lee (2001) proposed the worst-case cost as the control measure to be minimized together with the expected cost in chemical process design and planning problems with demand uncertainty. Chen and Lee (2004) focused on a tactical planning of a SC system with uncertain product prices and demands, and applied the *lower partial mean* as a measure to reduce the variability of multiple objectives to product demand uncertainties.

2.4.1 Risk management

Robust optimization provides the means to account for alternative decision-maker preferences, thus capturing different perspectives of risk when making decisions under uncertainty. Therefore, the so called *risk management* approaches, which usually manage the trade off between risk and return, can be categorized within the robust optimization domain.

Some contributions to risk management have also been reported. One of the first discussions was presented by Eppen et al. (1989) in the framework of capacity planning for the automotive industry. The concept of *downside risk* was proposed to measure the cost variability, and to obtain risk-averse investor solutions. This measure was recently used by Cheng et al. (2004b) to address coordinated capacity planning and inventory control under uncertain product demands and technology developments. For a technology selection problem faced by a firm undertaking a market-based pollution abatement initiative with emission and market uncertainties, Gupta and Maranas (2003b) discussed three alternative approaches to actively manage the risk exposure of the firm (variance control, probabilistic analysis, and worst-case analysis).

Considering the scheduling problem of multiproduct chemical batch processes, Sand and Engell (2003, 2004) extended the objective function in terms of expected profit for two-stage stochastic integer programming models with the concept of *minimum risk criterion* as a measure of the probability to obtain profit values below a certain threshold. A similar criteria was studied by Barbaro and Bagajewicz (2004b) to include *financial risk* management in the framework of two-stage stochastic programming for planning capacity expansion problems. The effect of using inventory and option contracts to manage risk in the same framework was further examined in Barbaro and Bagajewicz (2004a).

Within the area of SCM, and from an enterprise-wide perspective, Applequist et al. (2000) recognized that the simple optimization of expected returns could lead to riskier solutions, and introduced the concept of *risk premium* as a measure of risk for an investment relative to alternative financial investments in a SC.

2.5 Commercial packages

A growing number of advanced planning and scheduling systems (APS) are available for the industry to support decision making for operational applications. The first commercial packages appeared in the late 1980s, and focused generally on finite-capacity shop floor scheduling problems solved using simulation-based techniques (Sadowski, 1998). A boost in APS systems occurred in the 1990s as an extension of materials requirements planning (MRP), enterprise resource planning (ERP), and manufacturing execution systems (MES). From then on, and promoted by the advances in information technology, numerous applications with improved computational and optimization capabilities have been developed, which have significantly reduced the burden of implementation and enhanced return of investment (ROI).

Sadowski (1998) estimated APS systems revenues above $3 billion anually by the year 2000. According to a recent study reported by Advanced Process Combinatorics, Inc. (Pekny, 2005), an effective planning and scheduling system leads to a decrease in process costs, as well as to an increase in process throughout, implying an improvement about 5 % to 15 %.

However, the application of computer-aided decision-support systems for operational analysis appears quite limited in the industrial practice. Several factors were highlighted by Honkomp et al. (2000) as obstacles for a successful computerization of scheduling systems. Firstly, standard software tools are pursued, easy of use, and flexible for customization; however, and as suggested by Sand and Engell (2004), planning and scheduling operations can hardly be standardized due to the complex and highly plant specific interactions involved. Secondly, assumptions are made to avoid the formulation of complex large-size models, which may eventually lead to operation infeasibilities. In addition, external consultants for model development are usually required due to the lack of internal expertise, thus leading to maintenance costs beyond the original software cost. The integration capabilities with other applications (ERP, MES, forecasting) has also been identified by companies as a critical factor.

Furthermore, the inability of much scheduling systems to address the general issue of uncertainty is also cited as a major reason for the lack of influence of scheduling research in industrial practice (Aytug et al., 2005). This idea was also emphasized by McKay and Wiers (1999), who suggested that assumptions underlying scheduling research activities were inadequate for real world scheduling, and a change of principles was claimed to avoid the gap between theory and practice; otherwise, *"academia will continue to model and solve nonexistent problems, and practitioners will continue to move around in the dark"*. Besides, uncertainty was presented as the essential concept to understand and formalize the problem in the scheduling domain.

In spite of these claims, most commercial APS packages available rely on deterministic modeling systems. As suggested by Shapiro (2004), managers have only recently been exposed to deterministic optimization models, whereas their extension to stochastic programming is still restricted to academic research.

The problem of the uncertainty is, therefore, so far not well solved in commercial software. Most tools claim to provide real-time scheduling capabilities and *what if* scenario analysis. In general, they are able to generate updated schedules as disruptions occur, and use interactive Gantt charts which allow to drag and drop operations for manual rescheduling; however, the incorporation of robustness issues within the reasoning procedure is not considered at all.

Generally, commercial APS systems differ in philosophy, user interface and technology. For planning models, mathematical programming formulations become more and more the state-of-the-art in the chemical, food and pharmaceutical industry, as well as in refineries; instead, the majority of scheduling packages are still based on pure heuristics (Kallrath, 2002). Some simple systems are designed around an electronic and interactive Gantt chart that supports the users for deciding the appropriate allocation and sequencing of activities based on their knowledge of the process. More sophisticated systems incorporate analysis tools and handle process constraints such as storage policies, labor patterns, maintenance periods, and sequence-dependent changeovers.

Commercial APS systems built on mathematical modeling approaches are OSS Scheduler[1], VirtECS^{TM} Scheduler[2], ProSched[3], and ILOG Scheduler[4]. Other pack-

[1] OSS Scheduler, from Process Systems Enterprise Ltd., <www.psenterprise.com>, [29 May 2005]

[2] VirtECS^{TM} Scheduler, from Advanced Process Combinatorics Inc., <www.combination.com>, [Jan. 2006]

[3] ProSched, from Ingenious Inc., <www.ingenous.cc>, [6 Mar. 2006]

[4] ILOG Scheduler, from ILOG Inc., <www.ilog.com>, [6 Mar. 2006]

ages to be worth mentioning include PREACTOR[5], SchedulePro®[6], and ASPROVA[7]. A survey of APS software was provided by Elliott (2000).

Several corporations offer also APS systems as modular components of an integrated decision-support suite of applications for SCM, covering from strategic to operational planning functionalities. For example, infor:Scheduling, from Infor Business Solutions[8], supports planning, programming and optimization for small and medium industrial companies; Aspen Plant Scheduler™ is the application for short-term scheduling of the Aspen SCM™ suite of solutions[9]; SAP® SCM solution uses the application SAP® Advanced Planner and Optimizer (SAP® APO)[10], with its Production Planning and Detailed Scheduling (PP/DS) module; i2 Master Scheduling, i2 Production Scheduler, and i2 Sequencing are tools provided by i2 Technologies[11]; Oracle Manufacturing Scheduling and JD Edwards Production Scheduling modules are distributed by Oracle corporation[12]. Other companies providing scheduling solutions within their SC suite of solutions are Manugistics[13], TXT e-solutions[14], and Intentia[15].

Applications of such tools have been reported in the literature of PSE. For example, the commercial system AspenMIMI™ (now Aspen SCM™) from AspenTech was applied by Berning et al. (2004) as a collaborative planning platform to address the integrated planning and scheduling problem in a multi-site environment with interdependent multipurpose production plants; the system provided the means for transparency, collaboration, information sharing, and conflict management, and was customized to allow manual interaction. The VirtECS™ scheduling software was used by Jung et al. (2004) to solve the scheduling subproblems embedded in a simulation-based optimization framework proposed for SCM under demand uncertainty.

Besides the broad offer of commercial software available for SCM, there are generic packages for risk analysis to support the resolution of optimization problems under uncertainty. RISKOptimizer is a simulation optimization add-in for Microsoft Excel® that combines the Monte Carlo simulation technology of @Risk, a risk analysis add-in from Palisade[16], and the genetic algorithm optimization technology of Evolver™ to allow the optimization of Excel spreadsheet models containing uncertain data. The uncertainty is modeled using probability distributions from @RISK, and RISKOptimizer runs an optimization of simulations to find the best combination of parameters that optimizes some defined statistic function. Similarly, Risk Solver Engine[17], from Frontline Systems Inc., provides interactive Monte Carlo simulation models to support probability management in Microsoft Excel®.

[5] Preactor, from Preactor International, <www.preactor.com>, [22 Dec. 2005]
[6] SchedulePro, from Intelligen, <www.intelligen.com>, [6 Mar. 2006]
[7] ASPROVA, from Asprova corporation, <www.asprova.com>, [6 Mar. 2006]
[8] infor:Scheduling, from Infor Business Solutions, <www.inforiberica.biz>, [27 Feb. 2006]
[9] Aspen Plant Scheduler™, from AspenTech, <www.aspentech.com>, [27 Feb. 2006]
[10] SAP® APO, from SAP, <www.sap.com>, [27 Feb. 2006]
[11] i2 Technologies, <www.i2.com>, [27 Feb. 2006]
[12] Oracle and JD Edwards scheduling, from Oracle corporation, <www.oracle.com>, [27 Feb. 2006]
[13] Manugistics, <www.manugistics.com>, [27 Feb. 2006]
[14] TXT e-solutions, <www.txtgroup.com>, [27 Feb. 2006]
[15] Intentia, <www.intentia.com>, [27 Feb. 2006]
[16] @Risk, from Palisade, <www.palisade-europe.com>, [27 Feb. 2006]
[17] Risk Solver Engine, from Frontline Systems Inc., <www.solver.com>, [19 Apr. 2006]

2.6 Concluding remarks

Uncertainty is a general and somehow ambiguous term that can be defined and managed from different perspectives. The concept of uncertainty in the context of PSE has been initially presented, and a new taxonomy of different sources of uncertainty identified in PSE based on the strategic, tactical, and operational levels of decision making has been proposed, and is used as a reference throughout the thesis.

General techniques for the representation of the uncertainty in the area of PSE have been reviewed, along with different measures used in decision making to assess the performance of the system in uncertain environments. Stochastic and robust optimization methodologies have been further analyzed as powerful techniques for optimization under uncertainty, and several contributions reported in the field have been remarked.

A final analysis of commercial APS systems available for industrial practices reveals the lack of concern on uncertainty issues from a proactive perspective.

The state-of-the-art presented in this chapter addresses the first two questions formulated in Section 1.5, and establishes the basis for the analysis and discussion of the current situation and prospective research, which are examined in Chapter 3.

3.

Present and prospective analysis

> Why is it that such a vast amount of research is being conducted and financial and intellectual resources being wasted generating useless solutions to unrealistic problems?
>
> S.F. Hurley (Hurley, 1996)

This chapter discusses the main limitations and challenges that are inferred from the state-of-the-art survey in decision making under uncertainty, thus leading to the definition of the specific objectives pursued in this thesis. The basis of the formalism for schedule robustness used in this research work is then established; the sources of uncertainty considered are assessed in terms of disturbances, effects, consequences, and reactive actions implied; and the advantages and shortcomings of the modeling methodologies applied in the dissertation are finally discussed. All this analysis provides the common features of the overall research presented in the forthcoming chapters.

3.1 Scheduling under uncertainty: limitations and challenges

The progress on information technologies provides the means for a continuous improvement on the management and communication of all data available in a company, as well as for the development of modeling systems to support decision making. Successful and appealing results have been achieved so far, but limitations and challenges to be further considered are identified.

I. Significant research has been undertaken for the formulation and solution of reliable scheduling models. However, the possibility to analyze the problem from multiple points of view, with different assumptions, as well as the uncertain and dynamic operation environment, make difficult the **definition of a general modeling and solution methodology** to deal with all the features of the problem. In addition, numerous proactive operational approaches developed to deal with uncertainties have primarily been studied in a *machine scheduling* environment, thus omitting the properties of chemical processes such as tightly integrated equipment, simultaneous transfer operations, limited storage, unstable intermediate products, and limited recover abilities.

II. The **computational requirements** become a critical factor for the application of proactive models to solve practical problems with a large number of uncertain parameters. Large-scale optimization models are frequently obtained. As stated by Sahinidis (2004), the capability of simulation and optimization methods under uncertainty is still limited to fairly small problems due to the huge computational expense. Particularly, stochastic models can become computationally very expensive either because of the need to apply complex integration techniques when the uncertainty is represented by continuous distributions, or because of the large number of **scenarios** resulting from a discrete or scenario-based representation of the uncertainty. As it was observed in the previous chapter (see Section 2.3.5), expectations are usually approximated by the sum of performances in different scenarios, where each scenario or sample is just one possible set of realizations of the uncertain problem data. The number of scenarios taken determines the accuracy of the estimates of the actual performance and standard deviation, and their selection becomes a critical problem.

III. The concept of *schedule robustness* is generally used referred to the ability of a schedule to deal with stochastic events occurring at execution time and remain acceptable (minimum performance deterioration), without assuming rescheduling strategies beyond a simple right-shift of the altered operations. It has slightly been distinguished from the notion of flexibility, i.e., a *flexible schedule* denotes a responsive schedule, easy to be adapted to the environment. According to Honkomp et al. (2000), the challenge is to identify the optimum way to introduce slack time in a predictive schedule in order to increase robustness and extend forecasting capability, without sacrificing performance.

Though several formal definitions have been proposed, the attempts to generalize the concepts have not succeeded. Davenport and Beck (2000) identified the lack of agreement on a **formalism for schedule robustness** with the fact that there is no formal definition able to fit the multiple ways in which robustness can be defined for particular systems. In general, any system that hopes to address robustness in scheduling will have to allow a specific definition of robustness in different situations to which it is applied.

IV. The robust optimization methodology as defined by Mulvey et al. (1995) (Section 2.4) has largely been applied for design and planning analysis, but has not explicitly been extended to scheduling under uncertainty.

V. Concern on uncertainty issues is generally focused on product demands in strategic and tactical analysis. Relatively little attention is given to **operational uncertainties**, and they are commonly tackled from a reactive point of view (Section 1.4). The identification and characterization of the uncertainty from a proactive perspective impliy a knowledge of the process and its external inputs. However, sometimes only **limited information** is available and **assumptions** are made to draw a formal description.

VI. Unpredictable product **demands** in strategic and tactical studies, as well as variable **operation times** and **equipment breakdowns** in operational analysis, are the most common sources of uncertainty covered so far for their major impact on the performance of the system. However, only **one source of uncertainty** is usually considered in the models developed and simplifications are made, thus limiting their applicability in real industrial scenarios.

As pointed out by Aytug et al. (2005), it is impossible to address all sources of uncertainty explicitly, and may be even worthless since some of the events might be too improbable or minor; but an attempt has to be made in considering the most significant ones to achieve reasonable successful executions. Furthermore, it is important to keep an industrial focus to develop relevant techniques, so instead of developing exact solutions to somewhat idealized problems, research should first try to capture the problem in all its complexity and then explore rigorous or approximate solution procedures (Shah, 1998).

VII. In general, proactive modeling systems developed up to this point simply consider the stochastic value of some input parameters, whereas **disruptions** occurring at execution time as a consequence of the realization of the uncertainty, as well as the **reconfiguration procedure** to be implemented, are not explicitly addressed. An improvement in the system's performance could be eventually achieved if information about the effects of disruptions and the rescheduling strategy was modeled, thus being incorporated in the reasoning stage.

VIII. In the operational level of analysis, a production schedule is generally determined assuming an instantaneous delivery of goods, thus ignoring **transport requirements** between sites in a multi-site system. With the recent practices focused on globalization and integration of activities, transport constitutes a prominent source of uncertainty, as well as a central activity to be considered for the distribution of products (Sauer and Appelrath, 2000). The detailed production and distribution scheduling problems have extensively been analyzed. However, both problems have been dealt with primarily decoupled and independent from a supply chain (SC) environment (Chandra and Fisher, 1994) and Ertogral et al. (1998).

All the aspects mentioned above reveal that the ability to develop reliable decision-support systems for operational analysis under uncertainty is still limited, and it is recognized as one of the main challenges in the area of process operations.

In general, the *high computational requirements*, the *multiple sources of uncertainty*, and the *multiple and conflicting objectives* involved in a process system are identified as the main critical points for the agreement on a formal definition of schedule robustness, as well as for the development of standard and efficient modeling techniques taking into account all the features of the problem.

3.2 Objectives

Although the main concern nowadays seems focused on the area of enterprise management, robustness and flexibility of individual entities are essential to improve the efficiency of the overall sustem. The points discussed in the previous section pose the basis of this research work. The general objective can be stated as:

> *The development of a general decision-support framework for operational analysis of process systems under uncertainty, which exploits their flexibility and takes advantage of some knowledge of the uncertainty proactively (at decision time) to determine efficient and robust predictive schedules.*

This objective implies the development of modeling and resolution strategies taking into account the critical points highlighted in the previous discussion. Stochastic optimization (Section 2.3) has been selected as the basic modeling system for the underlying research. The stochastic domain, despite its current limitations, constitutes a practical platform to incorporate the uncertainty in a decision-making process. As also recognized in Shapiro (2000), a stochastic model provides the means to assess the performance of a system under several scenarios before they occur, thus denoting the need to identify and incorporate prospective options for different types of situations.

The objective pursued involves the consideration of the following issues:

a. Study of different sources of uncertainty and their effects both in terms of risk and opportunities.

b. Evaluation of some measures of robustness used mainly in tactical and strategic analysis in the context of scheduling under uncertainty. Proposal of a formalism for schedule robustness.

c. Consideration of the eventual effects of the uncertainty revealed at execution time in the decision-making procedure.

d. Extension of the methodology from production to distribution scheduling in a multi-site system, with the aim to assess the flexibility and improve the interoperability between different nodes sites a SC.

e. Analysis of equation-based and procedure-oriented approaches.

f. Assessment of different sampling techniques to incorporate the information about the uncertainty efficiently.

This thesis focuses mainly on the modeling viewpoint of the problem, rather than on the development of efficient solution algorithms. By analyzing different sources of uncertainty (a.), a better insight and guidance on the performance of the system is pursued. The following three points (b., c. and d.) are addressed to establish a general formalism of robustness, a proper definition of the problem, as well as to develop practical modeling systems for operational analysis under uncertainty. The last two issues (e. and f.) aim at the study and consideration of computational aspects in the development of the strategies. However, this is a critical aspect that deserves an own and more extensive analysis, which is out of the scope of this research work.

3.3 Research overview and prospective remarks

The points developed for achieving the objective pursued in this research answer the question formulated initially in Section 1.5, that is: *"How can schedule robustness be improved? What are the benefits?"*. In order to provide a global view of the common features addressed in the following chapters, the concept of schedule robustness used as well as the disturbances and modeling systems examined are next outlined as a whole.

3.3.1 Schedule robustness

The notion of *schedule robustness* defined in Section 3.1 (III.) is considered in all the contributions of this thesis as the main objective function to be improved.

A general formalism of the concept is stated as a trade off between the effects of uncertainty and the efficiency of the system, defined either in temporal or economical terms. Based on this formalism, quantitative measures are defined to assess the robustness of the predictive schedule; the effects of disruptions occurring at execution time as a consequence of the information about the uncertainty available at the time of reasoning are considered proactively and incorporated in the model.

3.3.2 Analysis of disturbances

As a consequence of the inherent uncertainty when deciding a predictive schedule, disruptions may appear at execution time affecting the implementation of the schedule. Disruptions may be complex, multiple in nature, and appear randomly over the span of the schedule.

In this thesis, four types of disturbances are assessed and considered proactively when addressing the scheduling problem: process time variations; machine breakdowns; travel time variations; and demand variations. For each of these perturbations, the main sources of uncertainty, effects, consequences, and reactive actions to be implemented are summarized in Table 3.1.

From the survey in Table 3.1, it is observed that the problems encountered either in production or transport scheduling due to operational uncertainties (variable operation times, resources availability, non-uniform quality of raw materials, poor performance of control systems), and often also combinations of various indeterminate reasons, lie mainly on the timing of the scheduled operations. *Wait* and/or *idle times* may be eventually generated, along with the subsequent delays, customer dissatisfaction, and/or quality problems implied.

These effects are illustrated in Figure 3.1. On the one hand, and given a predictive schedule, if the actual processing time is shorter than the scheduled one, idle times appear and subsequent equipment under-utilization and productivity losses occur (Figure 3.1 (b)). Scheduling the process using time estimates shorter than the nominal ones would keep the plant utilization high, at the expense of increased batch wait times.

On the other hand, if the actual processing time of a task is longer than the scheduled one, the time spent by batches waiting for the next unit to become available increases (Figure 3.1 (c)). Wait times may lead to unexpected delays and eventually result in quality problems for sensitive or unstable materials, which may even force the rejection of batches. This situation can also be encountered with the breakdown of an equipment unit (Figure 3.1 (d)), with the consequent increase of operational costs. Scheduling the operations with time estimates longer than the nominal ones, inserting idle time and extra resources, would eliminate the batch wait times, but at the expense of poorer plant utilization, larger cycle times, and higher inventory costs.

Therefore, from a system performance point of view, a trade off exists between high plant resources utilization, and low batch wait times. This trade off between schedule efficiency and robustness was also noticed by Herroelen and Leus (2004b).

The analysis provided reveals also the influence in operational decisions of disturbances occurred as a consequence of tactical uncertainties such as variable product demands. This point is already discussed in Section 2.1,

Some of the effects underlined here can be observed in the comprehensive example illustrated in Chapter 1 (Section 1.3).

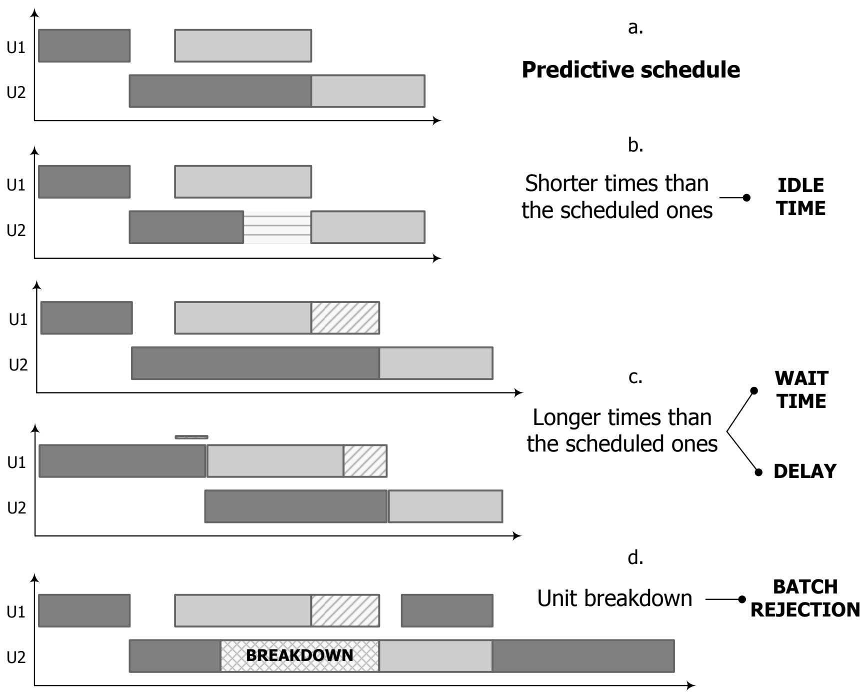


Figure 3.1: Illustration of the effects of operation times variability.

3.3.3 Modeling systems

A general classification of modeling systems is presented in Chapter 1 (Section 1.1.1). With the aim to manage the uncertainty in the reasoning procedure, rather than merely processing information, two analytical systems within the stochastic domain are contemplated throughout this research work: equation-based and procedure-oriented approaches.

Mathematical programming is considered a standard equation-based method to determine optimal schedules and assure feasibility, and allows a relatively easy modeling of particular operation modes of the production system.

Using mathematical programming, the optimality of a solution is guaranteed within reasonable CPU time for small to medium-size models with linear and convex constraints. Significant computational advances have been presented during the last few years, and more are expected in the near future. As analyzed by Advanced Process Combinatorics Inc. (Pekny, 2005), while computers increased in capability by about a factor of ten from 1990 to 1996, engineering efforts applied to scheduling and planning problems have increased the power of mathematical programming algorithms by several factors of ten; mixed-integer linear programming (MILP) technology has

Table 3.1: Survey of disturbances.

Disturbance	Uncertainty sources	Effects	Consequences	Reactive actions
Processing time variation	Operation conditions Resources availability Resources quality Yield ratios Absenteeism	Change in end times	Upstream wait times Downstream delays Idle times Quality problems Customer dissatisfaction Batch rejection	Retiming Maintenance task Schedule new batch
Machine breakdown	Resources availability Control system performance	Machine unavailable for a period	Upstream wait times Downstream delays Idle times Quality problems Customer dissatisfaction Batch rejection	Retiming Maintenance task Schedule new batch
Travel time variation	Transport conditions Resources availability Vehicle speed	Change in delivery time	Delays Customer dissatisfaction Idle times	Retiming Rerouting
Demand variation	Market demands Misjudgments Canceled orders Rush orders	Change in production requirements	Underproduction Missed sales (loss of profit, loss of market share and customer dissatisfaction) Overproduction Excessive inventory (holding costs)	Increase/reduce production Storage

been rapidly developed, whereas the area of mixed-integer non-linear programming (MINLP) is still limited to small problems.

In the context of uncertainty, the advances in stochastic programming methods are very promising. However, further research is required for the resolution of large-scale optimization models derived not only from industrial problems, but also from simple process systems. Multiple features and computational requirements additionally implied by modeling systems involving uncertainty favor the current development of procedure-oriented approaches.

Within the procedure-based methods, *simulation optimization*, defined by Fu (2001) as the optimization of performance measures based on outputs from stochastic simulations, couples both descriptive and optimization methodologies, and emerge as a promising strategy to address such problems.

A trade off usually exists between solution quality and computational effort. In this sense, it is important to consider the value of obtaining optimal solutions for a particular scenario at the expense of high computational effort, if decisions may eventually turn out infeasible due to the uncertainty.

Proactive systems for production scheduling are developed in Chapters 4 and 5 as decision-support systems to improve schedule robustness for operational uncertainties. **Stochastic programming** is considered in Chapter 4 as a first approach to cope with uncertain operation times. The unavailability of an equipment unit is further addressed in Chapter 5. This implies the simultaneous incorporation of novel scheduling features in the decision-making procedure, and a **simulation-based optimization** strategy is finally developed.

Using a similar procedure-oriented approach, the problem is extended to operational transport scheduling in Chapter 6 with the analysis of the integration of production and distribution activities, and the effect of travel times uncertainties.

The concern on uncertain product demands and their effect in the lower operational level of production scheduling is the center of interest in Chapter 7. With the same formal idea of schedule robustness, but expressed in economical terms, the ability of different measures to manage the risk of performing below a selected target is assessed.

The research overview provided above attempts to be a reference for the common characteristics of the contributions presented in the following chapters.

4.

Robust scheduling focused on operational uncertainties: First approach with uncertain operation times

The greatest loss of time is delay and expectation, which depends upon the future. We let go the present which we have in our power, and look forward to that which depends upon chance, and so relinquish a certainty for an uncertainty.

Seneca (5 BC - 65 AD)

After a retrospective and prospective survey on uncertainty in the area of Process Systems Engineering (PSE), this chapter presents the first contribution of this research aimed at identifying robust predictive schedules able to face the major effects driving the operation of batch processes with operation times variability. It is an initial attempt to formalize the short-term scheduling problem with operational uncertainties. The chapter starts with an introduction and the definition of the problem addressed. The use of *stochastic programming* as the modeling system is adopted, and a *multi-objective two-stage stochastic* formulation is first developed and next extended to explicitly manage the risk of poor performances. With this purpose, three different robustness criteria are analyzed and optimized. The effectiveness of the approach as a decision-support tool is shown and discussed through its application to academic and industrial-based examples, to finally conclude with some remarks.

4.1 Introduction

Numerous sources of uncertainty are identified with a direct effect on short-term decisions (Section 2.1). Time deviations as a consequence of processing time variations and/or machine breakdowns appear as the most common and costly effects of disruptions encountered in this stage, making difficult the prediction of exact production times and rates in industrial processes. The degree of variability is a function of the process itself, but deviations from 5 % upward of the estimated processing times are usual (Cott and Macchietto, 1989). The sources of uncertainty and effects of the disturbances caused are analyzed in Chapter 3, and wait times and idle times are identified as their critical consequences (see Section 3.3.2).

The traditional approach to minimize the effects of processing times uncertainty consists of introducing intermediate storage devices before the bottleneck processing units to maintain reserve material for downstream processing. This allows decoupling the operation of the processing units, avoiding the propagation of unexpected events, and allowing the execution of the predictive schedule without modifications. However, as exposed in the introduction of this dissertation (Section 1.4), the production of reserve material is often expensive, inefficient, and/or technically difficult to maintain, and dedicated storage units could be required for each product or intermediate with an additional cost. Furthermore, if materials leaving a processing unit are unstable, and therefore consecutive operations must be performed under a zero wait (ZW) transfer policy, intermediate storage is not a viable solution. These approaches use rough estimates or simply averages of the processing times observed in previous runs.

Relatively few works incorporate information about uncertain operation times proactively in the decision stage. Though contributions published in the literature are already reviewed in Chapter 2, some specific works are worth mentioning here.

Kouvelis and Yu (1997) described a mathematical programming framework and solution procedures for robust discrete optimization problems, and defined alternative minimax regret criteria to differentiate the robustness of various solutions over a given set of potential scenarios. Based on this framework, Daniels and Kouvelis (1995) focused on a single-machine scheduling environment with uncertain processing times represented using the scenario-based approach, and used the flow time as a performance criterion; exact branch-and-bound as well as heuristic algorithms were implemented to solve the problem. A similar proactive scheduling approach was developed in Kouvelis et al. (2000) for a two-machine flow shop environment, where the scenario-based and intervals representations of processing times were discussed, and the makespan was adopted as the performance measure.

Herrmann (1999) presented a two-space genetic algorithm as a general technique for solving robust discrete optimization problems using a minimax criterion; the algorithm was applied to identify a schedule with the minimum worst-case makespan for a parallel machine scheduling plant with uncertain processing times.

Recently, Herroelen and Leus (2004a) developed a mathematical programming model to determine robust predictive schedules in a project scheduling environment with uncertain operation times represented with discrete scenarios; the robustness measure to be minimized was defined as the expected weighted deviation of the actual from the predicted start times, when only the disruption of one operation time was anticipated; three additional heuristics related to existing algorithms were also presented and compared with the proposed model. Using the same robustness criterion in the same scheduling environment, Van de Vonder et al. (2005) developed and validated heuristic and metaheuristic procedures to allocate time buffers and generate a robust predictive schedule with acceptable makespan; the heuristic algorithms inserted the slack time in a deterministic predictive schedule with minimum makespan, keeping the assignment of resources fixed; a tabu search algorithm and an improvement heuristic were also developed to search for the best insertion of time by exploiting the neighborhood solutions.

In general, the proactive scheduling approaches proposed so far pursue the identification of predictive schedules with optimal expected performances, or schedules that guarantee a minimum performance with a certain probability. Simple production models are usually assumed (e.g., flow shop, single stage) and/or the main effects of the uncertainty are not considered in the modeling system. Therefore, critical situations that can arise during the execution of a predictive schedule due to deviations from the estimated operation times are not explicitly addressed, not even analyzed. For example, with the generation of considerable wait times the quality of sensitive or unstable materials can decrease and become even unacceptable, thus forcing the rejection of batches with the consequent increase of operating costs. Furthermore, completion times larger than those expected can lead to delays in the promised delivery dates, and hence to customer dissatisfaction.

This chapter focuses on general multipurpose multi-stage batch plants with uncertain operation times, and presents a proactive scheduling approach based on a stochastic programming formulation. The underlying idea is to improve the robustness of the predictive schedule by taking into account, in the reasoning procedure itself, wait times and idle times that may eventually occur at execution time as a consequence of the uncertainty.

4.2 Problem statement

The short-term scheduling problem is addressed for a multipurpose multi-stage batch plant with uncertain operation times. The *process-stage-operation* hierarchy defined by the standard ANSI/ISA S88 (International Soc. for Measurement and Control, 1995, 2001) is used to model the data (see Section 1.1.2). Following this standard, each order has associated a production process, i.e., a set of activities or stages required to transform the input materials into products. Furthermore, each stage involves an ordered set of operations that must be executed one immediately after another and assigned to the same equipment unit. Based on this structured information, given are the set of production orders to be fulfilled, the set of processing stages required in each order, a set of units where they can be processed, the operations required in each stage, and the processing time of each operation represented by a probability distribution.

The objective is to identify a robust predictive schedule. According to the formalism for schedule robustness proposed in Chapter 3 (Section 3.3.1), the **robustness criterion** for the underlying problem is formally defined as the expected value of a weighted combination of **makespan** and **wait times** generated during the execution of a predictive schedule. This measure balances the trade off between the need for high plant efficiency, evaluated in terms of makespan, and the low wait times, which account for the eventual effects arising due to the uncertainty. To avoid the generation of wait times is particularly important with unstable intermediate products, and when ZW transfer policies are applied. In addition, the reduction of idle times to keep reasonable plant utilization is implicitly considered with the minimization of the makespan.

Due to the uncertain operation times, there is no sense in determining detailed start and end processing times for each operation in the predictive schedule, but only the minimum information required to start the production in the plant, i.e., the sequence, the assignment of units to stages, and the initial processing time of each process or batch.

The following assumptions are made:

- From the predictive schedule, the lower control level only requires as a guidance information related to the sequence, the assignment of units to stages, and the processes start times. Then production proceeds according to the control recipe, without rescheduling considerations beyond a simple right-shift of eventual altered operations.

- The non-intermediate storage policy (NIS) between stages is assumed, that is, an intermediate product remains in the processing unit after its production until the unit assigned to the next stage is available.
- Within a stage, all the operations must be executed without interruption.
- Three sort of links are differentiated to describe temporal constraints between operations within a process: simultaneous, instant, and sequential. *Simultaneity* accounts for those operations from different stages that have to start and end at the same time. *Instant* requirements are defined between those operations that have to be produced one immediately after the other. *Sequential* links establish a relationship between the end time of an operation and the start time of another operation, i.e., they are defined between operations that have to be performed consecutively without immediacy requirements.
- To simulate the execution of a predictive schedule when operation times are uncertain, wait times are introduced at the end of a processing stage, or before a transfer operation, if the next unit is not available. To account for the generation of these wait times, sequential links are established in each process between the last operation of a stage (if it is not a transfer operation) and the first operation of the following stage, and between a transfer operation and the preceding one in the same stage.
- If an equipment unit is available before the time determined for the next batch, and idle time appears, i.e., processes cannot start before their start time in the predictive schedule (see Figure 3.1 in Section 3.3.2).
- For modeling purposes, a distinction is made between *wait times* between stages (wt^s) due to the blockage or unavailability of a unit, and *start wait times* (wt^0) due to delays on the predicted processes start times.

4.3 Modeling approach

An equation-based modeling system is considered in this study for the development of the proactive scheduling approach. Particularly, a **multi-objective two-stage stochastic programming model** is formulated to describe the features of the problem. This rigorous optimization approach is appropriate since decisions related to the production sequence, assignment, and start times of each process must be taken to start production, before the actual values of operations times are revealed, whereas the eventual effects of the uncertainty and the efficiency of the system are not disclosed until the execution of the predictive schedule. With a two-stage stochastic modeling, scenarios of possible operation times are anticipated to take into account different outcomes at the time of scheduling (refer to Section 2.3 for a review of stochastic techniques).

A *pure* stochastic formulation is first presented using the robustness criterion defined in Section 4.2 as objective function. The model is next extended to explicitly manage the risk of obtaining highly suboptimal schedule performances. Uncertainty associated with operation times is represented indistinctly by discrete or continuous probability distributions. Monte Carlo sampling is then applied over the probability space to generate a finite set of representative scenarios and approximate the expectation of the objective function (see Section 2.3.5).

4.3.1 Scheduling model

A two-stage stochastic mixed-integer linear programming (MILP) formulation is developed based on the concept of precedence relationship between stages introduced by Méndez et al. (2001), and Méndez and Cerdá (2003). Decision variables related to the production sequence, the assignment of units to stages, and the processes start times are modeled as first-stage decisions to be taken *here-and-now*, independently of the realization of the uncertainty. With the predictive schedule fixed in the first-stage, a detailed executed schedule, with the makespan and wait times generated due to deviations from the nominal operation times, is computed in a second stage and for each anticipated scenario, i.e., for each realization of processing times. As assumed (Section 4.2), the processes start times in the predictive schedule act as lower bounds in the executed schedules, i.e., the start time of each process in each scenario is constrained to be at least the start time in the predictive schedule.

Material balances, as well as features such as batch mixing and splitting, can also be contemplated in the model, but have been excluded from the scope of this research in order to focus on the problem of the uncertainty, and to avoid additional computational complexities arising from the discrete or continuous -time representation.

The model developed (SCHED1) is described next from equations 4.1 to 4.12 (the notation is related below, but refer to the Nomenclature chapter in page 153 for an overall reference). To identify a robust predictive schedule the expectation function to be minimized is written as a sum of the weighted combination of makespan (mk) and wait times (wt^s, wt^0) for each scenario k (eq. 4.1).

Equation 4.2 is a first-stage constraint that establishes the assignment of one of the alternative equipment units u to each processing stage j for every process i. The binary variable Y_{iju} is used for this purpose, which takes the value of 1 if stage j of process i is assigned to unit u, or 0 otherwise. The other variables related to decisions to be made independently of the final unveiled scenario (i.e., sequence and initial batch processing times) are derived from equations 4.3 - 4.12. These constraints (referred to as second-stage constraints) are defined for all the scenarios k to evaluate a detailed executed schedule for each instance.

(SCHED1)

$$\min \sum_k \left[\omega_k \cdot \left(\rho_1 \cdot mk_k + \rho_2 \cdot \left(\sum_i \sum_{j \in J_i} \sum_{o \in O_j} wt^s_{oik} + \sum_i wt^0_{ik} \right) \right) \right] \tag{4.1}$$

$$\sum_{u \in U_{ij}} Y_{iju} = 1 \qquad \forall i, j \in J_i \tag{4.2}$$

$$\begin{gathered} Tinr_{o'i'k} \geq Tfnr_{oik} + wt^s_{oik} - M \cdot (1 - X_{iji'j'}) - M \cdot (2 - Y_{iju} - Y_{i'j'u}) \\ \forall k, i, i', j \in J_i, j' \in J_{i'}, o \in O^l_j, o' \in O^f_{j'}, u \in (U_{ij} \cap U_{i'j'}), i < i' \end{gathered} \tag{4.3}$$

$$Tinr_{oik} \geq Tfnr_{o'i'k} + wt^{s}_{o'i'k} - M \cdot X_{iji'j'} - M \cdot (2 - Y_{iju} - Y_{i'j'u}) \qquad \forall k, i, i', j \in J_i, j' \in J_{i'}, o \in O^{f}_{j}, o' \in O^{l}_{j'}, u \in (U_{ij} \cap U_{i'j'}), i < i' \tag{4.4}$$

$$Tinr_{o'i'k} \geq Tfnr_{oik} + wt^{s}_{oik} - M \cdot (2 - Y_{iju} - Y_{i'j'u}) \qquad \forall k, i, i', j \in J_i, j' \in J_{i'}, o \in O^{l}_{j}, o' \in O^{f}_{j'}, u \in (U_{ij} \cap U_{i'j'}), i = i', j < j' \tag{4.5}$$

$$Tinr_{oik} = Tin_i + wt^{0}_{ik} \qquad \forall k, i, j \in J^{f}_{i}, o \in O^{f}_{j} \tag{4.6}$$

$$Tfnr_{oik} = Tinr_{oik} + Top_{oik} \qquad \forall k, i, j \in J_i, o \in O_j \tag{4.7}$$

$$Tinr_{oik} = Tinr_{o'ik} \qquad \forall k, i, j \in J_i, j' \in J_i, o \in O_j, o' \in O_{j'}, (o, o') \in O^{sim} \tag{4.8}$$

$$Tfnr_{oik} = Tfnr_{o'ik} \qquad \forall k, i, j \in J_i, j' \in J_i, o \in O_j, o' \in O_{j'}, (o, o') \in O^{sim} \tag{4.9}$$

$$Tfnr_{oik} = Tinr_{o'ik} \qquad \forall k, i, j \in J_i, o \in O_j, o' \in O_j, (o, o') \in O^{zw} \tag{4.10}$$

$$Tfnr_{oik} + wt^{s}_{oik} = Tinr_{o'ik} \qquad \forall k, i, j \in J_i, j' \in J_i, o \in O_j, o' \in O_{j'}, (o, o') \in O^{seq} \tag{4.11}$$

$$mk_k \geq Tfnr_{oik} \qquad \forall k, i, j \in J^{l}_{i}, o \in O^{l}_{j} \tag{4.12}$$

Constraints 4.3 - 4.5 are sequencing constraints that express the completion time of the last operation o of a stage j from process i in scenario k ($Tfnr_{oik}$) as a lower bound for the start time of the first operation o' of any later stage j' from process i' ($Tinr_{o'i'k}$) assigned to the same unit u. The binary variable $X_{iji'j'}$ is used to define the production sequence; it takes the value of 1 if stage j of process i is processed before stage j' of processi' in some unit u, or 0 otherwise. Equation 4.5 is imposed only for those stages j and j' from a same process i that are processed in the same unit u; since their sequence is already established by the recipe, the sequencing variable always takes the value of 1. These sequencing constraints become redundant whenever the production stages j and j' are not allocated to the same unit u.

The start time of a process i in the predictive schedule (Tin_i) is determined with constraint 4.6, which expresses the delay of process i in scenario k (wt^{0}_{ik}) as the difference between its actual start time in that scenario ($Tinr_{oik}$), and the predicted one decided in the first stage. Equation 4.7 relates the start and end times of the operations o of each process i for each scenario k through the actual operation time in the scenario (Top_{oik}).

Simultaneous requirements in process i between operation o in stage j and operation o' in stage j' are defined through constraints 4.8 and 4.9. Equation 4.10 establishes the instant links between operations o and o' in the same stage j of process i that must be performed one immediately after the other (O^{zw}). For those operations o and o' of process i that have to be processed sequentially (O^{seq}), without immediacy requirements, constraint 4.11 is provided; through this constraint, wait times generated in process i and in scenario k after processing operation o (wt^s_{oik}) are computed. Finally, the makespan of the executed schedule in scenario k (mk_k) is defined in equation 4.12.

4.3.2 Robust scheduling model

The formalism of robustness used in the previous stochastic model is based on the expected value of makespan and wait times over the set of anticipated scenarios. To avoid the identification of predictive schedules with highly suboptimal performances in some of the scenarios, criteria based on the worst-case scenario, and defined by Kouvelis and Yu (1997) in general terms as *absolute robustness*, *robust deviation* and *relative robustness* criteria, are assessed and optimized.

The **absolute robustness** criterion (Z_{AR}) is a *minimax* criterion that attempts to determine the predictive schedule with simply the best of the worst performance over all the scenarios. The **robust deviation** (Z_{DR}) and **relative robustness** (Z_{RR}) criteria are concerned with how the actual system performance compares with the optimal performance that could have been achieved if certain information about the scenario realization had been available at scheduling time. These criteria are known as *minimax regret* criteria, where regret is defined as the difference or the ratio, respectively, between the performance of the executed schedule and the performance of the optimal predictive schedule that would have been attained if the scenario had been known at decision time. Therefore, these criteria allow, respectively, the identification of the schedule with the best worst-case deviation or the best worst-case percentage deviation from optimality over all the scenarios.

For the problem under consideration, and based on the concept of schedule robustness used so far in terms of makespan accounting for the efficiency of the system and wait times measuring the effects of the uncertainty, the worst-case scenario implies the scenario with a maximum combination of makespan and wait times. Therefore, given a predictive schedule, the absolute robustness measure is formally defined as the maximum sum of makespan and wait times over all the anticipated scenarios, expressed according to equation 4.13. Similarly, the robust deviation and the relative robustness criteria are formalized as the maximum difference or ratio, respectively, over all the scenarios between the makespan and wait times generated in the realized scenario, and the makespan and wait times of the optimal schedule to be executed if the scenario had already been known at decision time (OF^*_k). These criteria are formalized as stated in equations 4.14 and 4.15, respectively.

$$Z_{AR} = \max_k \left\{ \rho_1 \cdot mk_k + \rho_2 \cdot \left(\sum_i \sum_{j \in J_i} \sum_{o \in O_j} wt^s_{oik} + \sum_i wt^0_{ik} \right) \right\} \tag{4.13}$$

$$Z_{DR} = \max_k \left\{ \left(\rho_1 \cdot mk_k + \rho_2 \cdot \left(\sum_i \sum_{j \in J_i} \sum_{o \in O_j} wt^s_{oik} + \sum_i wt^0_{ik} \right) \right) - OF^*_k \right\} \quad (4.14)$$

$$Z_{RR} = \max_k \left\{ \left(\rho_1 \cdot mk_k + \rho_2 \cdot \left(\sum_i \sum_{j \in J_i} \sum_{o \in O_j} wt^s_{oik} + \sum_i wt^0_{ik} \right) \right) / OF^*_k \right\} \quad (4.15)$$

Note that both robust deviation and relative criteria require the computation of the optimal performance in each scenario sampled (OF^*_k), and hence a deterministic problem for each realization of processing times is to be solved. This deterministic model derives simply from the stochastic model developed in Section 4.3.1 (SCHED1) considering only one scenario with the corresponding operation times. It is worth noting that when the actual scenario is already known at the time of scheduling, no delays in the processes start times are expected during the execution of the schedule. Therefore, only the wait times between stages arising from the application of the NIS policy are considered in the wait times term of the objective function, and constraint 4.6 is excluded.

The minimum absolute robustness Z^{min}_{AR}, robust deviation $Z^{min}_{textrmDR}$ and relative robustness $Z^{min}_{textrmRR}$ values can be evaluated by solving the SCHED1 model, but minimizing one of the alternate measures (eqs. 4.13 - 4.15) instead of equation 4.1. For modeling environments such as GAMS (Brooke et al., 1988) that do not support *minimax* functions, the definition of these metrics is handled by inequality constraints.

It is important to notice that the associated scenario probabilities are not used with these formulations. Besides, a predictive schedule with a minimum *worst-case* is identified, but some degree of flexibility to fix the temporal decisions exists in the second stage for the evaluation of those executed schedules that show a lower performance than the worst-case. Therefore, to be able to compute the proper executed schedules in the second stage of the solution algorithm, model SCHED1 is extended with the incorporation of two additional constraints: the worst-case formalism in terms of absolute robustness (eq. 4.13), robust deviation (eq. 4.14), or relative robustness (eq. 4.15); and the upper bound constraint 4.16, 4.17 or 4.18, respectively. A robust predictive schedule is then determined, with a maximum expected combination of makespan and wait times (eq. 4.1), and a minimum worst-case defined in terms of absolute robustness, robust deviation, or relative robustness.

This new model (SCHED2) can be regarded as a *robust optimization* approach (see Section 2.4) with preference for risk-averse decisions. Note that the stochastic model SCHED1 is extended with the incorporation of the absolute robustness, the robust deviation, or the relative robustness as a measure of the risk of obtaining highly poor performances.

(SCHED2)

min (eq. 4.1)

subject to

eqs. 4.2 - 4.12

eq. 4.13, 4.14 or 4.15

eq. 4.16, 4.17 or 4.18

$$Z_{\mathrm{AR}} \leq Z_{\mathrm{AR}}^{min} \tag{4.16}$$

$$Z_{\mathrm{DR}} \leq Z_{\mathrm{DR}}^{min} \tag{4.17}$$

$$Z_{\mathrm{RR}} \leq Z_{\mathrm{RR}}^{min} \tag{4.18}$$

The criterion to be applied is up to the decision-maker concern about risk. The absolute robustness criterion tends to lead to conservative decisions, since it attempts to hedge against the worst possible outcome. On the other hand, robust deviation and relative robustness criteria tend to be less conservative when making a decision, and also look at uncertainty as an opportunity to be exploited rather than just as a risk to be hedged against. The deviation from optimality can be used as an indicator of the improvements that can be achieved if part or all of the uncertainty can be resolved (Kouvelis and Yu, 1997).

4.4 Case Studies

The methodology developed to handle the operation times uncertainty proactively has been applied to an academic and an industrial-based case studies. The first case is the motivating example introduced in Chapter 1 (Section 1.3) involving a five-product three-stage flow shop plant. The industrial-based example consists of the scheduling of a washing subprocess of a more complex single-product production process; four orders have been considered for this problem. Both examples are described in appendices B.1 and B.4, respectively.

The multi-objective two-stage stochastic model (SCHED1) is first solved, and Pareto curves are then obtained by parametrically varying the weight values of both criteria (makespan and wait times) in the objective function. With fixed and selected weight values, the deterministic problem is also solved for comparison purposes, and to assess the suitability of the stochastic modeling system (as indicated previously, the deterministic model derives directly from the stochastic one considering only one scenario with the nominal operation times, and excluding constraint 4.6). The deterministic predictive schedule thus obtained is then evaluated in front of the set of scenarios, i.e., the production sequence, the assignment, and the processes start times in the predictive schedule are fixed, and the makespan and wait time values of the executed schedule in each scenario are computed. The extension of the model to the robust optimization approach (model SCHED2) is finally analyzed with the alternate measures of risk defined in terms of absolute robustness, robust deviation, and relative robustness.

For both examples, a set of 100 scenarios with equal probability is considered and derived from the probability distributions of processing times using Monte Carlo sampling. The models have been implemented in GAMS (Brooke et al., 1988), and solved using the MILP solver of CPLEX(7.5) on a AMD Athlon 2000 computer. Computational times about 150 s CPU time for the first example, and about 2000 s CPU time for the second case study, are required. Model sizes and computational requirements for the *pure* stochastic formulations (SCHED1) of both examples are reported in Table 4.1; the computational results provide an idea of the complexity of the model; nevertheless, note that the main purpose is to suggest a strategy for managing uncertainty in the operation level, rather than to develop the most efficient solution algorithm.

Table 4.1: Model sizes and computational requirements.

	Flow shop (section 4.5.1)	Washing subprocess (section 4.5.2)
Constraints	9536	28449
Binary variables	45	96
Continuous variables	11106	24505
OF	116.2	428.4
CPU time*	144.5	1820.6

*seconds with GAMS 20.5/CPLEX(7.5), on a AMD Athlon 2000 computer.

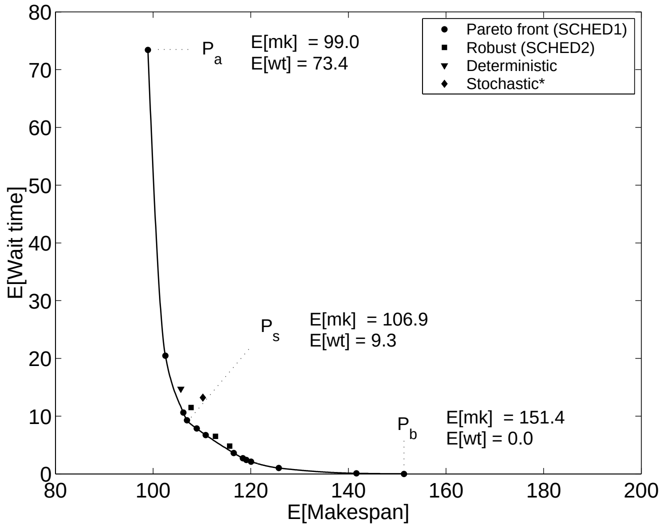
4.5 Results and discussion

Wait times between stages (wt^s_{oik}) and start wait times (wt^0_{ik}) have been distinguished for modeling purposes. However, and for the sake of clarity, the notation wt is used in the remaining of the chapter referred to the wait times as a whole.

4.5.1 Motivating example

The Pareto curve between the expected wait time and makespan values obtained with the resolution of model SCHED1 is depicted in Figure 4.1. Each Pareto point identifies a predictive schedule with different preferences for wait times and plant utilization. Solutions obtained using the three alternative control measures (model SCHED2) with weight values fixed at 1 for the makespan and wait times are also illustrated, along with the results obtained from the evaluation of the deterministic predictive schedule and the schedule with minimum expected makespan obtained by Balasubramanian and Grossmann (2002). If the minimum makespan is pursued, the predictive schedule identified by the Pareto point $\mathrm{P_a}$ ($\rho_1 = 1, \rho_2 = 0$) would be implemented; otherwise, if wait times have to be avoided, the predictive schedule determined by the Pareto point $\mathrm{P_b}$ ($\rho_1 = 0, \rho_2 = 1$) would be executed, which guarantees null expected wait times over the set of selected scenarios at the expense of poor plant utilization.

The predictive schedule obtained by fixing the weight values for the makespan and the wait time measures at 1 (Pareto point $\mathrm{P_s}$) balances both objectives. According to



* Point resulting from the evaluation of the schedule with optimum expected makespan identified in Balasubramanian and Grossmann (2002) ($\rho_1 = 1, \rho_2 = 1$).

Figure 4.1: Pareto curve between the expected wait times and expected makespan values for example 4.5.1 ($\mathrm{P_s} : \rho_1 = 1, \rho_2 = 1$; $\mathrm{P_a} : \rho_1 = 1, \rho_2 = 0$; $\mathrm{P_b} : \rho_1 = 0, \rho_2 = 1$).

this solution, the Gantt charts of the schedules executed in the nominal scenario and in one of the randomly-generated scenarios are represented in Figure 4.2 (the operation times for the random scenario are reported in Appendix B.1, Table B.7). Note that decisions related to the production sequence (A-C-E-B-D), the assignment of units to stages (fixed for this flow shop plant example in u1-u2-u3), and the processes start times (0-8-20-39-44 TU) are solved in a first stage and therefore, they are fixed and independent of the scenario unveiled.

Table 4.2 reports and compares the results obtained related to the expected sum of makespan and wait times ($\mathrm{E}[mk + wt]$), expected makespan ($\mathrm{E}[mk]$), expected wait times ($\mathrm{E}[wt]$), the processes start times (Tin_i), the absolute robustness (Z_{AR}), the robust deviation (Z_{RD}), and the relative robustness (Z_{RR}) values for the predictive schedules determined with the different modeling systems. The makespan and wait time values of the executed schedule in the nominal scenario according to each predictive schedule are also included (mk_{nom} and wt_{nom} in the table).

It is important to note from Table 4.2 that the decisions made using the deterministic formulation with nominal processing times poorly face the uncertainty, and overestimate the performance of the system. Although the makespan and wait time values of the predictive schedule thus obtained are optimal in the nominal scenario, when the deterministic decisions are used to face the uncertainty, i.e., an executed schedule is assessed in each scenario, the expected makespan raises nearly 5 % from the optimum one (from 101 to 105.7 TU), and the generation of significant wait times is expected (14.7 TU). On the other hand, the stochastic modeling with weight values fixed at 1 for both criteria in the objective function ($\mathrm{ST_{P_s}}$) allows the identification

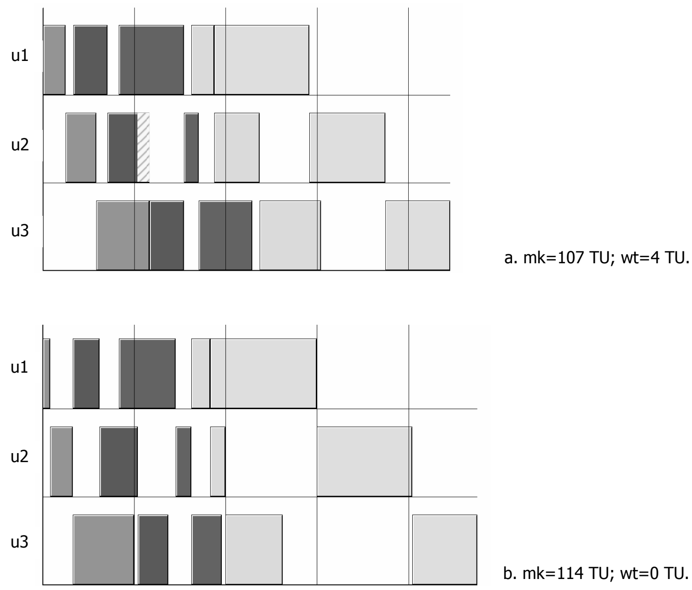


Figure 4.2: Gantt charts of executed schedules for case study 4.5.1 according to the predictive schedule determined with model SCHED1 in the : a) nominal scenario; b) random scenario (Table B.7) (Production sequence: A-C-E-B-D; assignment: u1-u2-u3; processes start times: 0-8-20-39-44 TU).

of a predictive schedule with expected wait times reduced nearly 37 % (from 14.7 to 9.3 TU), and with acceptable expected makespan (106.9 TU).

Using the robust optimization approach with the *minimax* criteria, alternative predictive schedules are identified with reduced risk of poor performances, while still maintaining improved robustness with respect to the deterministic approach. Using the absolute robustness measure (AR), for example, a predictive schedule is determined with a worst-case performance reduced by 14 % (from 152.0 to 131.6 TU), and with an expected wait time value about 56 % lower with respect to the deterministic schedule (6.5 vs. 14.7 TU). The reduction in expected wait times is even higher with the predictive schedule identified considering the relative robustness metric (nearly 67 %), despite the increase in the expected makespan and the poor performance in the nominal scenario.

The suitability of the proactive scheduling approach developed in this first contribution can be further supported considering the comprehensive analysis presented in Section 1.3. The predictive schedules determined using deterministic models for the nominal and the random scenarios show poorer robustness features than the predictive schedule identified with the proactive approach. Note the suboptimal performance of the *deterministic* predictive schedules when they are executed in a different scenario. For example, using the predictive schedule identified for the nominal scenario (Figure 1.4 (a)), the executed schedule in the random scenario has a makespan of 104 TU, and 19 TU of wait times are generated (Figure 1.4 (b)). With the robust predictive schedule, the makespan of the executed schedule in the random scenario increases up to

Table 4.2: Results for case study 4.5.1 with different modeling approaches: Deterministic (DET); SCHED1 (ST); SCHED2 with absolute robustness (AR); SCHED2 with robust deviation (DR); SCHED2 with relative robustness (RR).

	DET	ST_{P_s}*	AR	DR	RR	ST_{P_a}*	ST_{P_b}*	ST†
$E[mk+wt]$	120.4	**116.2**	119.3	119.2	120.5	166.0	153.0	123.4
$E[mk]$	105.7	106.9	112.8	107.8	115.7	**99.0**	151.4	110.2
$E[wt]$	14.7	9.3	6.5	11.5	4.8	73.4	**0.0**	13.2
mk_{nom}	**101.0**	107.0	111.3	107.0	115.8	99.0	153.0	105.0
wt_{nom}	**0.0**	4.0	1.0	6.5	0.8	67.0	0.0	0.0
Tin_A	0.0	0.0	0.0	0.0	0.0	0.0	0.0	68.0
Tin_B	10.0	39.0	30.2	30.0	47.8	2.0	119.0	0.0
Tin_C	75.0	8.0	85.3	75.5	28.7	29.0	92.0	79.0
Tin_D	16.0	44.0	35.2	35.0	53.0	8.0	34.0	6.0
Tin_E	57.0	20.0	8.8	8.0	9.3	41.0	15.0	47.0
Z_{AR}	152.0	135.0	**131.6**	142.5	138.1	‡.	‡.	165.0
Z_{DR}	45.0	38.0	43.5	**32.5**	35.1	‡.	‡.	60.0
Z_{RR}	0.62	0.43	0.59	0.45	**0.35**	‡.	‡.	0.57

mk_{nom}: makespan in the nominal scenario; wt_{nom}: wait times in the nominal scenario; $E[mk]$: expected makespan; $E[wt]$: expected wait times; Tin_i: processes start times; Z_{AR}: absolute robustness; Z_{DR}: robust deviation; Z_{RR}: relative robustness.

*$P_s : \rho_1 = 1, \rho_2 = 1$; $P_a : \rho_1 = 1, \rho_2 = 0$; $P_b : \rho_1 = 0, \rho_2 = 1$.

†Results obtained from the evaluation of the predictive schedule with optimum expected makespan identified in Balasubramanian and Grossmann (2002) (different assumptions are taken, see text).

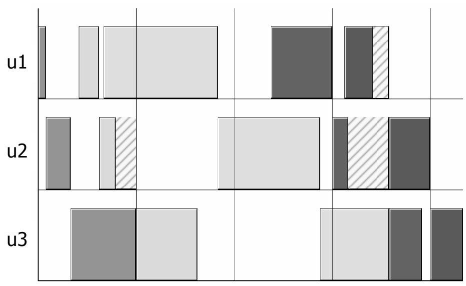
‡Values not given for being not comparable since different weight values are used.

114 TU (Figure 4.2 (b)), but any wait times are expected; in terms of the robustness criterion used (mk+wt), the value decreases from 123 to 114 TU with the proactive approach developed. A similar behavior occurs when comparing the robust predictive schedule with the predictive schedule identified for the random scenario (Figure 1.4 (c)). Whereas the execution of the robust schedule leads to an executed schedule in the nominal scenario with 107 TU of makespan and 4 TU of wait times (Figure 4.2 (a)), the *deterministic* schedule performs with a makespan of 114 TU, and 14 TU of wait times are generated (Figure 1.4 (d)).

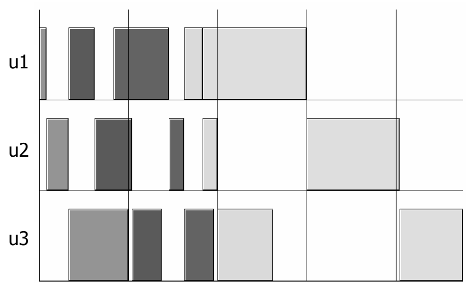
Expected makespan and wait times vs. expected makespan

The adoption of the expected makespan as the formalism for schedule robustness, without considering the effects of the uncertainty, is also analyzed. With the model developed (SCHED1), using only the makespan term in the objective function, a predictive schedule with a minimum expected makespan value of 99 TU is obtained; this is at the expense of an important increase in the expected wait times in the executed schedules (ST_{P_a} results in Table 4.2). Notice that this predictive schedule differs from the one identified in the contribution by Balasubramanian and Grossmann (2002) with optimum expected makespan. In this sense, it is important to mention that their work did not consider the NIS policy but the ZW one, thus leading to a higher expected makespan value (106.1 TU instead of 99 TU). Moreover, the processes start times were not taken into account when evaluating the schedule in different scenarios, i.e., they were not fixed but adjusted for each scenario to follow the ZW policy. This is not always feasible in a real procedure; generally, an increase in the operation times can not be detected prior to execution, so the production of a batch starts according to the start time in the predictive schedule (if possible), before knowing if the processing times of the stages in the preceding batch deviate from the nominal ones. Therefore, the ZW policy can not be followed at all, and unavoidable wait times are generated (refer to Figure 3.1 in Chapter 3 for illustrative purposes).

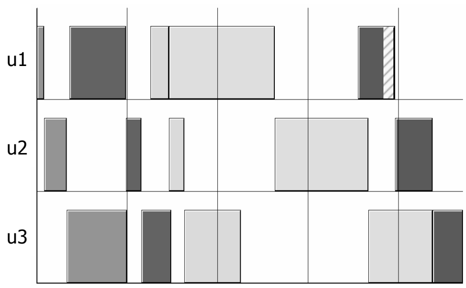
Despite both approaches can not be compared directly, it is interesting to analyze them to remark the usefulness of considering the start times in the predictive schedule for developing more realistic modeling approaches and for reducing the generation of wait times. With this purpose, the predictive schedule identified by Balasubramanian and Grossmann (2002) is fixed and evaluated in front of the different scenarios with the assumptions considered in this research work (see Section 4.2). The results are appended in the last column of Table 4.2. As it can be observed, the predictive schedule neglects the wait and idle times that can be generated during its execution. Considerable expected wait times appear (13.2 TU), and the expected makespan increases about 4 % with respect to the optimum expected makespan value reported (110.2 vs. 106.1 TU). Note that both the expected wait time and makespan values are about 42 % and 3 % higher, respectively, than those obtained by executing the predictive



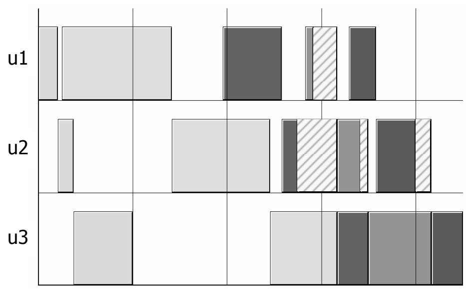
a. mk: 104 TU; wt: 19 TU.



b. mk: 114 TU; wt: 0 TU.



c. mk: 113.8 TU; wt: 2.8 TU.



d. mk: 108 TU; wt: 22 TU.

Figure 4.3: Gantt charts of executed schedules in a random scenario (Table B.7) for case study 4.5.1, following predictive schedules determined using different modeling approaches: (a) deterministic; (b) SCHED1; (c) SCHED2 with absolute robustness; (d) predictive schedule with optimum expected makespan identified in Balasubramanian and Grossmann (2002).

schedule determined with the proactive scheduling approach developed in this work. Moreover, the variability of outcomes is also noteworthy as can be observed from the absolute robustness value (165.0 TU), which is about 25 % higher than the minimum one (131.6 TU).

Finally, to illustrate the role of the uncertainty in decision making, the Gantt charts of the schedules executed in the random scenario defined in Appendix B.1(Table B.7) using different predictive schedules as a guidance are represented in Figure 4.3. Note that each executed schedule has its own production sequence and minimum processes start times (see Table 4.2). Other results in terms of production efficiency would be obtained in other scenarios. The predictive schedule to be finally executed is up to the decision-maker preferences or organization policies.

4.5.2 Washing subprocess

The Pareto curve illustrating the trade off between the expected wait time and makespan values for this second case study using the SCHED1 model is shown in Figure 4.4. The points obtained evaluating the predictive schedules identified with the deterministic formulation and the SCHED2 model using the alternative robustness measures are also included (for these evaluations, the weight values ρ_1 and ρ_2 are fixed at 1).

According to the predictive schedule determined with model SCHED1, fixing the weight values of both criteria at 1, the Gantt charts of executed schedules in the nominal scenario and in one of the randomly-generated scenarios (Table B.19 in Appendix

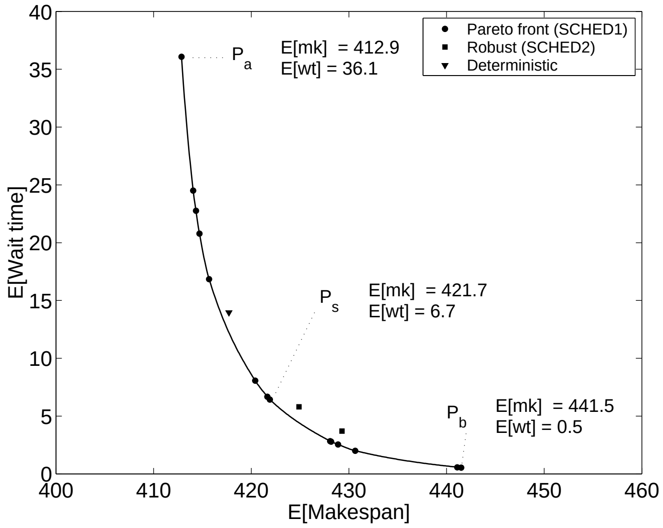


Figure 4.4: Pareto curve between the expected wait time and expected makespan values for case study 4.5.2 ($\mathrm{P_s} : \rho_1 = 1, \rho_2 = 1$; $\mathrm{P_a} : \rho_1 = 0.95, \rho_2 = 0.05$; $\mathrm{P_b} : \rho_1 = 0.06, \rho_2 = 0.94$).

B.4) are represented in Figure 4.5.

Results of the expected sum of makespan and wait times, expected makespan, expected wait times, processes start times (Tin_i), absolute robustness (Z_{AR}), robust deviation (Z_{RD}), and relative robustness values (Z_{RR}) for the predictive schedules determined with different modeling approaches are reported in Table 4.3. The makespan and wait time values that would be attained following the alternative predictive schedules in the nominal scenario are also included. It is worthwhile to note that for this particular example, and except for the case when only the minimization of the expected makespan is pursued ($\mathrm{ST}_{\mathrm{P_a}}$), the schedule executed in the nominal scenario proceeds without the generation of wait times for any of the predictive schedules determined.

As it is also underlined in case study 4.5.1, the predictive schedules determined with the stochastic models developed (SCHED1 and SCHED2) perform better over the uncertain space than the predictive schedules based on nominal values (DET). Observe in Table 4.3 that the predictive schedule identified with the stochastic approach (SCHED1), and weight values fixed at $\rho_1 = \rho_2 = 1$ for both criteria in the objective function, leads to expected wait times reduced 52 % (from 14.0 to 6.7 TU), and to an acceptable expected makespan (1 % increase) compared with the schedule based on deterministic operation times (DET). Furthermore, a predictive schedule

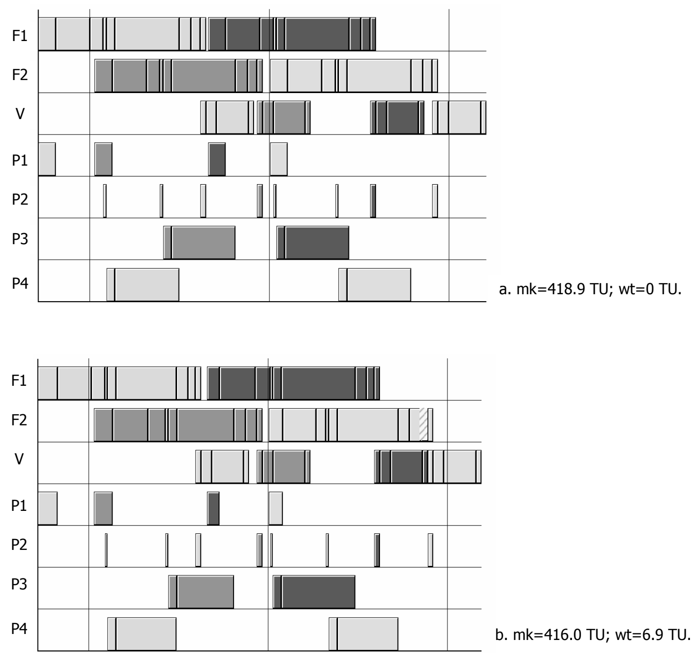


Figure 4.5: Gantt charts of executed schedules for case study 4.5.2 according to the predictive schedule determined with model SCHED1 in the: a) nominal scenario; b) random scenario (Table B.19) (Production sequence / assignment / process start time: 1 / F1-V-P1-P2-P4 / 0 TU; 2 / F2-V-P1-P2-P3 / 52.9 TU; 3 / F1-V-P1-P2-P3 / 158.9 TU; 4 / F2-V-P1-P2-P4 / 216.9 TU).

Table 4.3: Results for the washing subprocess case study with different modeling approaches: Deterministic (DET); SCHED1 (ST); SCHED2 with absolute robustness (AR); SCHED2 with robust deviation (DR); SCHED2 with relative robustness (RR).

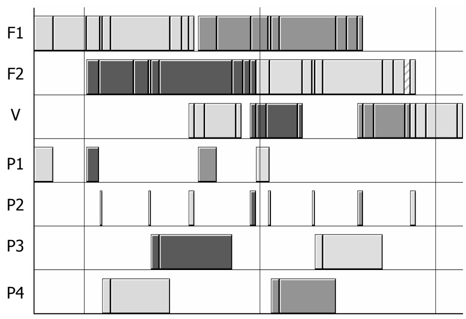
	DET	$\mathrm{ST}_{\mathrm{P_s}}{}^*$	AR	DR	RR	$\mathrm{ST}_{\mathrm{P_a}}{}^*$	$\mathrm{ST}_{\mathrm{P_b}}{}^*$
$\mathrm{E}[mk + wt]$	431.7	**428.4**	433.0	430.7	430.7	449.0	442.14
$\mathrm{E}[mk]$	417.7	421.7	429.3	424.9	424.9	**412.9**	441.6
$\mathrm{E}[wt]$	14.0	6.7	3.7	5.8	5.8	36.1	**0.54**
mk_{nom}	**409.3**	418.9	426.1	422.1	422.1	409.3	441.3
wt_{nom}	0.0	0.0	0.0	0.0	0.0	35.2	0.0
Tin_1	157.0	52.9	58.6	164.9	165.0	197.6	239.3
Tin_2	0.0	0.0	170.5	220.1	220.1	0.0	174.0
Tin_3	50.3	158.9	224.1	59.4	59.4	34.8	65.0
Tin_4	207.3	216.9	0.0	0.0	0.0	147.0	0.0
Z_{AR}	475.9	486.4	**449.1**	460.2	460.0	†.	†.
Z_{DR}	76.3	72.7	57.0	**43.9**	44.1	†.	†.
Z_{RR}	0.19	0.18	0.15	0.11	**0.11**	†.	†.

mk_{nom}: makespan in the nominal scenario; wt_{nom}: wait time in the nominal scenario; $\mathrm{E}[mk]$: expected makespan; $\mathrm{E}[wt]$: expected wait time; Tin_i: orders start times; Z_{AR}: absolute robustness; Z_{DR}: robust deviation; Z_{RR}: relative robustness.

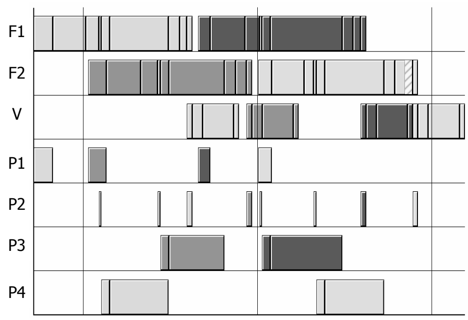
*$\mathrm{P_s}: \rho_1 = 1, \rho_2 = 1$; $\mathrm{P_a}: \rho_1 = 0.95, \rho_2 = 0.05$; $\mathrm{P_b}: \rho_1 = 0.06, \rho_2 = 0.94$.
†Values not given for being not comparable since different weight values are used.

with a relatively small increase in the expected makespan and expected wait times reduced 74 % (from 14.0 to 3.7 TU) is identified using model SCHED2 with the absolute robustness criterion.

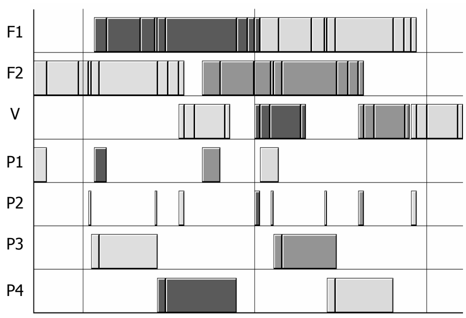
Finally, schedules executed according to alternate predictive schedules in the particular scenario defined in Table B.19 (Appendix B.4) are represented in Figure 4.6. Note again the different production sequences, assignments of units to tasks, and processes start times of each schedule. The suitability in terms of production efficiencies depends on the final revealed scenario. Therefore, first-stage decisions concerning the information to be released to the control system imply a trade off to be solved by the decision maker according to the risk acceptability policy.



a. mk: 410.1 TU; wt: 10.5 TU.



b. mk: 416.9 TU; wt: 6.9 TU.



c. mk: 419.6 TU; wt: 1.2 TU.

Figure 4.6: Gantt charts of executed schedules in a random scenario (Table B.19) for case study 4.5.2, according to predictive schedules determined using different modeling approaches: (a) deterministic; (b) SCHED1; (c) SCHED2 with robust deviation.

4.6 Concluding remarks

The variable and unpredictable operation times appear as one of the most common sources of operational uncertainty, which has usually been faced through reactive scheduling mechanisms without taking into account any information available at the time of reasoning. Instead, a proactive scheduling approach is developed in this study to account for this uncertainty in general multipurpose multi-stage batch plants, considering in the decision stage itself the main consequences driving the execution process.

The proactive approach consists of an optimization model based on a multi-objective two-stage stochastic formulation. The notion of *schedule robustness* is formalized as the expected weighted combination of makespan and wait times, thus accounting for the efficiency of the system and for the eventual effects of the uncertainty, respectively. More robust predictive schedules are identified, with significantly reduced expected wait times and acceptable line occupation.

The use of the expected makespan as the formalism for schedule robustness is also assessed by evaluating the predictive schedule thus derived. The analysis shows that ignoring the eventual effects arising at execution time is not realistic, and leads to a significant increase in the expected wait times and/or plant under-utilization.

Additionally, criteria based on the concepts of absolute, robust deviation and relative robustness are also analyzed and used as control measures to manage the risk of poor performances. This robust optimization approach imposes the worst-case value of these measures as an upper bound, i.e., the predictive schedule determined will perform with a sum of makespan and wait times lower than the worst-case in all the scenarios. The method could be further extended by incorporating these metrics in the objective function, along with the expected criterion, and analyzing the trade off between them. Alternative robust predictive schedules are obtained.

The study presented in this chapter is a first approach aimed at the formalization of the scheduling problem with operational uncertainties, addressing explicitly and proactively the major disruptions occurring at execution time. The results obtained highlight the importance of managing the uncertainty, as well as its consequences in decision making to perform effectively in an uncertain environment. However, a single source of uncertainty has been considered up to this point, and further research is required to improve the performance of stochastic programming models for applications of industrial size and complexity.

5.

Robust scheduling focused on operational uncertainties: Proactive incorporation of rescheduling strategies

> It is change, continuing change, inevitable change, that is the dominant factor in society today. No sensible decision can be made any longer without taking into account not only the world as it is, but the world as it will be.
>
> Isaac Asimov

A first proactive approach for scheduling with operational uncertainties has been developed so far, and different measures for schedule robustness have been assessed. Useful insight on the performance of the system with variable operation times has been obtained, as well as promising strategies to deal with this source of uncertainty. In this chapter, the goal is to step forward in the modeling and resolution of the problem by taking into account, proactively, uncertainty in the availability of equipment units, along with information regarding the rescheduling procedure to be implemented at execution time.

A *simulation-based optimization* strategy is developed as a proactive approach to cope with the new features of the problem, and to identify a robust predictive schedule with the flexibility to absorb disruptive events without major consequences when rescheduling. After an introduction and definition of the problem, the modules of the system (*optimizer*, *stochastic modeler*, and *scheduling model*) are described. The approach is tested in three different case studies, and overall remarks are finally summarized.

5.1 Introduction

Process time variations and machine breakdowns are identified as the most common disturbances occurring due to the uncertainty in an operational level of analysis, with a direct impact on predicted time activities. This is also remarked in the previous chapter (see Section 4.1), and their effects are analyzed in Chapter 3 (see Section 3.3.2). As discussed elsewhere (Section 3.1), it is difficult, if not impossible, to cope with all sources of uncertainty proactively, and may be even worthless for the improbability of some events. However, it is important to exploit some knowledge of the uncertainty available at the time of scheduling, as it is also deduced from the studies presented in the preceding chapter.

Most of the contributions reported in the literature of production scheduling to deal with the eventual effects of variable operation times and breakdowns address the problem from a reactive point of view (reactive approaches are introduced in Section 1.4). In general, rescheduling systems based on a predictive schedule aim at generating feasible updated schedules relatively quickly, while minimizing deviations from the predictive plan. A reference work in this field is that of Cott and Macchietto (1989), where an algorithm for on-line schedule modification was proposed to deal with processing time and batch size variations; the algorithm detected the deviations between the target and the predictive schedule at short intervals, and shifted the operations without sequence modifications. Kanakamedala et al. (1994) described an heuristic strategy for reactive schedule modification of multipurpose plant schedules subject to processing time deviations and unit unavailabilities, based on the selection of the solution with a minimum impact on the rest of the schedule. Numerous works have been published from then on. See for example the works of Vin and Ierapetritou (2000); Méndez and Cerdá (2004); and the review by Aytug et al. (2005).

Some other contributions analyze the effects of the sources of uncertainty on predictive schedules based on a Monte Carlo simulation framework. For example, Mignon et al. (1995) defined schedule robustness as the standard deviation of a profit-based function weighted by the absolute value of the deterministic objective to assess the robustness of schedules obtained from deterministic methods when they were executed in the presence of uncertainty. Basset et al. (1997) considered the uncertainty in processing times and equipment availability to define and assess operating policies related to production lead times, maintenance protocols, and inventory profiles.

These latter procedures provide insight on the actual performance of a predictive schedule, though any knowledge of the uncertainty is explicitly used in the decision stage of the simulation algorithm in order to generate schedules which can better handle the uncertainties.

Relatively few works have been reported in the literature incorporating the uncertainties proactively. Refer to Section 4.1 for a survey of contributions considering uncertain operations times, and to Chapter 2 for a general review.

In addition, several studies have been reported in a *machine scheduling* environment based on robustness measures that manage the incorporation of slack time into the schedule, and consider the right-shifting rescheduling policy after a breakdown. In this line, Leon et al. (1994) developed and evaluated robustness measures, formalized as a linear combination of expected makespan and expected delay, to address job shop scheduling with machine breakdowns or processing time variations; the problem was modeled using graph theory, and a genetic algorithm was presented for its resolution. Within the same scheduling environment, Mehta and Uzsoy (1998) focused on the minimization of the expected job completion time deviations; the problem was modeled using a disjunctive graph representation, and two heuristics were proposed to insert slack time based on the production sequence of an initial schedule determined by minimizing the maximum lateness.

A similar approach was proposed by O'Donovan et al. (1999) for a single-machine environment with stochastic breakdowns; heuristic and rescheduling approaches were proposed using the total tardiness as a performance measure. Davenport et al. (2001) examined three different slack-based heuristic techniques in a job shop scheduling environment with machine breakdowns; the problem was first solved to optimality using the summed tardiness as a performance measure; the execution of the schedule thus obtained was then simulated under uncertainty to evaluate robustness in terms of the mean simulated tardiness, or the mean absolute difference between the predicted and the simulated tardiness.

In a series of contributions by Jensen (Jensen, 2001, 2003), different measures were considered to examine robustness and flexibility of job shop schedules subject to machine breakdowns, and the minimization of lateness instead of tardiness was proposed as a way to increase the slack of the schedules; alternative rescheduling methods were analyzed, and genetic algorithms were implemented as a solution approach. In general, the results obtained revealed that no single best method existed to address all problem instances, but the performance of the robust scheduling methods was highly dependent on the problem size, the rescheduling strategy, and the machine downtime.

In the area of Process Systems Engineering (PSE), Sanmartí et al. (1996) proposed a method combining the generation of robust schedules with reactive procedures for scheduling multipurpose batch chemical plants under equipment failure uncertainty; schedule robustness was quantified using a reliability index; the schedule with minimum makespan was initially generated, and then used in an evolutionary algorithm to determine schedules with higher reliability while maintaining the makespan below the time horizon; the schedule with the best combination of high reliability/low makespan was finally identified by simulating a set of random equipment failures and analyzing the efficiency of rescheduling procedures in terms of deviation of completion times and number of reassignments.

Later, Honkomp et al. (1999) presented a simulation-based optimization framework, which coupled an optimizer based on nominal process data with a Monte Carlo simulator, to assess and compare strategies for generating robust schedules, as well as rescheduling techniques when processing times and equipment availability were uncertain.

In a multiproduct batch scheduling environment, Lee and Malone (2001a,b) proposed a strategy based on a combination of Monte Carlo simulation and simulated annealing (SA) to determine a predictive schedule with an optimal degree of flexibility, defined as the amount of free time inserted into a schedule to be adapted to future changes; the expected profit was to be maximized, and tactical and operational uncertainties were considered; a reactive schedule adaptation algorithm was applied based on local search techniques that used the incorporated flexibility to respond to changes during the execution time.

In general, most proactive scheduling approaches proposed so far assume simple flow shop or single-stage production processes, and deal with a single source of uncertainty. Multiple sources of uncertainty have been considered with simplifying considerations, and mainly using simulation-based optimization techniques due to the multiple features and high computational requirements implied. In addition, the effects of disruptions occurring at execution time are hardly addressed, and breakdowns are assumed to occur just before the start time of a batch, so batch rejection is avoided, and simple reassignments and/or resequencing strategies are implemented.

Chapter 4 focuses on short-term scheduling with uncertain processing times, and a first formalization of the problem in the stochastic programming domain is developed. However, the need to reduce the gap between theory and the industrial practices claims for a more realistic view of the problem. In this sense, this chapter considers the equipment availability as a source of uncertainty along with the processing times. In addition, not only a set of anticipated scenarios for the uncertain parameters is used in the decision stage, but also information concerning the reactive scheduling approach to be taken during schedule execution. A robust predictive schedule is pursued, with the flexibility to incorporate disruptive events arising at execution time with minimum effect on planned activities, while achieving an acceptable performance.

5.2 Problem statement

The short-term scheduling problem is considered in a general multipurpose multi-stage batch plant with uncertainty in the form of variable processing times and equipment availability. The input data defined for the approach developed in the previous chapter (Section 4.2) is required. In addition, information related to the expected breakdown time and breakdown duration for each fallible equipment unit is also specified in terms of probability distributions obtained using statistics from historical data.

A robust predictive schedule is again pursued. To balance the trade off between schedule efficiency and the eventual effects arising because of the uncertainty, the **robustness** formalism defined in the previous chapter (Section 4.2) as the expected weighted combination of the **makespan** and **wait times** resulting from the execution of a predictive schedule is also adopted.

Several **reactive scheduling** techniques can be assumed to adjust a predictive schedule in front of a disruptive event and compute its actual performance. This study focuses on the extreme strategies of *right-shifting* and *complete rescheduling*. Right-shifting consists of a simple move forward in time of all the operations altered by a disruption, without introducing sequencing or assignment changes. Contrary, complete rescheduling involves the possible resequencing of batches and/or reassignment of units for those stages not yet executed.

The same assumptions considered in the previous chapter (see Section 4.2) apply in this study. It is worth remembering:

- A detailed predictive schedule is not required, but only information to be released to the control system and related to the production sequence, the assignment of units to stages, and the processes start times.
- The non-intermediate storage (NIS) policy between stages is assumed.
- Two different sources of wait times generated during execution are assessed: wait times between stages due to the blockage or unavailability of a unit; and wait times due to deviations from the predicted processes start times.
- During schedule execution, wait times are introduced at the end of a processing stage, or before a transfer operation, if the next unit is not available. Moreover, processes cannot be started before their start time in the predictive schedule.

In addition, the following issues are assumed:

- Only one equipment unit is subject to failure. The unavailability of more than one unit could also be contemplated taking into account that the effect of a breakdown depends on the outcome of the preceding ones. However, it has been excluded from the scope of this research work to focus on the problem of the uncertainty itself, and to avoid additional modeling and computational complexities.

- Any batch can be processed in the broken unit during a disruption; if breakdown occurs during the production of an operation, the complete batch is rejected and it must be restarted from the beginning.

5.3 Modeling approach

The use of mathematical programming to capture all the features of the underlying problem implies the formulation of a complex stochastic mixed-integer model. To avoid major simplifying assumptions and to reduce computational requirements, a **simulation-based stochastic optimization framework** is developed as the proactive scheduling approach incorporating the new modeling features of the problem.

Research on simulation-based optimization is very large, not only in production scheduling, but particularly in tactical and strategic analysis, as well as in other research directions within PSE. For example, Subramanian et al. (2001) addressed the pipeline management problem and presented SIMOPT, an architecture that combined mathematical programming and discrete event simulation to assess the effect of uncertainty and support decision making. The SIMOPT architecture was further discussed by Pekny (2002) for decision making in general process management applications involving combinatorics, uncertainty, and risk management.

In the context of supply chain management (SCM) with uncertain product demands, Jung et al. (2004) developed a simulation-based optimization approach to determine safety stock levels and achieve a customer satisfaction level with minimum expected value of the cost of supply chain (SC); the strategy involved an outer optimization on the safety stock levels, which minimized the weighted sum of deviations from the target customer satisfaction levels, and an inner problem comprising repeated simulations, each with a given Monte Carlo sample of the demands and a series of imbedded planning and scheduling subproblems solved in a rolling horizon scheme. For another application of simulation-based optimization in SCM, as well as a review in the area, refer to Mele (2006).

The simulation-based optimization framework developed in this research comprises three interdependent modules (an optimizer, a stochastic modeler, and a scheduling model), and involves two recursive loops (Figure 5.1).

The outer optimization loop directs the search for alternative predictive schedules with improved schedule robustness, i.e., better expected sum of makespan and wait times. From this loop, the scheduling model and the stochastic modeler are viewed as a *blackbox* that returns a performance measure (expected sum of makespan and wait times value) as output, given a set of decision variables (sequence, assignment, and initial batch times) as input. The optimizer uses this performance measure to adjust the decision variables and improve the objective.

The inner sampling loop manages the stochastic features of the problem. In the stochastic modeler module, uncertainty associated with operation times, equipment breakdown times, and breakdown durations is represented indistinctly by discrete or continuous probability distributions. The *scenario-based representation* of the uncertainty is adopted, and a set of probable scenarios is anticipated by sampling over the probability distributions of the uncertain parameters. Each scenario specifies a value

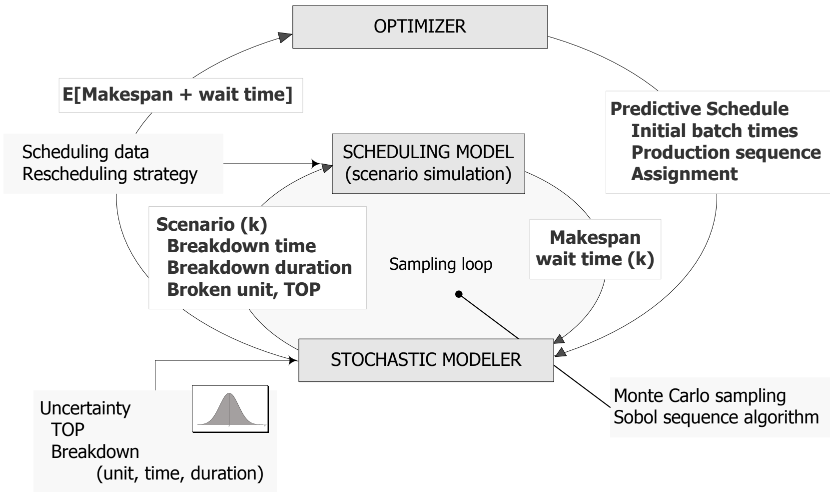


Figure 5.1: Stochastic modeling framework.

for the breakdown time, a breakdown duration, the broken unit, and the operation times.

Given an scenario generated by the stochastic modeler, the rescheduling strategy to be followed in front of disruptions, and implementing the decisions (sequence, assignment, and initial batch times) derived from the outer optimization loop, the scheduling model simulates the execution of the predictive schedule and computes the makespan and wait times generated; this step is repeated for each of the scenarios sampled. After all the simulation runs, the robustness performance (expected sum of makespan and wait times) is evaluated and returned to the optimizer.

The procedure proceeds iteratively until decision variables converge to their optimal values, or some other stopping criterion is satisfied. The framework has been implemented in C++ using the Borland C++Builder 6.0 programming environment.

5.3.1 Optimizer

Different procedures, either rigorous or heuristic-based, can be implemented for optimization purposes within the stochastic framework. As already discussed, the representation of the problem with equations and inequalities would lead to a complex stochastic mathematical model with high computational requirements. Instead, heuristic-based procedures are developed in this research.

Meta-heuristics, and genetic algorithms (GAs) in particular, have proved suitable for solving deterministic scheduling problems with relatively small computational effort. Several applications have been reported in the manufacturing industry, although few publications exist in the process industry (Wang et al., 2000; Graells et al., 2000; Björkqvist, 2005). Some other works rely on simulated annealing (SA) algorithms to efficiently optimize a probabilistic objective function. Kim and Diwekar (2002) focused on improving the efficiency of a SA-based stochastic algorithm by using the more uniform Hammersley sequence sampling (HSS) technique (see Section 2.3.5, both in the inner sampling and in the outer optimization loops. The application of GAs to scheduling under uncertainty is very limited, but they can easily be adapted to the requirements of an stochastic formulation Leon et al. (1994) and Sevaux and Sörensen (2004).

Stochastic Genetic Algorithm (stochGA)

An stochastic GA (stochGA) has been designed and implemented as optimization procedure in the outer loop of the modeling framework to search for more robust predictive schedules. The Galib C++ library (Wall, 1996) is used with customized chromosome classes. The algorithm proceeds following the common steps of a GA (Goldberg, 1989), but incorporates an embedded inner sampling loop to evaluate the probabilistic objective function (Figure 5.2). A number of generations is specified as a termination criterion, and a *linear scaling* function is used, along with the *roulette wheel selection* scheme to choose the chromosomes from a population for mating. Additional parameters to be defined involve the population size, the overlapping percentage, the crossover and mutation probabilities, and the crossover method.

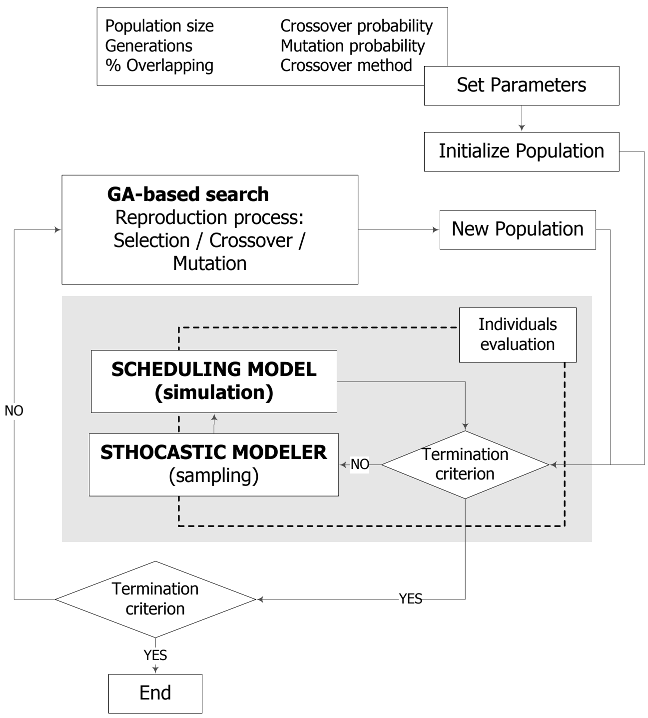


Figure 5.2: Stochastic GA-based search procedure.

Representation

The representation of a solution is one of the important issues of a search algorithm. For the problem under consideration, each chromosome or individual of the population of solutions identifies a predictive schedule, and hence it consists of both continuous times and discrete sequence and assignment decision variables. To avoid the generation of infeasible solutions, each individual is encoded using a mixed representation involving the following strings (refer to Figure 5.3 for illustrative purposes):

a. A *real-valued* vector for the processing times, where each item of the string identifies the minimum start processing time of the batch assigned to the position of the item.

b. A *permutation* of integer values for the sequencing decisions; each item corresponds to a batch, and denotes its position in the production sequence.

c. An *integer* representation for the assignment; items from this array match the stages in the batches, and identify the alternative unit assigned to that stage.

To illustrate this encoding consider the example represented in Figure 5.3. According to this representation, the second batch identified in the list of batches will be executed in the fourth position of the production sequence, starting at least at time point 22. Moreover, it consists of two stages: the first stage will run on its second alternative unit, whereas the second stage will be processed in the first one.

From the operators involved in a GA, initialization, mutation, and crossover are explicitly customized. Suitable procedures are implemented for each string of the solution vector, and are reported in the following sections. For a detailed description of these and other available operators refer to Baeck et al. (1997).

Initialization

The initialization procedure implemented to generate the first population of solutions uses a feasible initial predictive schedule, determined with the scheduling module described in Section 5.3.3 below, using nominal values for the processing times, and assuming no breakdowns. The sequence, assignment, and start times from this predictive schedule define the first individual of the population; the other solutions derive from these initial variables introducing random exchanges of positions in the sequence, random assignments of the alternative units, and taking the start processing times of the batches from a temporization of a schedule with the new random sequence and assignment decisions, and using nominal operation times.

Mutation

The mutation operator pursues the introduction of new solutions, as well as the modification of the existing ones.

The *deviation-based mutation* (Baeck et al., 1997) is implemented as operator for the string of real values. Based on this operator, each item of the string is modified by generating at random a number between upper and lower bounds determined as a predefined deviation from the current value.

In the integer permutation vector of a chromosome, a *reciprocal exchange mutation* (Baeck et al., 1997) is used. This operator selects two positions of the permutation array randomly, and then swaps the values in these positions.

Mutation in the integer string is performed by selecting randomly one stage of each batch, and changing also randomly the integer value among the number of alternative units available for that stage.

Crossover

The crossover operator defines the procedure for generating a new solution from two parent solutions. Unlike mutation, it involves multiple chromosomes.

Two alternative operators are implemented for the real-valued encoding: *intermediate recombination* and *line recombination* (Chipperfield et al., 1994). Both operators generate the new real-valued vectors based on the rule stated in equation 5.1. The intermediate recombination operator uses a factor f different for each pair of items of the parent vectors, and can generate any point within a hypercube slightly larger than that defined by the parent strings. On the other hand, line recombination uses the same value of f for each pair of parent strings combined together, and can generate any point on a slightly longer line than that defined by the parent solutions within the limits of the perturbation f.

$$Offspring = Parent_1 + f \cdot (Parent_2 - Parent_1) \tag{5.1}$$

The *partially mapped crossover (PMX)* (Baeck et al., 1997) operator is used in the integer permutation string of a solution. Based on this operator, two crossover sites selected at random in each parent string define a matching section that is directly copied to the new vectors. PMX proceeds by position-wise exchanges, where the remaining parts are taken from the other parent string.

Finally, the *single-point crossover* (Baeck et al., 1997) is applied to the integer array. This operator involves selecting an integer position of the string at random, and swapping the items of both parents from that point.

5.3.2 Stochastic modeler

The stochastic modeler acts as a central module controlling the generation and evaluation of a finite and representative set of scenarios from the probability distributions that describe the uncertain parameters in order to approximate the probability space.

The selection of the number of samples required in a stochastic optimization procedure to estimate the performance with a given accuracy is recognized as a challenging problem (Diwekar, 2003). It depends not only on the types of uncertainty distributions, but also on factors such as the sampling technique, the values of the decision variables, and the characterization of the error.

As reviewed in Chapter 2 (Section 2.3.5), different techniques can be applied for sampling, from the widely used Monte Carlo sampling (MCS) to quasi-Monte Carlo methods. Two techniques are implemented in this framework using the GNU scientific library (GSL) (Galassi et al., 2001): a **MCS** procedure, and the **Sobol sequence** algorithm, which seems to maintain good properties as the number of dimensions increases (Kocis and Whiten, 1997). The MCS technique uses the default *MT19937 generator*, and the seed is initialized as a random value between 0 and 99999. On the other hand, the generator using the *Sobol sequence algorithm* evaluates the dimension at runtime based on the number of uncertain parameters established.

The sampling procedure is described in Figure 5.4. The number of scenarios sampled (nk) is assessed at runtime in order to evaluate the actual mean μ and standard deviation σ of the performance measure with a given accuracy γ. However, a minimum number of scenarios is initially fixed (NK_0) to avoid the unnecessary

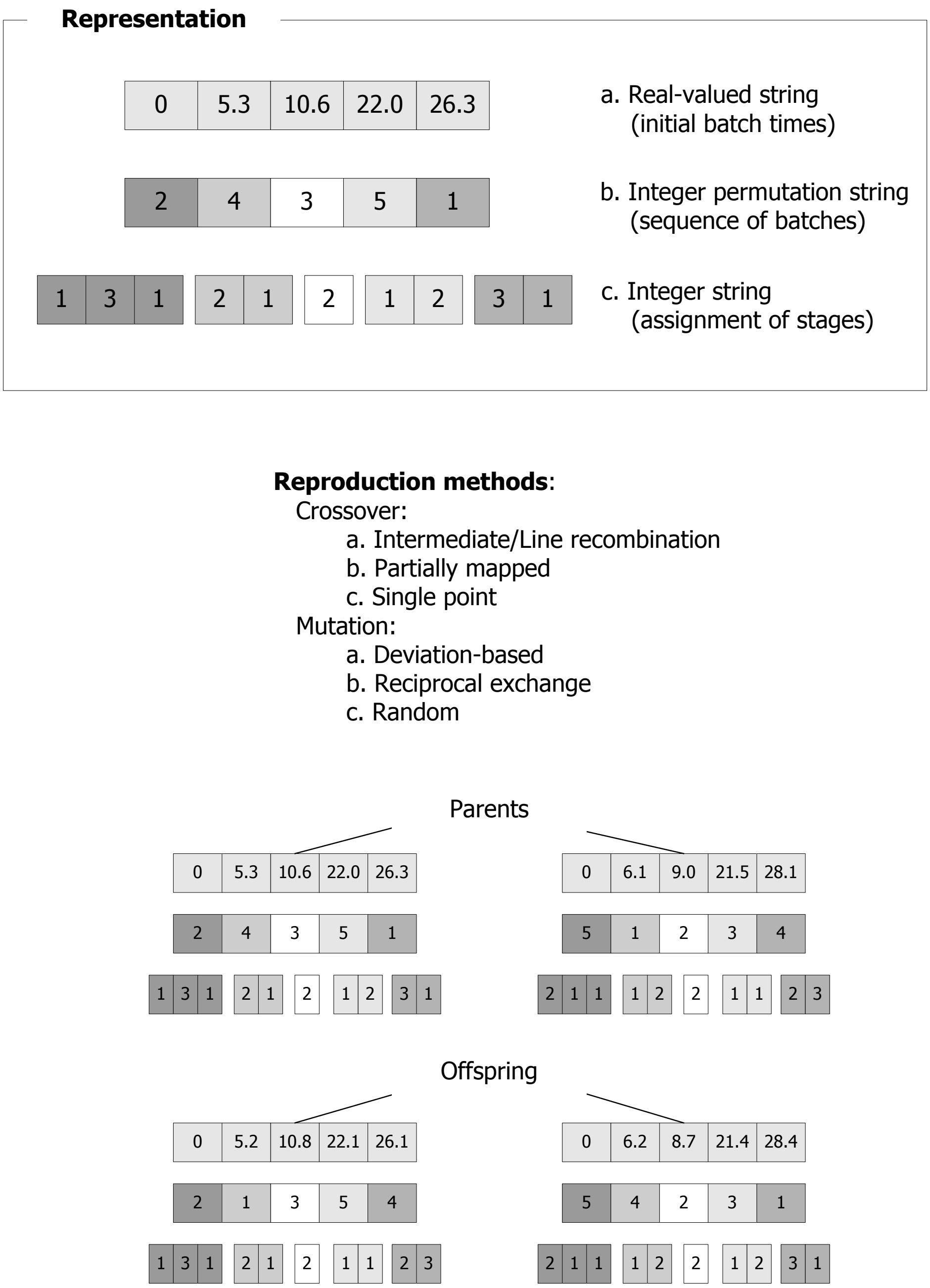


Figure 5.3: Representation of a chromosome (solution) in the stochGA.

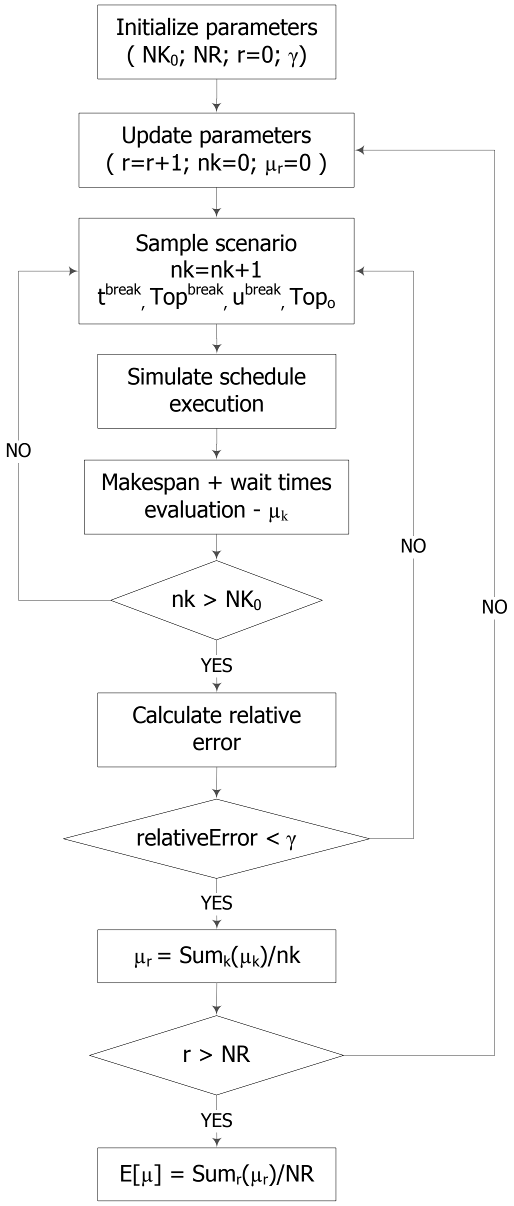


Figure 5.4: Sampling algorithm implemented in the stochastic modeler.

evaluation of the relative error during the first iterations of the algorithm, when the number of scenarios sampled is still low.

The relative error is approximated with a probability of $(1 - \alpha)$ using the half-length confidence interval $(\delta_{nk,\alpha})$ as stated in equation 5.2 (the sample average and standard deviation are computed using expressions 5.3 and 5.4) (Law and Kelton, 2000).

Using the Monte Carlo method, and due to the randomness of the uniform generator, the overall sampling procedure is repeated for a given number of replications (NR). The objective function is then approximated as the mean value of the expected performances of all the replications.

$$\gamma = t_{nk-1,1-\frac{\alpha}{2}} \cdot \frac{\sqrt{\frac{\sigma^2}{nk}}}{\overline{\mu}} = \frac{\delta_{nk,\alpha}}{\overline{\mu}} \tag{5.2}$$

$$\overline{\mu} = \frac{\sum_k \mu_k}{nk} \tag{5.3}$$

$$\sigma^2 = \frac{\sum_k (\mu_k - \overline{\mu})^2}{nk - 1} \tag{5.4}$$

Classical statistical methods make use of the central limit theorem to assume a normal distribution of the random variables. They appear to provide good estimates of the confidence interval only for truly random MCS, while tending to overestimate the bounds for other sampling techniques. Some studies were conducted by Shapiro and Homem-de-Mello (2000) concerning the convergence of Monte Carlo simulation-based approximations for a class of stochastic programming problems. However, and as stated by Diwekar (2003), there is a lack of a systematic procedure to quantify the accuracy for non-Monte Carlo techniques. Therefore, classical statistical methods are applied in the stochastic modeler module of the framework to approximate the average of the performance measure.

5.3.3 Scheduling model

The integrated support system for planning and scheduling of multipurpose batch chemical plants developed by Cantón (2003) is used for modeling the scheduling problem and simulating the execution of a predictive schedule. The system is based on heuristic procedures commonly used in commercial packages, and it has been designed in a modular way allowing the implementation of alternative heuristic or mathematical algorithms, as well as additional functionalities to solve and further optimize the problem as needed.

Given a set of product demands, rule-based algorithms establish the number of batches to be processed, the sequence, and the assignment of production stages to specific units. These algorithms are applied in combination with the Event Operation Network (EON) model proposed by Cantón (2003) to perform the timing of the operations. This temporization model takes into account complex storage and resource constraints, and it is based on a graph representation involving a network of events (time instants at which some change occurs), and operations (time intervals to be observed between start and end events).

The scheduling package serves two purposes. First, and as reported in Section 5.3.1, it allows the identification of a feasible predictive schedule, used to initialize the population of solutions in the stochGA. Secondly, it is the module used in the inner loop to simulate and evaluate the execution of a predictive schedule derived from the optimizer in each of the scenarios sampled by the stochastic modeler.

Given the predictive schedule, the rescheduling strategy to be followed, and a particular scenario (breakdown time, breakdown duration, broken unit, and operation times), the scheduling system reproduces the situation that would actually occur at execution time according to the following steps:

STEP 1. Check the status of the batches in the predictive schedule at breakdown time.

STEP 2. Fix the batches already finished or running.

STEP 3. Reject the operations not yet executed from the batch, if breakage occurs during batch production.

STEP 4. Incorporate a maintenance task in the broken unit, at breakdown time, and with an operation time equal to the breakdown duration.

STEP 5. Include a new batch in the production sequence if batch rejection occurred.

STEP 6. Reschedule the non yet executed batches. With complete rescheduling strategies, as any scheduling problem, different objective functions can be considered.

An example of the evaluation of a predictive schedule in a particular scenario is represented in Figure 5.5. The Gantt chart of the executed schedule is illustrated assuming both right-shifting and complete rescheduling strategies (Figures 5.5 (d) and (e)). Note the generation of wait times and the incorporation of a new batch, due to batch rejection, in order to meet the requested demands. Following a right-shifting policy, the sequence and assignment of the predictive schedule are preserved, and the new batch is introduced at the end of the production sequence (Figure 5.5 (d)). Instead, complete rescheduling allows sequencing and assignment changes, and hence a new schedule is determined for the non yet executed batches based on the objective function selected (Figure 5.5 (e)).

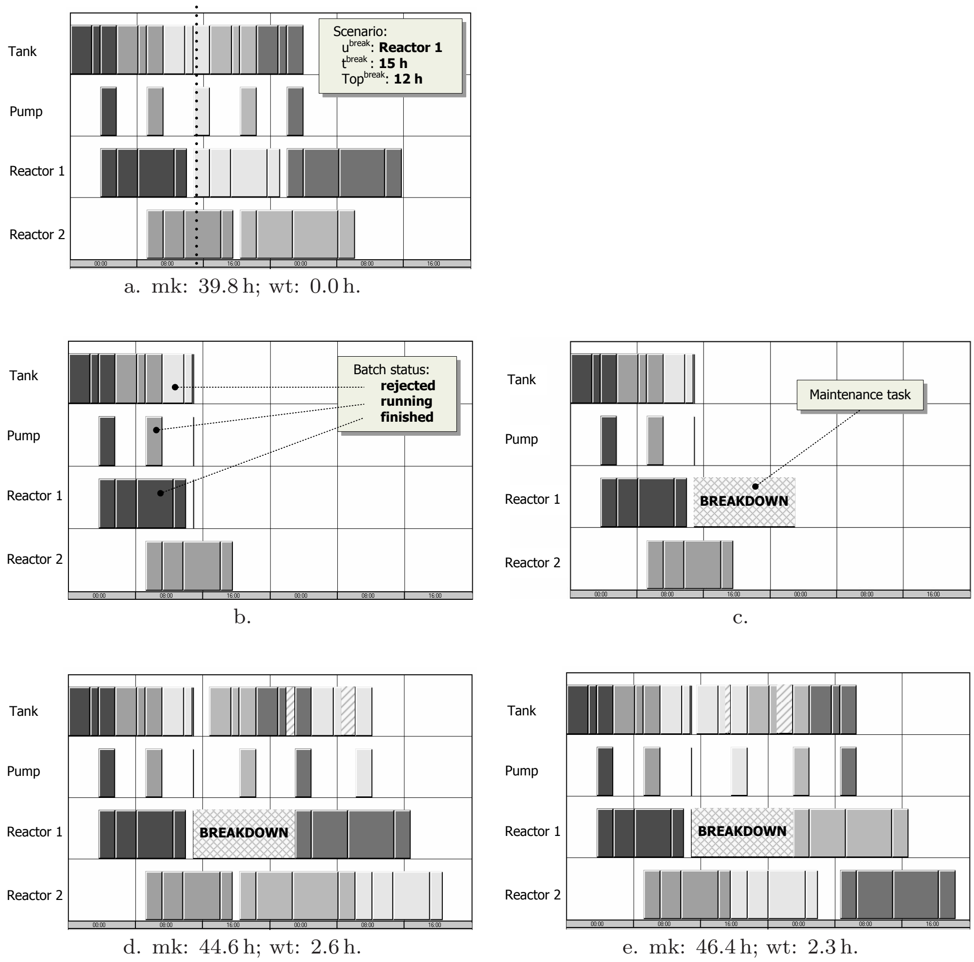


Figure 5.5: Gantt charts illustrating the simulation steps of the execution of a predictive schedule in a particular scenario: a) predictive schedule determined assuming certainty; b) status of the batches at breakdown time; c) incorporation of a maintenance task; d) executed schedule assuming right-shifting rescheduling; e) executed schedule adopting complete rescheduling.

5.4 Case studies

The simulation-based stochastic optimization framework developed for the generation of robust predictive schedules has been applied to two academic and one industrial-based case studies. The first case study is again the comprehensive example used in the thesis and described in Appendix B.1. The second example concerns a batch production facility, referred to as Procel, which involves three production stages and eight operations; it is detailed in Appendix B.3. Finally, the washing subprocess of a more complex single-product production process, analyzed also in the previous chapter (Section 4.5.2) and described in Appendix B.4, is adopted as a third case study. Except for the first example that uses a discrete distribution function to describe the uncertain processing times, variable operation times and breakdown durations are characterized with uniform probability distributions, whereas an exponential distribution function is used to represent the uncertain breakdown time.

Two particular scenarios have been distinguished. The first scenario, referred to as *faultless*, is a scenario with nominal operation times and no breakdown. Secondly, a scenario denoted as *nominal*, with mean values for the operation times and a failure occurring at the average breakdown time with a mean breakdown duration, is also considered. For comparison purposes, and to assess the suitability and robustness of the predictive schedules identified with the developed approach, the deterministic problem is also solved for the specific scenarios, and the predictive schedules thus determined are used as input to the inner sampling loop, i.e., they are evaluated in front of a set of scenarios and for the rescheduling strategies considered.

For the sampling procedure used in the stochastic modeler module, an initial number of 25 scenarios has been selected, and an accuracy γ of 0.05 approximated with a 90 % confidence interval is pursued. Concerning the sampling technique, both the Sobol sequence and MCS have been tested. Deviations of maximum 2 % are observed between the results obtained with both procedures, but the computational requirements of MCS increase considerably because of the number of replications used to account for its randomness (the evaluation of a single predictive schedule

Table 5.1: Computational requirements.

	Flow shop (section 5.5.1)	Procel (section 5.5.2)	Washing subprocess (section 5.5.3)
scenarios ; CPU time ; γ^*			
right-shifting	25 ; 1 ; 0.05	25 ; 1 ; 0.05	30 ; 2 ; 0.05
	550 ; 10 ; 0.01	500 ; 20 ; 0.01	800 ; 50 ; 0.01
complete rescheduling	-	30 ; 1 ; 0.05	60 ; 3 ; 0.05
	-	800 ; 30 ; 0.01	1500 ; 90 ; 0.01
CPU time†			
right-shifting	120	660	780
complete rescheduling	-	960	1200

*scenarios and seconds for 1 simulation run in the inner sampling loop with a precision γ.
†seconds required for the overall stochGA-based procedure with γ=0.05 on a AMD Athlon 2000 computer.

for the third example requires about 12 times more computational effort using MCS compared with the Sobol sequence algorithm).

For information purposes, the number of scenarios sampled in a simulation run using the Sobol sequence algorithm to evaluate the robustness measure of a predictive schedule are summarized in Table 5.1, based on the precision required and the rescheduling strategy considered. CPU time expended in the overall stochGA-based procedure is also reported.

5.5 Results and discussion

5.5.1 Motivating example

After preliminary tuning tests conducted to fix the values of the parameters used in the stochGA-based search procedure (Table 5.2), a first robust predictive schedule has been determined considering uncertainty only in the operation times (*RobustI*); this predictive schedule is next evaluated in the inner loop considering uncertainty in both the operation times and the availability of unit $U2$. On the other hand, a second predictive schedule has been identified (*RobustII*) using the developed proactive approach with variable operation times and uncertain equipment availability; the performance of this predictive schedule when only the operation times are uncertain is also assessed within the inner sampling loop.

Table 5.2: stochGA parameter values for case study 5.5.1.

Parameter	Value
Population size	10
Generations	100
Overlapping [%]	70
Crossover probability	0.9
Mutation probability	0.5

Table 5.3 reports the expected makespan and wait times (E[mk+wt]) for these predictive schedules, the makespan and wait time values of the executed schedules in the nominal and the faultless scenarios ($mk_{nominal}, wt_{nominal}, mk_{faultless}, wt_{faultless}$), as well as the start time of the batches (Tin_i). The results obtained using a deterministic modeling of the problem for the faultless scenario and evaluated in the two uncertainty contexts are also included. Right-shifting rescheduling has been assumed assumed in the simulation runs.

As it is also observed in the previous chapter (Section 4.5), the results obtained suggest that a deterministic modeling overestimates the performance of the system; although the predictive schedule from the deterministic approach (from now on *deterministic* predictive schedule) presents optimal makespan and wait time values if everything occurs as predicted (faultless scenario), its expected performance decreases significantly when it is executed in uncertain environments. Instead, the predictive schedules identified with the proactive approach (*RobustI* and *RobustII*) show better robustness properties over the anticipated scenarios.

Table 5.3: Results for case study 5.5.1.

	Predictive schedule		
	Deterministic	RobustI	RobustII
$\mathrm{E}[mk+wt]^*$	123.1	**118.2**	123.1
$\mathrm{E}[mk]^*$	106.2	108.9	118.0
$\mathrm{E}[wt]^*$	16.9	**9.3**	5.2
$\mathrm{E}[mk+wt]^\dagger$	152.3	152.5	**147.7**
$\mathrm{E}[mk]^\dagger$	121.4	121.0	131.5
$\mathrm{E}[wt]^\dagger$	30.9	31.5	**16.2**
$mk_{nominal}$	128.0	137.5	124.0
$wt_{nominal}$	9.0	2.7	18.2
$mk_{faultless}$	**101.0**	108.5	115.8
$wt_{faultless}$	0.0	2.7	0.0
Tin_A	0.0	0.0	77.0
Tin_B	10.0	39.1	0.0
Tin_C	75.0	8.3	89.8
Tin_D	16.0	46.5	8.3
Tin_E	57.0	20.3	52.8

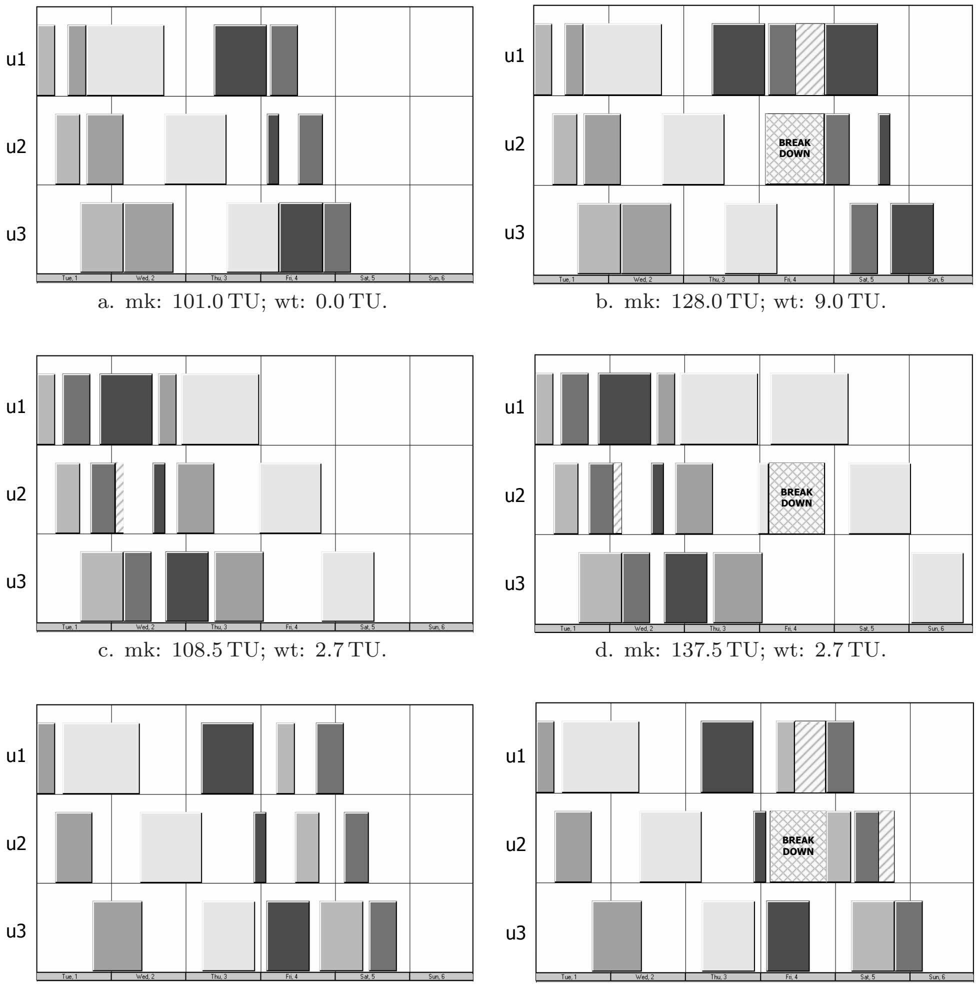
*Expected values obtained using a set of scenarios for the operation times uncertainty.

†Expected values assessed using a set of scenarios for both processing times uncertainty and equipment breakdowns.

Using only the information related to the uncertain operation times, the robust predictive schedule (*RobustI*) shows an expected wait time value about 45 % lower than its deterministic counterpart (9.3 vs. 16.9 TU), with a slight increase around 2 % in the expected makespan. Using information about the possible breakdowns in the decision stage itself, maintenance periods along with the incorporation of a new batch in the production sequence due to batch rejection are taken into account, thus leading to the identification of a more conservative predictive schedule (*RobustII*), with increased slack times. As it is expected, when this predictive schedule is evaluated in scenarios where breakdowns are excluded, it performs with low expected wait times (5.2 TU, which is about 70 % lower compared with the deterministic predictive schedule), but with an increased expected makespan (118 TU).

When the predictive schedules are evaluated in the scenarios that consider all the sources of uncertainty, the deterministic and *RobustI* schedules show a similar behavior (152.3 and 152.5 TU), whereas *RobustII* exhibits an improved expected performance (147.7 TU). The expected wait time value is about 48 % lower, at the expense of an acceptable increase in the expected makespan.

The Gantt charts depicted in Figure 5.6 illustrate the executed schedules in the faultless and nominal scenarios according to the deterministic and robust predictive schedules. Notice the different sequencing decisions, and the slack time introduced between the batches in the robust predictive schedules. Note also that the usage of information related to breakdowns leads to the identification of a more expanded schedule (Figure 5.6 (e)) in order to deal with the effects of the breakdown with a major flexibility. Despite its improved robustness, the predictive schedule *RobustII*



a. mk: 101.0 TU; wt: 0.0 TU.

b. mk: 128.0 TU; wt: 9.0 TU.

c. mk: 108.5 TU; wt: 2.7 TU.

d. mk: 137.5 TU; wt: 2.7 TU.

e. mk: 115.8 TU; wt: 0.0 TU.

f. mk: 124.0 TU; wt: 18.2 TU.

Figure 5.6: Gantt charts of schedules executed in the faultless (left-hand side, LHS) and nominal (right-hand side, RHS) scenarios for case study 5.5.1 using as a guidance the predictive schedules: a)/b) deterministic; c)/d) *RobustI*; e)/f) *RobustII*.

performs with poorer wait times in the nominal scenario (18.2 TU), though with better makespan than the deterministic one (124.0 TU). Instead, the predictive schedule *RobustI* performs with low wait times (2.7 TU), but with high makespan (137.5 TU).

The methodology developed is heuristic-oriented, so it is difficult to validate from an optimality point of view. However, the results obtained considering only uncertainty in the operation times can be compared with those reported in Chapter 4 using the stochastic programming approach, although it is important to note that different procedures are used to generate the set of scenarios. With the rigorous formulation, robustness measures of 120.4 TU and 116.2 TU are determined for the deterministic and robust predictive schedules, respectively (see Table 4.2). These results show only a difference of nearly 2 % with respect to those obtained with the simulation-based optimization framework (123.1 TU and 118.2 TU in Table 5.3). Moreover, the same production sequence is identified (A-C-E-B-D), and the processes start times are nearly equivalent (the assignment is fixed in this case study).

The use of the simulation-based optimization approach leads to a more agreeable modeling of the system. However, because of the simplicity of this example, its advantages in terms of computational effort cannot be fully justified. Nevertheless, the results obtained prove the suitability of the proposed proactive methodology, and the efficiency of the stochGA for the evaluation and identification of robust predictive schedules.

The results obtained so far show the quick lose of optimality when using a deterministic predictive schedule, neglecting the known uncertainty, and the inconveniences generated in terms of efficiency and quality properties. Because of the simplicity and the lack of alternative units in this case study, only a right-shifting rescheduling strategy has been assumed; the evaluation of alternative rescheduling policies is focused in the next examples.

5.5.2 Procel

The pilot plant facility Procel (Appendix B.3) is adopted as a second example, and five orders are considered for scheduling. Table 5.4 details the parameter values used in the stochGA-based search procedure and fixed after preliminary tuning tests. Table 5.5 reports the expected makespan and wait times, the batches start times, as well as the makespan and wait time values of the schedules executed in the faultless and the nominal scenario according to the deterministic and robust predictive schedules, for both right-shifting and complete rescheduling strategies.

Table 5.4: stochGA parameter values for case study 5.5.2.

Parameter	Value
Population size	10
Generations	100
Overlapping [%]	80
Crossover probability	0.8
Mutation probability	0.5

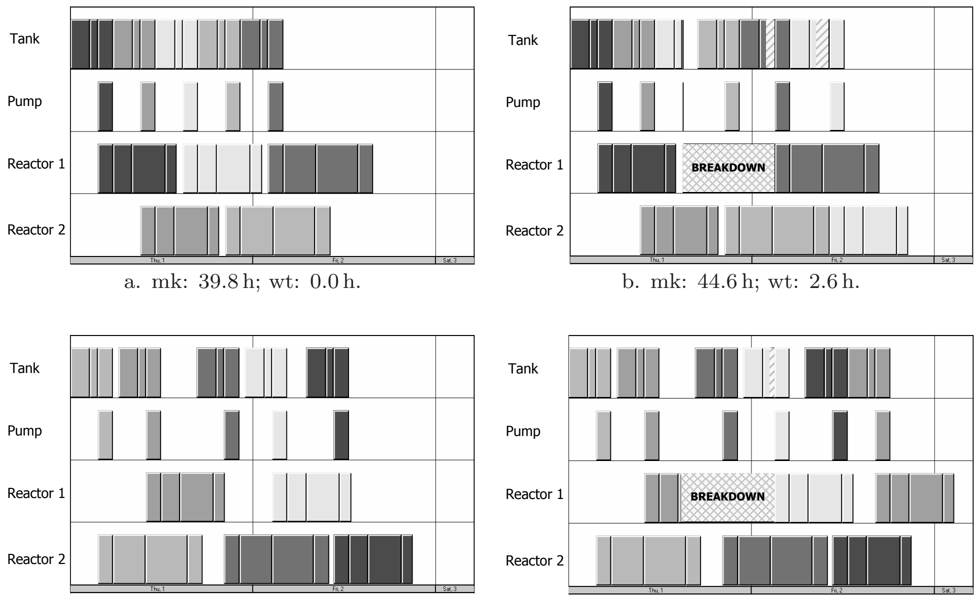
As already remarked in the previous example, these results show that the deterministic modeling overestimates the performance (schedule robustness) of the system. For example, the robust predictive schedule determined assuming right-shifting rescheduling (third column in Table 5.5) shows an expected makespan and wait time value about 20 % lower than its deterministic counterpart (57.2 h vs. 70 h); robustness improves at the expense of a relatively little increase in the makespan, as can be observed comparing the executed schedules in the faultless and nominal scenarios.

These trends are also observable in the Gantt charts depicted in Figures 5.7 and 5.8. They illustrate the actual executed schedules in the faultless and nominal scenarios using as an instruction the deterministic and robust predictive schedules evaluated assuming right-shifting and complete rescheduling policies, respectively.

Table 5.5: Results for case study 5.5.2.

	Predictive schedule			
	Right-shifting		Complete rescheduling	
	Deterministic	Robust	Deterministic	Robust
$\mathrm{E}[mk + wt]$	70.0	**57.2**	55.6	**53.5**
$\mathrm{E}[mk]$	49.3	48.9	49.6	48.4
$\mathrm{E}[wt]$	20.7	**8.3**	6.0	**5.1**
$mk_{nominal}$	44.6	50.6	46.4	52.0
$wt_{nominal}$	2.6	0.5	2.3	4.9
$mk_{faultless}$	**39.8**	45.0	**39.8**	44.7
$wt_{faultless}$	**0.0**	0.0	**0.0**	0.0
Tin_{batch1}	0.0	31.0	0.0	21.1
Tin_{batch2}	5.6	6.3	5.6	0.0
Tin_{batch3}	11.2	22.9	11.2	6.5
Tin_{batch4}	16.8	0.0	16.8	27.3
Tin_{batch5}	22.4	16.6	22.4	12.9

Notice the different sequencing decisions and the insertion of slack time. In the nominal scenario, the robust predictive schedule leads to an executed schedule with significantly lower wait times than the deterministic one when assuming a right-shifting



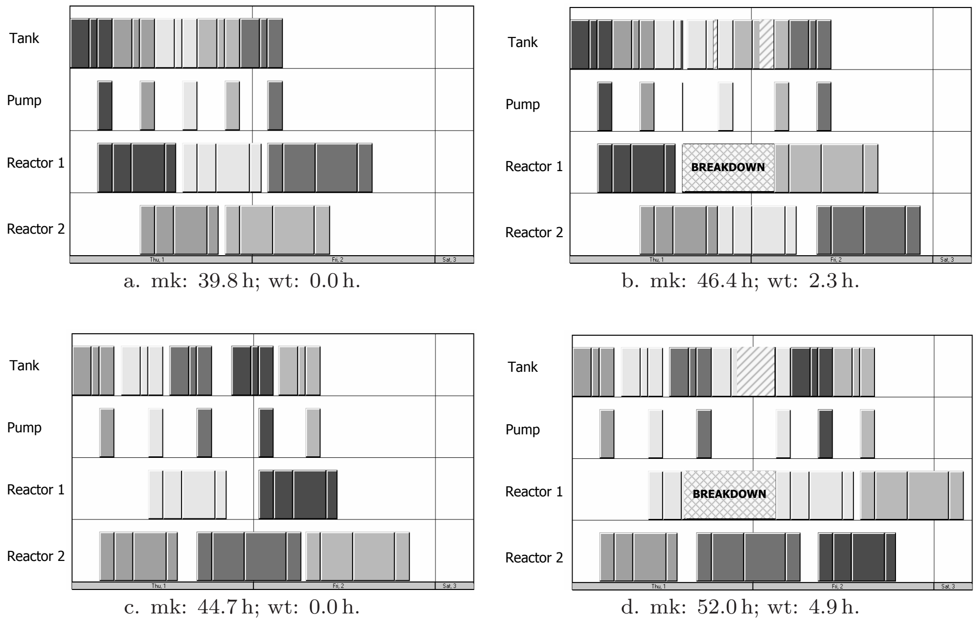
a. mk: 39.8 h; wt: 0.0 h.

b. mk: 44.6 h; wt: 2.6 h.

c. mk: 45.0 h; wt: 0.0 h.

d. mk: 50.6 h; wt: 0.5 h.

Figure 5.7: Gantt charts of schedules executed in the faultless (LHS) and nominal (RHS) scenarios for case study 5.5.2 assuming a right-shifting rescheduling strategy and using as a guidance the predictive schedule: a)/b) deterministic; c)/d) robust.



a. mk: 39.8 h; wt: 0.0 h.

b. mk: 46.4 h; wt: 2.3 h.

c. mk: 44.7 h; wt: 0.0 h.

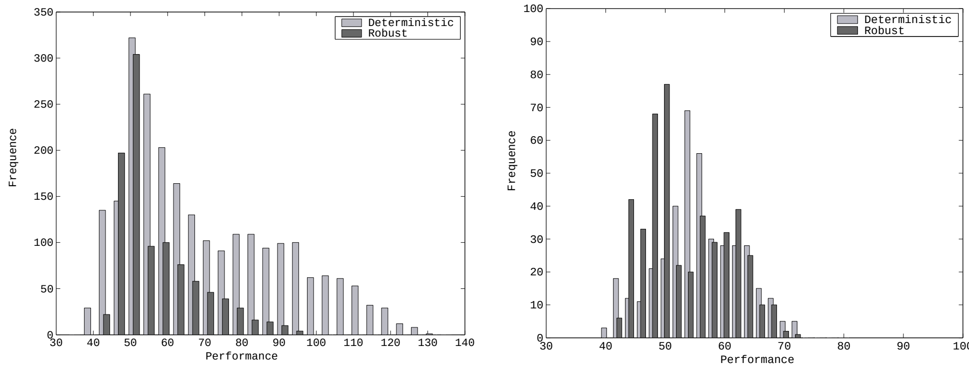
d. mk: 52.0 h; wt: 4.9 h.

Figure 5.8: Gantt charts of schedules executed in the faultless (LHS) and nominal (RHS) scenarios for case study 5.5.2 assuming a complete rescheduling strategy and using as a guidance the predictive schedule: a)/b) deterministic; c)/d) robust.

rescheduling strategy (0.5 vs. 2.6 h), and at the expense of a slight increase in the makespan (Figure 5.7 (b) and (d)). When considering complete rescheduling, the robust predictive schedule executed in the nominal scenario turns to perform poorer than the deterministic one despite the better expected performance (Figure 5.8 (b) and (d)).

Concerning the rescheduling policies, interesting remarks can be presumed comparing the strategies examined. Assuming complete rescheduling, the improvements on robustness in the predictive schedules appear to be less significant than using right-shifting rescheduling. This observation seems reasonable; complete rescheduling allows the introduction of sequencing and assignment changes in the predictive schedule once the uncertainty is revealed; with the possibility to modify all the non-executed batches with hindsight, robustness features become less critical than if adopting a right-shifting strategy with which some modifications in the schedule and during execution are restricted. It is worthwhile to note that robustness is not considered in the rescheduling procedures. Hence, no idle time is introduced within the new scheduled batches, as can be observed for example in the Gantt charts of the executed schedules in the nominal scenario (Figure 5.8 (c) and (d)).

Finally, the distribution of the expected performance for both the deterministic and the robust predictive schedules is represented in Figure 5.9. It is worthwhile to notice the higher variability of the deterministic predictive schedule when considering right-shifting rescheduling; the more robust predictive schedule shows not only a better expected performance, but also a smaller variability of possible outcomes. Moreover, and as observed before, the advantages of a robust predictive schedule using complete rescheduling become less significant.



a. Right-shifting rescheduling. b. Complete rescheduling.

Figure 5.9: Distributions of the expected performance of the deterministic and robust predictive schedules for case study 5.5.2.

5.5.3 Washing subprocess

The more complex washing subprocess (Appendix B.4) is finally tested in the framework of the proactive approach developed in this chapter to corroborate the results obtained so far. Four orders are considered for scheduling. After tuning tests of the stochGA-based search procedure, and since the convergence in this case study proved faster, the termination criterion is fixed after 80 generations, and a 70 % overlapping is selected; the other stochGA parameters are the same as those reported for the previous example in Table 5.4.

The expected makespan and wait time values of the deterministic and robust predictive schedules determined assuming both right-shifting and complete rescheduling are reported in Table 5.6, along with the start times of the batches, and the makespan and wait time values that would arise from their execution in the faultless, nominal, and a random scenarios (see Tables B.21 and B.20 in Appendix B.4). Gantt charts of the predictive schedules executed in the faultless scenario and in the scenario selected randomly are depicted in Figure 5.10.

The same trends remarked in the previous examples can also be observed. The predictive schedules identified with the proactive approach show a better expected performance (schedule robustness) over the anticipated scenarios. The robust predictive schedule determined assuming right-shifting rescheduling presents nearly a 12 % improved expected performance (518.0 vs. 523.9 TU); an improvement can also be appreciated adopting the complete rescheduling strategy, though it is not so significative. Again, the results show that the robustness features become less critical when complete rescheduling is adopted, but significant improvements can be obtained if reschedule limitations are established. These results remark the benefits of introducing information about the rescheduling strategy to be adhered to at execution time in the decision stage itself.

Focusing on a particular scenario, the performance of the deterministic and robust predictive schedules appears to be the same in the nominal scenario (see Table

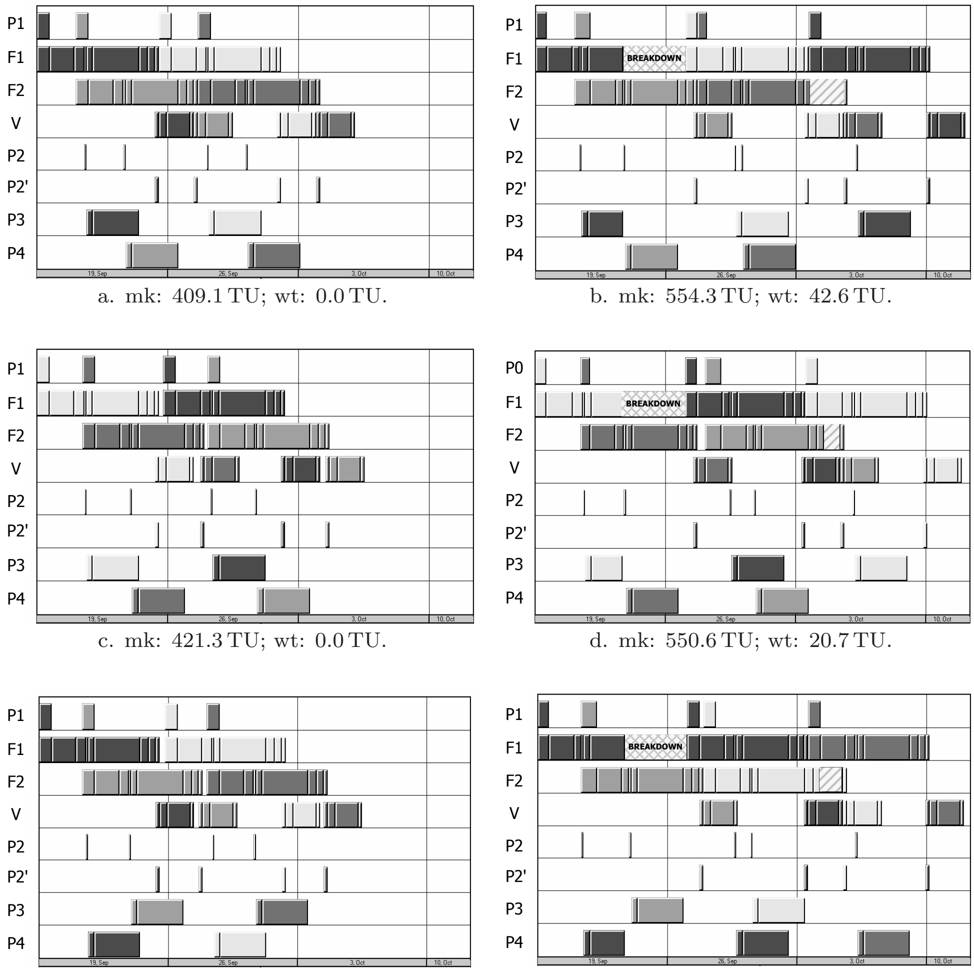
Table 5.6: Results for case study 5.5.3.

	Predictive schedule			
	Right-shifting		Complete rescheduling	
	Deterministic	Robust	Deterministic	Robust
E$[mk + wt]$	523.9	**518.0**	498.1	**495.2**
E$[mk]$	497.1	500.7	485.7	488.6
E$[wt]$	26.8	**17.3**	12.4	**6.6**
$mk_{nominal}$	525.9	525.9	525.9	525.9
$wt_{nominal}$	0.0	0.0	0.0	0.0
$mk_{faultless}$	409.1	421.3	409.1	420.0
$wt_{faultless}$	0.0	0.0	0.0	0.0
mk_{rnd}	554.3	550.6	552.6	552.6
wt_{rnd}	42.6	20.7	33.8	29.5
Tin_{batch1}	0.0	162.4	0.0	0.0
Tin_{batch2}	50.3	219.4	50.3	55.9
Tin_{batch3}	156.9	0.0	156.9	163.9
Tin_{batch4}	207.2	58.8	207.2	218.3

5.6), whereas the flexibility of the robust schedules can clearly be observed in the reduced generation of wait times and improved makespan values of the random instance reported. Notice that the different sequencing decisions and the slack time introduced between the batches of the robust predictive schedule determined with the right-shifting policy lead to an executed schedule in this scenario with not only significantly decreased wait times (20.7 TU instead of 42.6 TU), but also a reduced makespan (550.6 TU). See also Gantt charts (b) and (d) in Figure 5.10.

Finally, this example further illustrates the effects of using proactively the information about the uncertain equipment availability, as well as the rescheduling procedure to be implemented in front of a disruption, underlined above in case study 5.5.1. The comparison between the results obtained using all the available information (Table 5.6) and those reported in the previous chapter when considering only variable processing times (see the third column in Table 4.3) reveals the increased slack times introduced in the robust predictive schedules. With the anticipation of possible breakdowns in the reasoning procedure, maintenance periods along with the production of an additional batch if rejection occurs are considered, thus leading to more conservative decisions. Note the increased value of the expected makespan and wait times (518.0 TU, or 495.2 TU if complete rescheduling is assumed, instead of 428.4 TU determined with the proactive approach developed in Chapter 4), as well as the slightly increased start times of the batches. However, notice also that the performance of the predictive schedules in the faultless scenario (denoted as nominal in the previous chapter) is almost equivalent; the small differences can be due to the different modeling systems applied, i.e., rigorous and procedure-based approaches.

Again, these results prove the suitability of the proactive methodology developed using information about equipment breakdowns and rescheduling procedure to be implemented, as well as the improved robustness of the predictive schedules thus determined, and its acceptable performance even in a faultless or nominal scenario.



a. mk: 409.1 TU; wt: 0.0 TU.

b. mk: 554.3 TU; wt: 42.6 TU.

c. mk: 421.3 TU; wt: 0.0 TU.

d. mk: 550.6 TU; wt: 20.7 TU.

e. mk: 420.2 TU; wt: 0.0 TU.

f. mk: 552.6 TU; wt: 29.5 TU.

Figure 5.10: Gantt charts of executed schedules in the faultless (LHS) and a randomly (RHS) selected scenario (Tables B.21 and B.20) for case study 5.5.3 using as a guidance the predictive schedule: a)/b) deterministic and right-shifting rescheduling; c)/d) robust assuming right-shifting rescheduling; e)/f) robust adopting complete rescheduling.

5.6 Concluding remarks

The proactive system developed in Chapter 4 to address the short-term scheduling problem with uncertain operation times has been extended to deal simultaneously with uncertain equipment availability, as well as to consider proactively not only the stochastic features of the input parameters, but also information related to the reactive scheduling strategy followed at execution time. Valuable information is then used in the decision stage, which provides a good insight and leads to a more detailed and realistic modeling system for the operational analysis.

All the new features of the problem are captured with the development of a simulation-based stochastic optimization framework instead of a rigorous equation-based approach. The formalism for robustness defined in the previous chapter in terms of makespan as the efficiency of the system and wait times to manage the eventual effects of the uncertainty is also applied. This allows the comparison of the features of the predictive schedules determined with the different proactive methods. However, the robustness metric could be easily extended to account for the cost of rescheduling, using some measure such as the number of jobs reassigned, or the deviations from the predictive schedule.

The framework developed has been proved suitable for the identification of robust and flexible predictive schedules. Actually, more conservative schedules with increased slack times are identified, thus assuring an improved performance when they are executed in an uncertain environment. In addition, the robust predictive schedules not only guarantee improved expected makespan and wait times in the context of the uncertainty, but their performance when they are executed in a scenario with nominal operation times and no breakdowns is as well acceptable. On the other hand, it has been proved once again that a deterministic modeling of the problem does not consider the proper idle times to improve flexibility and robustness, and tends to overestimate the performance of the process.

The results obtained suggest that the efficiency of the proactive approach highly depends on the problem instance, as well as on the rescheduling method adopted. From the strategies analyzed in this study it has been shown that robustness is essential when restrictive rescheduling policies are used, but it becomes less critical with the possibility to modify the predictive schedule at execution time.

The case studies illustrated in this research work are quite simple, and relatively little variability is associated with the uncertain parameters. Because of this, the advantages of the procedure-oriented approach in terms of computational requirements cannot be fully justified. Moreover, robustness features are not considered when rescheduling. Therefore, further improvements can be achieved by introducing the robustness criterion also in the reactive scheduling approach. However, it is important to notice the consequences of neglecting the known uncertainty, the different decisions that can be determined based on the strategy assumed in the plant, and the quick loose of optimality when implementing a deterministic schedule.

This study completes the formalization of the short-term production scheduling problem with operational uncertainties, covering not only the major disruptions occurring due to the uncertainty at execution time (i.e., process time variations and machine breakdowns), but also incorporating the rescheduling procedures proactively in the decision stage of scheduling. In general, the proactive modeling approach developed appears as a promising framework to provide visibility for future actions and a more practical model of the real problem. Interesting directions exist for improvements in applications of industrial size and complexity, thus providing the appropriate support for remaining effective and competitive within a dynamic and uncertain SC environment.

6.

Extension to transport scheduling: Coordinated production and distribution activities

It's astonishing in this work how things don't turn out at all the way you expect them to.

Agatha Christie

Within the development of proactive modeling systems to deal with uncertainties in the operational level of analysis, the focus of interest is extended in this chapter from production to distribution scheduling in a multi-site context. The efficient coordination of production and distribution systems becomes a challenging problem as companies move towards higher collaborative and competitive environments. The idea is to support the coordination of short-term production and transport activities in uncertain conditions to properly manage the inventory profiles and material flows between sites, thus improving the flexibility and interoperability between different nodes in a supply chain (SC).

The chapter starts with an introduction to Supply Chain Management (SCM) from an operational perspective, and the proper definition of the problem addressed. The modeling and resolution approaches are then described relying on a *procedure-oriented methodology*. Special attention is centered on the modeling of the *transport scheduling* problem, and uncertainty is considered in the travel times, thus taking into account eventual delays and/or exceeded due dates due to unpredictable transport events. Two case studies are presented and discussed, to finally conclude with some remarks.

6.1 Introduction

SCM focuses on the combination of strategies and tools to integrate all the entities of a SC (suppliers, production plants, distribution centers, retailers, markets) and achieve a common objective.

Most of the work published in the literature addresses the SC problem from an strategic or tactical point of view to optimally configure and manage the system according to some economic objective (refer to Shapiro (2000) and Mele (2006) for an extensive survey of SCM). Some models considering product demands uncertainty in these domains are reviewed in Chapter 2.

From an operational perspective, and as discussed in Chapter 3 (Section 3.1), numerous contributions have been reported so far to analyze short-term production scheduling and distribution problems, although both problems have been dealt with primarily decoupled and independent from any SC environment (Chandra and Fisher, 1994; Ertogral et al., 1998). Generally, a production schedule is developed assuming a constant delivery of goods, thus ignoring the transport requirements between production sites in a SC. However, the problem in which a number of vehicles available in a site of the SC has to serve a set of geographically dispersed locations (either distribution centers or final markets) can be identified in most of the production sites. Assignment, routing and timing decisions are involved. In addition, transport tasks have to cope with a highly dynamic and uncertain environment. Transport failures or the unexpected unavailability of vehicles are common events that may lead to eventual delays in downstream sites, and/or to exceeded due dates. Furthermore, disruptions occurring in the production lines may also imply delays in transport scheduling.

The *transport scheduling* problem, usually referred to as *pickup and delivery problem* (PDP), has been extensively analyzed in the area of Operations Research. Numerous exact and heuristic algorithms have been proposed for its solution, focusing mainly on individual and geographical aspects to reduce delivery costs (Hillier and Lieberman, 2001). Various problem types ranging from the basic traveling salesman problem (TSP) to the multi-vehicle pickup and delivery problem with time windows (PDPTW) are distinguished as special cases of the general PDP (Savelsbergh and Sol, 1995). They are summarized in Table 6.1.

Table 6.1: Taxonomy of transport problems according to Savelsbergh and Sol (1995).

Problem type	Definition	Decisions
Traveling Salesman Problem (TSP)	Find the shortest route through a set of cities, visiting each city exactly once and returning to the start city.	routing
Pickup and Delivery Problem (PDP)	All vehicles depart from and return to a central depot to deliver transport requests between a given origin and destination.	assignment routing
Pickup and Delivery Problem with Time Windows (PDPTW)	PDP in which transport requests additionally specify pickup and delivery time windows.	assignment routing timing
Vehicle Routing Problem (VRP)	PDP in which either all the origins or all the destinations are located at the depot.	assignment routing
Vehicle Routing Problem with Time Windows (VRPTW)	VRP in which transport requests have to be served within a given time window.	assignment routing timing
Dial-a-Ride Problem (DARP)	PDP in which the loads to be transported represent people.	assignment routing

An extensive review of heuristic solution techniques for vehicle routing problems (VRP) and TSP problems was presented in Marinakis and Migdalas (2002). Other contributions can be found in Solomon and Desrosiers (1988), and Thangiah et al. (1996). Recently, Karimi et al. (2005) addressed a tank container management problem in the chemical process industry (CPI) to minimize logistic costs; a two-stage event-based order-driven approach with a continuous time representation was presented, where the container movements were first identified, and a linear programming (LP) formulation was then proposed to determine the events that minimized the schedule cost. The logistics problem was addressed from a tactical perspective, assuming an unlimited number of containers of the same type, and without addressing the scheduling/routing problem of limited resources.

New variants of the transport problem involve dynamic and stochastic routing problems. Verweij et al. (2003) proposed two-stage stochastic formulations for modeling three classes of routing problems with random travel times or vehicle failures; routing decisions were considered in the first stage, whereas the second stage involved a penalty or a rerouting decision as a resource; the overall objective was to minimize the sum of the first-stage routing cost and the expected recourse cost. The VRP was also considered by Kenyon and Morton (2003) in the stochastic programming domain with random travel and service times; vehicle routes were determined with minimum expected completion time and maximum probability of completing the project by a prespecified deadline.

The decoupled production and distribution processes rely on finished goods inventory to buffer both operations from each other. However, inventory costs and the trend to operate in a *just-in-time* (JIT) manner are putting pressure on firms to reduce inventories in their distribution chain. Coupling production and transport activities requires the consideration of additional features. Particularly, complex temporal and capacity interdependencies arising between production processes in a SC environment, due to load sizes, travel time allowances, and service time windows, place important constraints to be taken into account; moreover, the total of a product to be delivered at any time point cannot exceed the amount available as implied by the production schedule first determined.

The efficient *coordination of production and distribution systems* remains an open area for research, with an increasing interest as companies move towards into higher collaborative and competitive environments. Only few contributions have been reported so far in this direction, and most of them focus mainly on the integration of production-distribution systems in the strategic and tactical levels; moreover, the presence of uncertainty is neglected (existing literature was reviewed in Sarmiento and Nagi (1999), and Erengüç et al. (1999)).

Chandra and Fisher (1994) presented a computational study to assess the value of coordinating production and distribution scheduling; the production scheduling problem was mathematically formulated as a capacitated lot size problem to minimize the cost of setups and inventory holdings subject to meet total demand; the distribution problem was modeled as a multiperiod VRP, with a discretization of the time horizon into uniform time periods for which demands at each retail order had to be met in that period or earlier; no travel times were considered in that level of analysis.

Ertogral et al. (1998) addressed the integration of production and transport planning in SCs from the automotive and electronic industries; both problems were formulated as mathematical models to determine the loads to be pickup and delivered, and the travel time allowances that minimized the operational cost over both planning functions; transport planning was modeled as a PDPTW assuming a single depot and an homogeneous fleet of vehicles; transport times were considered as parameters of the model.

Recently, Méndez et al. (2006a) presented a rigorous mathematical mixed-integer linear programming (MILP) formulation based on a continuous-time representation to coordinate short-term production and transport scheduling.

In general, literature related to the integration of production and transport scheduling problems in the operational level of analysis is almost void, not only for SCs in CPIs, but also in a manufacturing environment. This integration, as well as the consideration of disturbances arising from the complex dynamic and uncertain SC environment, deserve further research. A first attempt in this direction is the purpose of the study presented in this chapter.

6.2 Problem statement

The coordination of production and transport activities is addressed from the perspective of a production plant of a multi-site system that owns, or leases on a long-term basis, a fleet of vehicles for its logistic needs. Particularly, the scenario considered concerns a multipurpose batch plant, which produces a number of products over time and maintains an inventory of finished goods that have to be distributed to a number of delivery centers or retail outlets. The work by Méndez et al. (2006a) is adopted as a reference. A scheme of the underlying problem is illustrated in Figure 6.1.

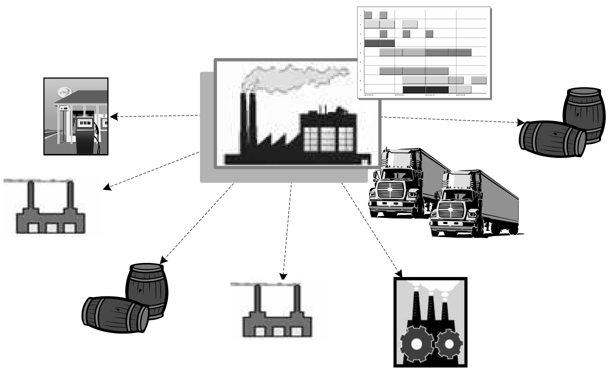


Figure 6.1: Representation of the coordinated production and transport scheduling problem.

Transport scheduling is devised as a general scheduling problem (see definition given in Section 1.2 from a production perspective), where vehicles are the resources available, equivalent to equipment units (*how*), and the routes define the specific allocation of vehicles to distribution activities between sites, similar to the assignment of units to production stages in a batch (*where*).

The data is again modeled according to the ANSI/ISA-S88 standard (International Soc. for Measurement and Control, 1995, 2001). Information is given for production scheduling related to the configuration of the plant with the available equipment units, the production recipes, and the set of production orders to be produced. For transport scheduling, data is required concerning the set of interconnected locations with a distances matrix, the fleet of available vehicles, and the set of transport orders to be fulfilled.

Note that a distinction is made between transport and production orders, which is especially useful when considering a decentralized SC. A *transport order* is defined for each amount of material to be delivered in a particular site at a requested due date. For production scheduling, *production orders* are considered from two different points of view. First, the efficiency of the system is defined irrespective of due dates for specific orders; this perspective reproduces a strategy of a manufacturing plant looking for its own benefits, neglecting the efficiency of the overall system. Secondly, a maximum customer satisfaction is pursued, thus due dates for specific orders are taken into account in production scheduling; this situation is typical in SC systems with a centralized management policy.

The problem consists of identifying detailed production (number of batches to be produced, assignment of units to production stages, sequencing and timing) and transport schedules (loads, assignment of vehicles to transport orders, routing and timing), so as to optimize some established objective function. Different criteria, from time considerations (delivery times to meet the due dates, flow time) to economical measures (cost of production setups, transport and inventory), can be considered for the evaluation of both production and transport schedules.

6.3 Modeling approach

Different methodologies, either equation-oriented or heuristic-based rules, could be implemented to develop a model and solution procedure for the underlying problem. An MILP mathematical representation was presented in Méndez et al. (2006a) . The formulation was based on a continuous-time representation, where the assignment and sequencing decision variables were managed independently. Even though the examples presented were based on simple SC configurations, they led to large-scale optimization problems, for which the identification of optimal production and transport schedules was not possible with reasonable computational effort.

The aptitude of *heuristic-based procedures* is assessed in this research. An overall framework has been designed adopting an object-oriented representation and in a modular way, thus allowing the implementation of alternative heuristic or mathematical algorithms, as well as additional functionalities to solve or further optimize the problem as needed. The framework has been implemented in C++ using the Borland C++Builder 6.0 programming environment.

The production and transport scheduling models are first described individually. Next, the coordination of both activities is addressed.

6.3.1 Production scheduling

Modeling architecture

The integrated support system for planning and scheduling of batch chemical plants developed by Cantón (2003), and used in Chapter 5 as the scheduling module in the simulation-based stochastic optimization framework (Section 5.3.3), is also used in this study for production scheduling. The data model allows the definition of different production recipes for the same material, as well as alternate units for each stage. For a detailed description of the object-oriented models used to characterize all the information required refer to Cantón (2003).

Different objective functions can be defined for optimization purposes to assess a short-term production predictive schedule. Common criteria to be considered involve the makespan, due date-based measures such as earliness and tardiness, or economical functions considering revenues and production costs. Robustness metrics defined and assessed in the previous research studies can be also applied. The results obtained so far highlight their advantages for the determination of more robust predictive schedules in uncertain operation environments.

Table 6.2: Priority rules implemented in the production scheduling module for process selection, assignment and sequencing decisions.

Process selection	AUP:	Already Used Process
	FP:	First Process
	HPP:	Highest Priority Process
Assignment	AUA:	Already Used Assignment
	FU:	First Unit
	HPU:	Highest Priority Unit
	LUU:	Less Used Unit
	MAU:	Most Available Unit
	SPTU:	Shortest Processing Time Unit
Sequencing	EDD:	Earliest Due Date
	HSL:	Highest Storage Level
	SCT:	Shortest Cycle Time
	SPT:	Shortest Processing Time
	LCT:	Longest Cycle Time
	LPT:	Longest Processing Time
	LSL:	Lowest Storage Level

Solution methodology

For production scheduling, a rule-based heuristic algorithm available in the scheduling system is used to establish the number of batches to be performed, the sequence, and the assignment of production stages to specific units.

For recipe selection and task to unit assignments, as well as for sequencing decisions, common dispatching rules used in commercial packages are applied in combination with the Event Operation Network (EON) temporization model (the main priority rules implemented in the module are reported in Table 6.2). Based on the characteristics of the problem and the objective function previously defined, different combinations of these rules can be selected.

The algorithm proceeds as shown in Figure 6.2. Given the production orders to be met, a material balance is first performed to draw a list of batches to be next sequenced and assigned to specific units. Assignment and sequencing decisions are made simultaneously based on the corresponding rules selected. The detailed timing of the operations is then calculated by means of the EON model. This procedure allows the identification of an initial feasible schedule, which can be further improved according to some objective function. Meta-heuristic algorithms such as simulated annealing (SA) and genetic algorithms (GA) have been implemented for this purpose within the module.

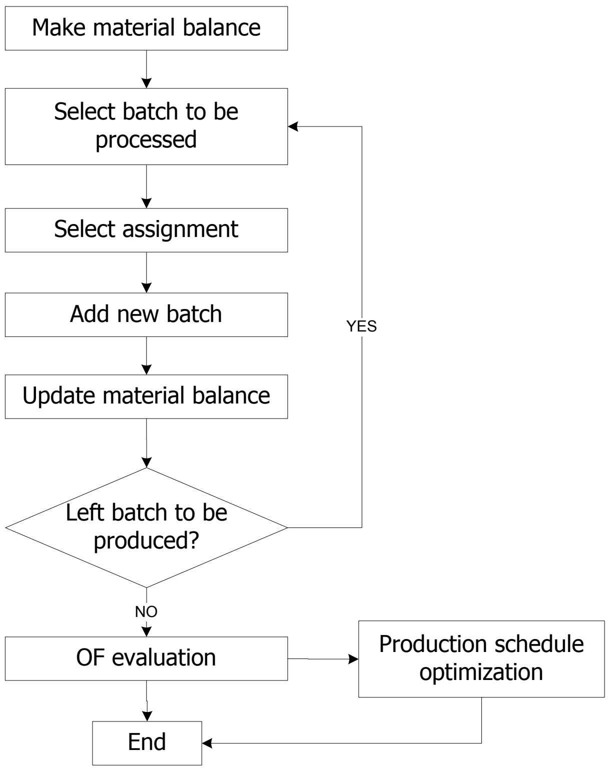


Figure 6.2: Rule-based heuristic algorithm for production scheduling.

6.3.2 Transport scheduling

Modeling architecture

The transport scheduling model is developed based also on a hierarchical organization of the information. Emulating the ANSI/ISA S88 standard (International Soc. for Measurement and Control, 1995, 2001), the entities of transport route, transport stage, transport operation, transport order, and vehicle are used referred to transport scheduling similarly to the objects of batch, unit procedure, batch operation, production order and unit used, respectively, in the production scheduling paradigm.

Different classes have been defined to identify these categories. A class diagram of the transport scheduling model is illustrated in Figure 6.3 using a UML (Unified Modeling Language) representation. The main entities are following described.

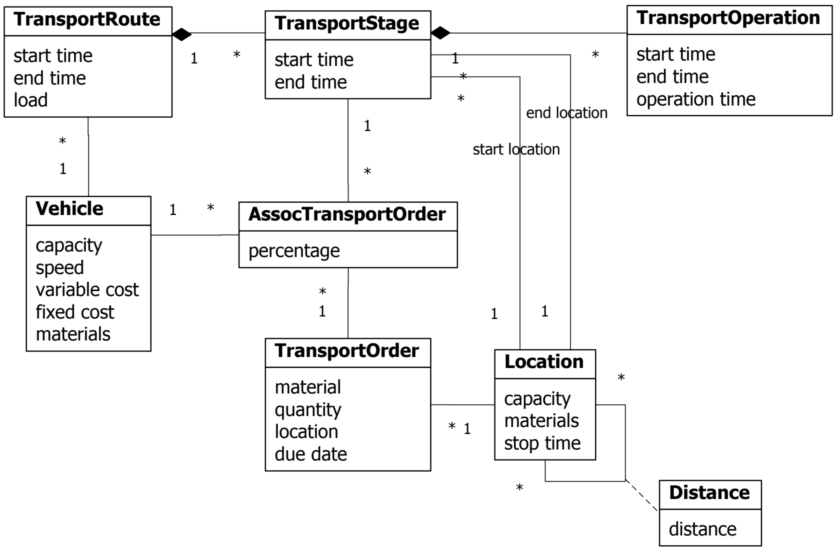


Figure 6.3: Class diagram of the transport scheduling model.

Model entities

TransportRoute. A transport route (tr) represents the distribution of a set of *transport orders* among different and dispersed *locations*. It consists of a sequence of *transport stages* that an assigned *vehicle* must perform when it leaves the plant. Each transport route must start and finish at the plant. Therefore, a route involves at least two transport stages: from the plant to a delivery center, and the return stage to the plant.

TransportStage. A transport stage (ts) identifies a distribution task between two locations, and consists of a set of *transport operations* to characterize the specific steps involved (charge of materials, transport, discharge, etc.), as well as a set of *associated transport orders* to be delivered.

TransportOperation. A transport operation (to) provides the detailed definition of the time required for each transport step. Particularly, the *travel* from the start to the end location, the *discharge* operation in the delivery center, and a *stop time* are distinguished as transport operations in the modeling framework developed.

For each transport stage, the operation time for the travel operation (Top_{ts}^{travel}) is computed based on the speed of the vehicle undertaking the corresponding route (s_v), and the distance ($dist_{ts}$) to be covered (eq. 6.1). The operation time for the discharge operation depends on the amount of material delivered in the stage (Q_{ts}^{d}); a transport factor $f_{v,l}^{tr}$ is used as unloading rate (eq. 6.2). The operation time for the stop operation is calculated with a fixed stop time specified for each site, which is considered a minimum stop time; some slack could be included to account for early deliveries or unexpected requirements.

$$Top_{ts}^{travel} = \frac{1}{s_v} \cdot dist_{ts} \tag{6.1}$$

$$Top_{ts}^{discharge} = f_{v,l}^{tr} \cdot Q_{ts}^{d} \tag{6.2}$$

TransportOrder. A transport order ($t\theta$) defines an amount of material to be delivered in a particular *location* at an specific due date.

AssocTransportOrder A transport order may need more than one transport stage to be fulfilled depending on the capacity of the vehicles available. Associated transport orders ($at\theta$) are defined to establish the percentage of a transport order associated to a stage.

Vehicle. A fleet of vehicles (v) is assumed to be available in the plant for its distribution needs. Each vehicle can operate on more than one transport route, and is characterized in terms of capacity (C_v), mean speed (s_v), variable and fixed costs (c_v^u, c_u^f), and materials that can be transported.

Location. A location (l) describes a delivery center or retail outlet where products have to be distributed. Each location is characterized by a capacity (C_l), a set of related materials, and a fixed stop time.

Performance measures

Because of the complexity and dynamics of a SC system, it is difficult, if not impossible, to define a general optimality criterion for transport scheduling that efficiently takes into account all the features of the problem. Multiple and even conflicting objectives, based either on time or economical attributes, can be considered depending on the preferences of each organization. In this thesis, the flow time (F), the due date-based measures of summed lateness (L), summed tardiness (T), and summed earliness (E) are examined, along with transport costs (c^{tr}), inventory costs (c^I), and the number of routes required ($Routes$). These criteria are defined as stated in equations 6.3 - 6.8.

Notice that the lateness criterion favors JIT deliveries, and seeks a transport schedule with minimum tardiness, while keeping order earliness at reasonable values. From a production scheduling point of view, by completing the production orders as closed to their due dates as possible, the system implicitly minimizes inventory costs and penalties for missed demands at the same time. However, from a transport scheduling perspective, the lateness criterion favors JIT transport schedules without accounting for the production inventory remaining in the plant waiting for distribution.

On the other hand, the transport cost associated with a transport schedule, and expressed in equation 6.7, is defined as the contribution of a fixed charge (c_v^f) and a variable cost (c_v^u) depending on the distance covered. Note that this cost only depends on transport decisions, whereas the due date-based measures are also subject to the release date of the vehicles implied by the production schedule. The inventory cost, defined in equation 6.8, accounts for the storage of all the materials in the plant and throughout the time horizon; this criterion couples both production and transport scheduling.

$$F = \sum_{tr} (Tfn_{tr} - Tin_{tr}) \tag{6.3}$$

$$L = \sum_{tr} \sum_{ts \in tr} \sum_{at\theta \in ts} |Tfn_{ts} - dd_{at\theta}| \tag{6.4}$$

$$T = \sum_{tr} \sum_{ts \in tr} \sum_{at\theta \in ts} \max(Tfn_{ts} - dd_{at\theta}, 0) \tag{6.5}$$

$$E = \sum_{tr} \sum_{ts \in tr} \sum_{at\theta \in ts} \max(dd_{at\theta} - Tfn_{ts}, 0) \tag{6.6}$$

$$c^{tr} = \sum_{tr} c_v^f + \sum_{ts \in tr} (c_v^u \cdot dist_{ts}) \tag{6.7}$$

$$c^I = \sum_{i} c_i^I \cdot Q_i^I \cdot t_i^I \tag{6.8}$$

In order to assess multiple objectives simultaneously, the measures of flow time (F), number of routes ($Routes$), summed earliness (E), and summed tardiness (T) are translated into economical terms and aggregated in a single multiple cost function (c^{sum}) as stated in equation 6.9. Transport and inventory costs can be also appended in the metric, but have been excluded and evaluated as mono-objectives to be able to compare the procedure-oriented methodology with the rigorous mathematical model proposed in Méndez et al. (2006a).

$$c^{sum} = \rho_1 \cdot F + \rho_2 \cdot Routes + \rho_3 \cdot E + \rho_4 \cdot T \tag{6.9}$$

Solution methodology

A **rule-based heuristic algorithm** is developed for transport scheduling to define the transport routes and associated transport stages, the assignment of vehicles, and the transport time intervals. Rules are used to establish the criteria to prioritize the requested transport orders, the assignment of vehicles, to charge a vehicle with free capacity, and to temporize the routes. The rules implemented are detailed in Table 6.3, and the heuristic algorithm is represented in Figure 6.4.

Given the set of transport orders to be fulfilled, and based on the orders selection rule, the transport scheduling algorithm starts with the definition of a prioritized list of associated transport orders, and the assignment of a vehicle to each of them based on the assignment rule. This selection directs the scheduling of transport routes. The algorithm proceeds with an iterative procedure to match the associated transport

Table 6.3: Priority rules implemented in transport scheduling for transport orders selection, vehicles assignment, vehicles loading, and routes temporization.

Orders selection	EDD:	Earliest Due Date
	HD:	Highest Demand
Vehicles assignment	BFV:	Best Fit Vehicle
	BUV:	Best Used Vehicle
	FFV:	First Fit Vehicle
	LUV:	Less Used Vehicle
Vehicles loading	DD:	Due Dates
	ML:	Maximum Load
	MRT:	Minimum Release Time
Temporization	BD:	Backward from due date
	FD:	Forward from earliest pick up

orders within routes. At each step, a transport route is defined to deliver the first associated transport order in the list, along with other remaining orders assigned to the same vehicle, provided that the capacity of the vehicle is not exceeded and the loading criterion selected is met. According to the due dates rule (DD), associated transport orders remaining in the list and assigned to the same vehicle will also be selected for transportation in that route while free capacity is available, and the release time of the vehicle does not exceed the due date of the first order selected. Instead, assuming the minimum release time rule (MRT) as a loading criterion, an associated transport order is also assigned to the route if free capacity is available and it does not imply a delay in the release time of the vehicle due to the unavailability of material in the storage. If the maximum load (ML) rule is adopted, a full load of the vehicle is pursued, irrespective of delays in the release time or exceeded due dates of the tranpsort orders involved.

The end sites of the associated transport orders appended to a route establish the number of transport stages associated, that is a transport stage is defined for each set of associated transport orders with the same end location; the direction is given by the priority of the orders. Once the route and its associated transport stages are defined, the detailed temporization of the transport operations is performed based on the temporization rule, the availability of all the materials to be released as implied by the production schedule, as well as the availability of the assigned vehicle.

Travel times uncertainty

The time-based measures defined before are based on estimated values of the speed of the vehicles and therefore, of the travel times. To account for the variability associated with transport times, mainly due to usual unpredictable events such as deviations and traffic jams, uncertainty is introduced in the speed of the vehicles, and it is characterized by a probability distribution function. The scenario-based representation of the uncertainty (refer to Chapter 2, Section 2.2.1) is then adopted by sampling over the probability space defined by the speed parameter.

Once the assignment and routing decisions are established following the solution procedure described above, the execution of the inferred transport schedule is simulated in each of the scenarios through a series of temporization runs. Different

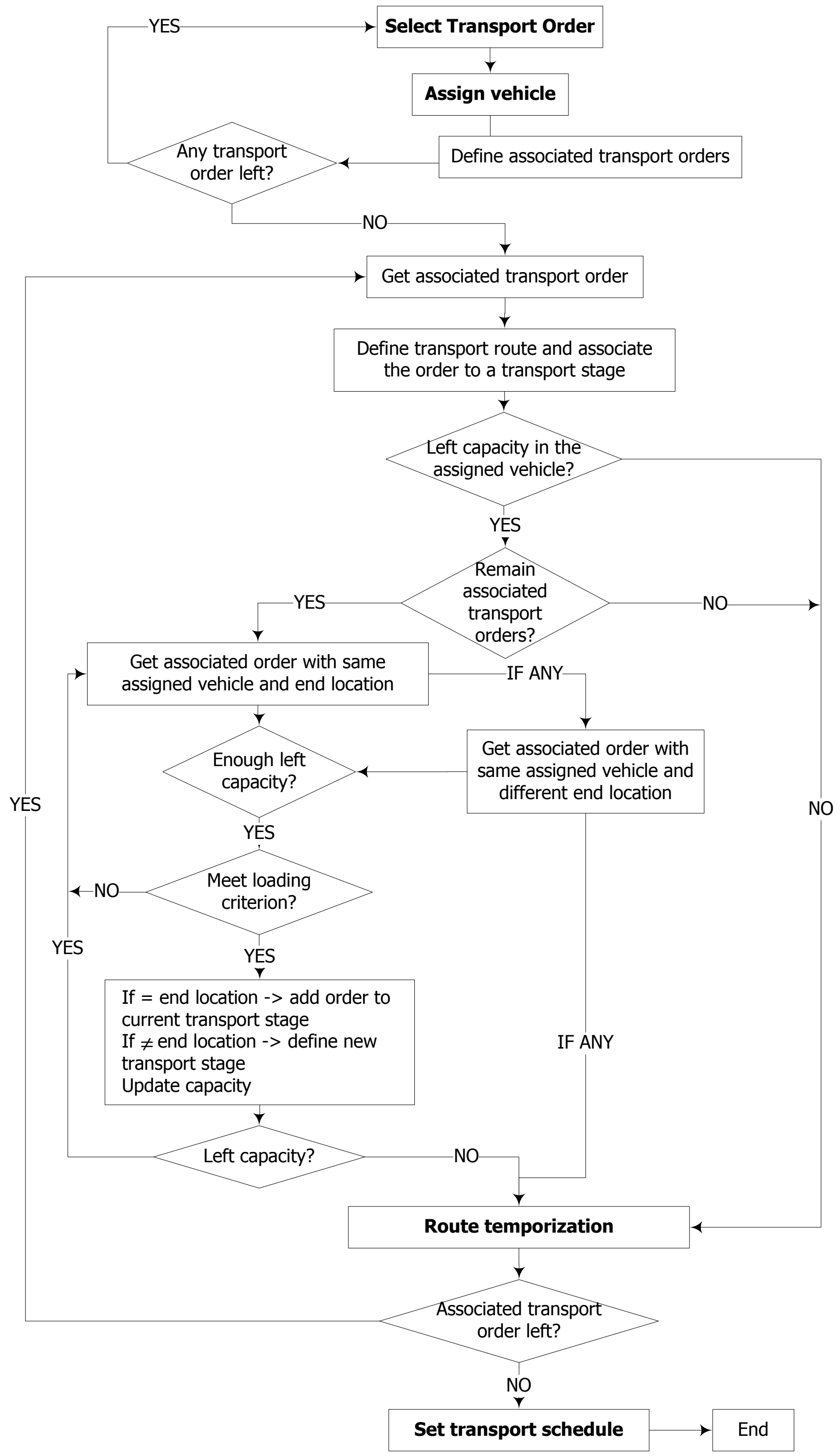


Figure 6.4: Rule-based heuristic algorithm for transport scheduling.

recourse actions, from a simple right-shifting to a complete rerouting of the pending transport stages, could be considered at execution time once disruptions or deviations occur due to the uncertainty. In this study, a retiming with right-shifting of the altered transport stages is assumed in the simulation step. The selected criterion is then computed for each scenario, to finally evaluate an expectation of the objective function. This evaluation procedure is equivalent to the inner sampling loop of the modeling framework developed in Chapter 5 (Section 5.3); the number of scenarios to be sampled (nk) is also assessed at runtime following the procedure described for the stochastic modeler module in Section 5.3.2.

New metrics are defined related to the expected flow time $\mathrm{E}[F]$, the expected summed tardiness $\mathrm{E}[T]$, and a general expected deviation $\mathrm{E}[Dev]$ based on the sum of delays from the predicted delivery times (Tfn_{ts}^{nom}) (eqs. 6.10 - 6.12, respectively). The predicted delivery times are obtained from the resolution of the transport scheduling problem using the mean value for the speed parameter, that is, nominal travel times.

$$\mathrm{E}[F] = \sum_{k} \omega_k \sum_{tr} (Tfn_{tr,k} - Tin_{tr,k}) \tag{6.10}$$

$$\mathrm{E}[T] = \sum_{k} \omega_k \sum_{tr} \sum_{ts \in tr} \sum_{at\theta \in ts} \max(Tfn_{ts,k} - dd_{at\theta}, 0) \tag{6.11}$$

$$\mathrm{E}[Dev] = \sum_{k} \omega_k \sum_{tr} \sum_{ts \in tr} \max(Tfn_{ts,k} - Tfn_{ts}^{nom}, 0) \tag{6.12}$$

6.3.3 Coordinating production & transport scheduling

Two different procedure-oriented methodologies are examined for coordinating production and transport activities: a sequential procedure and an integrated approach.

Sequential coordination

As a procedure commonly applied in the industry to coordinate the scheduling problems, a sequential approach is implemented using a *two-stage strategy*. A scheme of this approach is depicted in Figure 6.5.

The production scheduling problem is first solved as exposed in Section 6.3.1 to determine the production activities that fulfill a set of production orders. Then, the transport schedule is established according to the strategy described in Section 6.3.2. Temporal and capacity conditions implied by the production schedule constrain the start time of the transport routes, that is, the vehicle assigned to a route cannot be released until the full amount of transport orders to be delivered in its associated transport stages is available in the plant.

An **exhaustive enumeration procedure** is also implemented for the evaluation of all possible combination of transport rules in terms of the alternative criteria. This procedure consists of two recursive loops, similarly to the simulation-based stochastic optimization system developed in Chapter 5. There is an outer loop that explores the different combination of rules; an inner loop is embedded to determine the transport

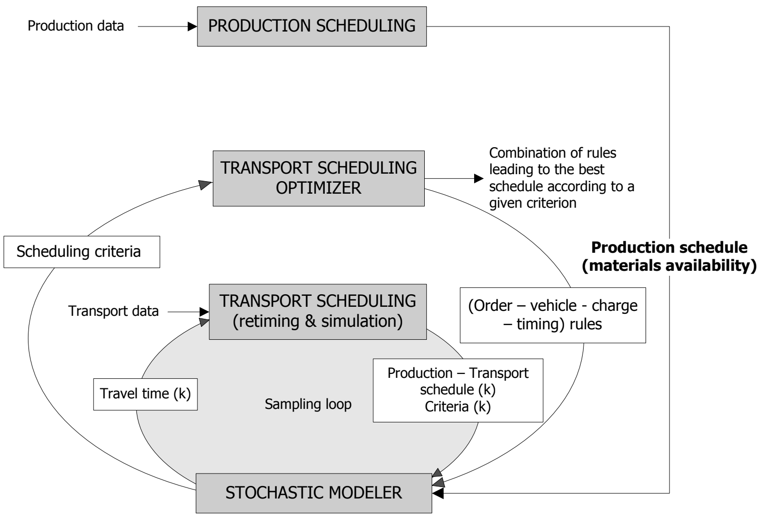


Figure 6.5: Sequential coordination for production and transport scheduling.

schedule for the combination of transport rules given by the outer loop, and to evaluate it in terms of the different criteria. For stochastic measures, a set of travel time scenarios is anticipated by sampling over the probability distribution describing the speed of the vehicles, and the performance of the transport schedule is simulated in each scenario to finally compute the probabilistic metric. For the evaluation of deterministic measures, only the scenario with nominal values for the speed parameters is considered.

Integrated coordination

With a sequential coordination of production and transport schedules, different criteria can be established for each problem, transport times are not considered in production scheduling, and the inventory in the plant is usually neglected. This approach may lead to critical inventory costs, and may be particularly unsatisfactory when due date-based measures are considered in transport scheduling since JIT deliveries are favored, thus neglecting the subsequent generation of stock in the plant.

By integrating production and transport scheduling decisions, the flexibility of the plants is exploited to improve the overall management of resources and material flows through multiple sites. Numerous strategies could be considered for this purpose. The definition of a general procedure is out of the scope of this research, but an attempt is made to imply the value of integrated decisions using the procedure represented in Figure 6.6.

The procedure is based on updating the production orders and due dates for production scheduling in accordance with temporal requirements implied by the transport schedule. Particularly, the algorithm developed starts with the resolution of the production and transport scheduling problems using the sequential procedure exposed above to derive an initial feasible coordinated schedule. The production schedule thus

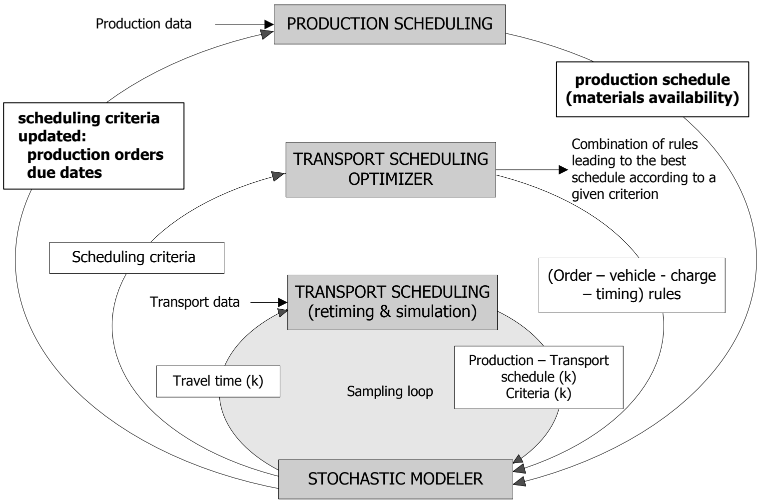


Figure 6.6: Integrated coordination for production and transport scheduling.

determined is allowed to change by redefining the production orders and related due dates according to the following steps:

STEP 1. A production order is defined for each of the associated transport orders established in the transport schedule.

STEP 2. The due date associated to each new production order is determined as the start time of the transport route that delivers the corresponding associated transport order, adjusted with the maximum tardiness originated in that route (or minimum earliness if all the orders are delivered in time).

The maximum tardiness (T_{tr}^{max}) of a transport route is evaluated as the major difference between the delivery time and the due date among all the transport orders distributed (eq. 6.13). Similarly, the minimum earliness of a route is calculated as stated in equation 6.14.

$$T_{tr}^{max} = \max_{at\theta \in ts, ts \in tr} [max(Tfn_{ts} - dd_{at\theta}, 0)] \tag{6.13}$$

$$E_{tr}^{min} = \min_{at\theta \in ts, ts \in tr} [max(dd_{at\theta} - Tfn_{ts}, 0)] \tag{6.14}$$

With the new production decisions, the production and transport scheduling problems are solved again. The strategy proceeds iteratively while improvements are obtained. Because of the features of the rule-based algorithm developed in this research work, the priority list of associated transport orders and the assignment of vehicles established in the first transport schedule remain fixed, thus reducing the possibilities for improvement. Therefore, the algorithm has been implemented with a single iteration. Nevertheless, the transport times, initially unknown in production scheduling, are now taken into account.

6.4 Case studies

Two different case studies are next presented to prove the flexibility and applicability of the framework developed to support and coordinate production and transport scheduling decisions.

The first case study has been adapted from the example proposed in Dondo et al. (2003), and involves the distribution of a single product in 10 different locations. A fleet of 2 vehicles is available in the plant. A description and problem data for this case study are reported in Appendix B.5. The production layout for this example is very simple, but the aim is to illustrate the modeling approach developed for transport scheduling and the coordination of production and transport activities from the operational perspective, rather than to focus on the well-known production scheduling problem.

The second case study is based on the Procel production facility (Appendix B.3), and involves two different products that have to be distributed in eight retail outlets geographically spread around 200 km from the production site. The example is detailed in Appendix B.6. This example illustrates the concept of associated transport order (notice that transport order 5, 800 WU, is higher than the capacity of the available vehicles, 500 and 700 WU, hence two associated transport orders need to be defined).

For both case studies, the sequential coordination of production and transport scheduling has been solved first. The production schedule has been determined to fulfill the required production orders. Then, the exhaustive enumeration procedure has been used to identify the transport schedule for each combination of transport rules and to evaluate it in terms of the alternative criteria defined.

The first example considers the distribution of a single product. Therefore, the application of the integrated approach to exploit the flexibility of the plant is irrelevant. For the second case study, and in order to improve the management of inventory and the coordination of the activities, the integrated approach is assessed with three criteria: summed lateness, flow time, and multiple cost. Weight values for the F, $Routes$, E and T criteria in the multiple cost function ($\rho_1, \rho_2, \rho_3, \rho_4$ in equation 6.9) have been fixed at 50, 100, 5 and 20, respectively.

Concerning the computational issues, the heuristic-based modeling approach developed in this research work has been compared with the rigorous formulation proposed in Méndez et al. (2006a). The results obtained are discussed in the next sections.

6.5 Results and discussion

6.5.1 Production & transport: single product facility

For the single product case study, selected results obtained from the exhaustive enumeration procedure (see Section 6.3.3), out of the 48 possible combination of rules, are detailed in Table 6.4. The Gantt charts of coordinated schedules identified with the minimum lateness value (schedule *3* in Table 6.4, 4.7 h) and with the minimum multiple cost (schedule *5* in Table 6.4, 592.53 €) are depicted in Figures 6.7 and 6.8, respectively. The latter presents also a minimum flow time (5.3 h).

These results illustrate the wide range of decisions that can be made based on the criterion selected, and valuable insight on the performance of the system can be drawn. On the one hand, it is important to note the effects of the temporization rule. As expected, the *Backward from due date* rule (BD) favors earliness at the expense of high inventory costs, whereas the *Forward from earliest pick up* rule (FD) leads to reduced storage costs due to the sooner release of products and the subsequent lower inventory maintained in the plant throughout the time horizon (this is observed, for example, in schedules *4* and *6* in Table 6.4). On the other hand, the *Highest Demand* policy (HD) for prioritizing the transport orders guarantees that the major orders are delivered first, but it ignores completely the due dates, thus leading to increased lateness values (see, for example, schedules *5* and*10* in Table 6.4).

Different schedule performances are also observed concerning the loading criterion of the vehicles. The *Maximum Load* rule (ML) associates orders within the same vehicle provided that enough capacity is available, even if the release date is delayed. This way, the number of routes required to fulfill the transport orders is reduced (see schedules *2*, *5* and *10* in Table 6.4).

Regarding the assignment of vehicles, since the vehicles available in this example have the same attributes, *First Fit Vehicle* (FFV) and *Best Fit Vehicle* (BFV) rules tend to assign always the first vehicle of the list to all the transport orders. Consequently, tighter transport schedules are determined, with less flexibility and an underutilization of the resources as can be observed from the high expected deviation and lateness values (note, for example, schedules *1* and *2* in Table 6.4).

Concerning the uncertainty, it is interesting to notice the different ability of the schedules to deal with variable travel times, and the increased expected performance measures when compared with criteria based on nominal parameter values. In addition, observe for example schedules *5* and *6* from Table 6.4. Schedule *5* would be preferably selected in front of schedule *6* due to its better performance in terms of lateness, tardiness or earliness; however, its expected deviation and tardiness values are significantly higher (about 40% and 30%, respectively) than those for schedule *6*. Therefore, the implementation of schedule *6* may not result in the optimal strategy, but it appears to be more flexible and perform better in an uncertain environment.

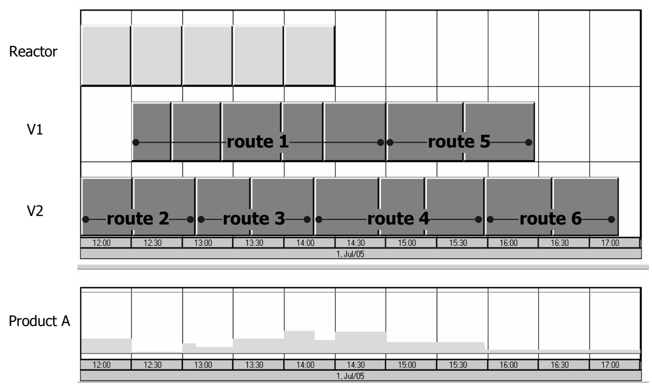


Figure 6.7: Gantt chart of the coordinated schedule with minimum lateness for case study 6.5.1 (4.71 h).

Table 6.4: Evaluation of transport schedules based on different combinations of transport rules for case study 6.5.1.

ID	Rules	c^{sum}	c^{tr}	c^{I}	L	T	E	F	E[Dev]	E[T]	E[F]	*Routes*
1	EDD - FFV - BD - MRT	1283.90	214.60	13340.03	18.2	18.2	0.0	8.4	19.8	30.1	10.4	5
2	EDD - BFV - FD - ML	686.70	91.10	6016.59	11.2	11.2	0.0	5.3	29.9	34.7	8.9	2
3	EDD - LUV - FD - DD	1136.23	252.85	3543.06	**4.7**	3.3	1.4	9.3	10.5	9.1	11.3	6
4	EDD - BAV - FD - MRT	1011.67	214.60	2053.54	8.3	3.3	5.0	8.4	11.2	9.2	10.4	5
5	EDD - BAV - FD - ML	**592.53**	91.10	2698.15	6.6	6.4	0.2	**5.3**	19.4	21.9	8.9	2
6	EDD - BAV - BD - MRT	1082.76	214.60	5093.56	9.1	7.8	1.3	8.4	11.4	15.4	10.4	5
7	EDD - BAV - BD - DD	753.55	135.75	5217.33	6.3	6.3	0.0	6.6	13.8	16.2	9.2	3
8	HD - BFV - FD - DD	1021.49	102.35	4980.89	27.3	25.6	1.7	6.0	23.2	43.2	8.8	2
9	HD - LUV - BD - MRT	976.13	179.60	5315.34	9.4	9.4	0.0	7.8	7.0	14.2	9.5	4
10	HD - BAV - FD - ML	869.31	102.35	2716.13	19.8	17.9	1.9	6.0	13.9	27.2	8.8	2

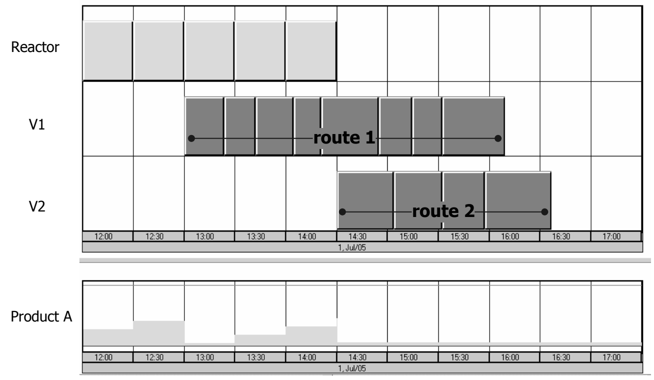


Figure 6.8: Gantt chart of the coordinated schedule with minimum multiple cost (592.53 €) and minimum flow time (5.3 h) for case study 6.5.1.

In general, however, when comparing the solutions from different combinations of rules, it is observed that a transport schedule with a good performance in the nominal scenario tends to perform also good when it is evaluated in terms of an expected performance. It is important to note that the modeling approach developed proceeds over a set of different rules using always the same input information, and the effects of the uncertainty are not managed proactively in the decision stage, but just evaluated. Therefore, it cannot be considered a proactive procedure to determine robust solutions. However, the analysis of simple measures in the context of the uncertainty, such as the expected deviation, can be used as valuable indicators of the most flexible schedules.

Generally, the results obtained provide powerful insight on the implications of the uncertainty and suggest that the deterministic criteria tend to overestimate the performance of the schedules, whereas the possibilities for making improved decisions when considering the uncertainty are very promising.

Rigorous vs. procedure-oriented modeling systems

With the use of an heuristic-based procedure to make decisions, there is no means to know how far they are from the optimal solution. To get a general idea of the effectiveness of the approach developed, this case study has also been solved using the mathematical formulation presented in Méndez et al. (2006a). The results obtained with both approaches for different objective functions are compared in Table 6.5.

The applicability of rigorous methods limited to quite small cases due to the inherent combinatorial nature of scheduling problems can be observed with the simple example examined. Note in Table 6.5 that the optimal solutions can not be found within reasonable computational time. For example, a multiple cost of 543.61 € is obtained after 10000 s CPU time with a relative gap of 14 %, whereas an approximated solution of 592.53 € is identified within 5 s using the rule-based heuristic algorithm.

Notice that the procedure-oriented approach required only 5 seconds to explore the overall combination of rules and identify the transport schedule based on the

Table 6.5: Comparison between heuristic and mathematical solution algorithms for case study 6.5.1.

	MILP*			Heuristic	
	criterion	% rel. gap	CPU [s]	criterion	CPU [s]
F	4.6	0.32	1000	5.3	5
L	1.3	0.46	1000	4.7	5
c^{sum}	616.25	0.38	1000	592.53	5
c^{sum}	543.61	0.14	10000	592.53	5

*MILP formulation presented in Méndez et al. (2006a), implemented in GAMS 20.5, and solved using the MILP solver of CPLEX(7.5) on a AMD Athlon 2000 computer.

criterion selected. The algorithm developed proves to be suitable on the generation of coordinated schedules with acceptable performance, particularly when considering flow time and multiple cost criteria. Additional heuristics may be further developed to improve the results when other objectives are pursued.

Concerning the uncertainty, the incorporation of variability in the travel times implies the reformulation of the MILP model into a stochastic programming problem (see Section 2.3), with the consequent increase in computational effort. An additional complexity is added in the model, which would hardly end up with a feasible solution; therefore, the extension of the rigorous formulation to the stochastic domain has not been contemplated.

6.5.2 Production & transport: Procel

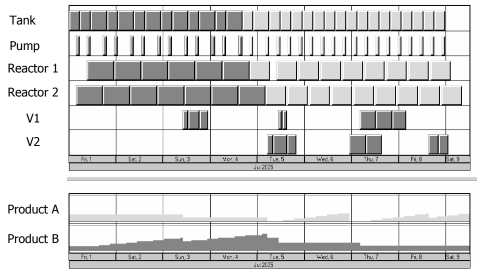
The second case study considered for production and transport scheduling concerns the Procel production facility (Appendices B.3 and B.6). The production scheduling problem is first addressed without taking into account the due dates of specific orders; the *Longest Processing Time* rule (LPT) is used for sequencing. With the subsequent application of the exhaustive enumeration procedure, alternative transport schedules are obtained. The trends observed in the previous example based on the combination of rules, as well as the analysis of uncertainty, are corroborated.

Table 6.6 summarizes the combination of rules and the values of the alternative criteria for transport schedules identified applying the sequential coordination and the integrated approaches (see Section 6.3.3) with minimum multiple cost (*s1, i11-i41*), minimum lateness (*s2, i12-i42*), minimum flow time (*s3, i13-i43*) and minimum inventory cost (*s4*). For example, for the integration considering the multiple cost criterion, the sequential approach is first solved, and the transport schedule with the best multiple cost ($s1$) is identified using the exhaustive enumeration procedure; this schedule is next used to update the production orders and derive a new production schedule that finally leads to the transport schedules *i11 - i41* depending on the desired criterion; the same is performed with the other objective functions.

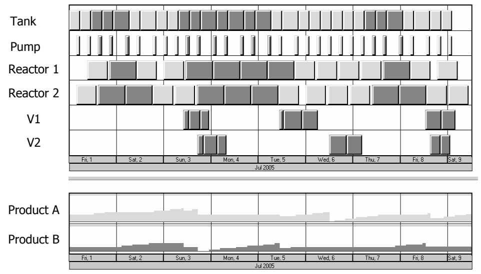
Figure 6.9 depicts Gantt charts of coordinated schedules identified with the best multiple cost, lateness, and flow time using the sequential and integrated methodologies. The transport routes of the transport schedule obtained with the minimum multiple cost (schedule *i11* in Table 6.6) are detailed in Table 6.7. Figure 6.10 depicts

Table 6.6: Evaluation of transport schedules based on different combinations of transport rules and determined using the sequential and integrated coordination procedures for case study 6.5.2 (due dates are neglected in the initial production scheduling problem).

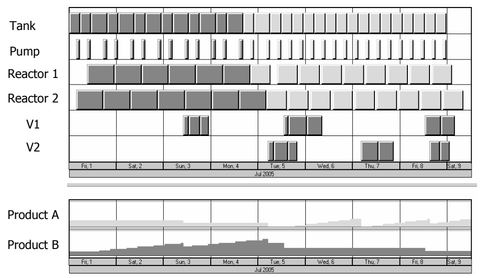
ID	Rules	c^{sum}	c^{tr}	c^{I}	L	T	E	F	E[Dev]	E[T]	E[F]	*Routes*
Sequential coordination												
s1	EDD - BAV - BD - MRT	**6201.30**	466.92	44908.47	89.8	64.7	25.1	83.6	13.4	69.6	88.6	6
s2	EDD - BAV - BD - ML	6337.70	530.20	47188.47	**77.0**	56.5	20.5	90.1	13.5	61.6	95.0	6
s3	HD - BAV - FD - DD	9562.80	434.76	34921.80	400.4	203.2	197.2	**78.3**	14.4	205.9	83.3	6
s4	EDD - lUV - FD - MRT	9072.40	532.00	**20868.91**	545.2	60.4	484.7	92.8	11.5	61.8	97.4	8
Integration using minimum multiple cost criterion												
i11	EDD - BAV - BD - MRT	**5390.50**	505.80	38657.00	57.1	0.0	57.1	90.1	13.5	4.2	95.0	6
i21	EDD - BAV - BD - ML	5390.50	505.80	38657.00	**57.1**	0.0	57.1	90.1	13.5	4.2	95.0	6
i31	HD - BAV - FD - DD	9202.30	434.76	25109.39	423.9	171.3	252.6	**78.3**	14.3	174.5	83.2	6
i41	EDD - BAV - FD - MRT	7438.70	479.76	**17380.49**	452.2	19.3	432.9	85.8	13.2	20.2	90.8	6
Integration using minimum lateness criterion												
i12	EDD - BAV - BD - MRT	**5390.50**	505.80	38519.23	57.1	0.0	57.1	90.1	13.5	4.2	95.0	6
i22	EDD - BAV - BD - ML	5390.50	505.80	38519.23	**57.1**	0.0	57.1	90.1	13.5	4.2	95.0	6
i32	HD - BAV - FD - DD	8747.30	434.76	22826.39	415.7	143.7	271.9	**78.3**	14.3	146.9	83.2	6
i42	HD - BFV - FD - MRT	9721.80	526.00	**17067.52**	486.0	123.4	362.6	92.8	12.8	124.6	97.6	8
Integration using minimum flow time criterion												
i13	EDD - BAV - BD - ML	**5768.20**	505.80	41439.89	73.42	19.7	53.7	90.1	13.5	23.7	95.0	6
i23	EDD - BAV - BD - ML	5768.20	505.80	41439.89	**73.42**	19.7	53.7	90.1	13.5	23.7	95.0	6
i33	HD - BAV - FD - DD	8550.8	434.76	23482.80	402.8	134.9	267.9	**78.3**	14.3	137.2	83.3	6
i43	HD - LUV - FD - MRT	10434.60	532.24	**15663.14**	562.6	145.3	417.3	92.8	13.2	146.1	97.6	8



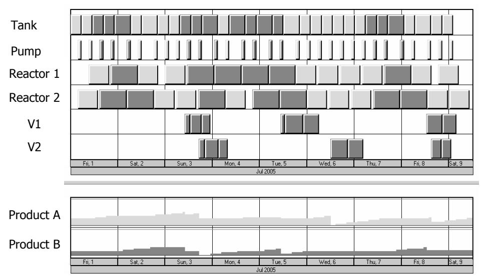
a. s1 (c^I: 44908.47 €).



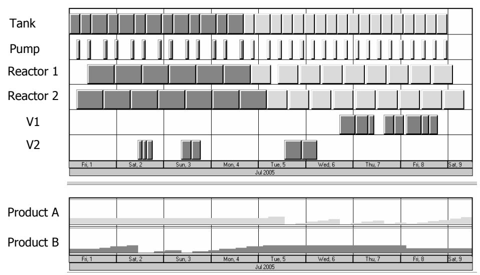
b. i11 (c^I: 38657.00 €).



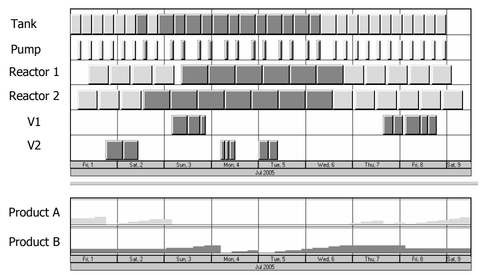
c. s2 (c^I: 47188.47 €).



d. i22 (c^I: 38519.23 €).



e. s3 (c^I: 34921.80 €).



f. i33 (c^I: 23482.80 €).

Figure 6.9: Gantt charts of sequentially (left-hand side, LHS) and integrated (right-hand side, RHS) coordinated schedules for case study 6.5.2 according to selected transport schedules in Table 6.6: a)/b) minimum multiple cost; c)/d) minimum lateness; e)/f) minimum flow time.

the corresponding transport routing.

The results obtained illustrate that the incorporation of information from the transport schedule in production scheduling allows to exploit the flexibility of the plant, thus leading not only to a better management of material flows between the plant and the distribution centers, but also to improved performances from different criteria point of view. Notice the reduced inventory costs of the schedules derived from the integrated approach as an indication of the improved inventory handling. For example, considering the lateness criterion, the best transport schedule obtained from the integrated approach (schedule *i22* in Table 6.6) shows lateness and inventory cost values reduced about 26 % and 18 %, respectively, compared with the schedule obtained in using the sequential procedure (schedule *s2*). The effects of integration

Table 6.7: Transport routes for transport schedule *i11* in Table 6.6.

Route	Vehicle	Start	End	Order	Site	Arrival	Departure	E	T
R1	V1	57.9	71.2	300	GIR	60.0	60.8	0.0	0.0
				200	LLE	65.9	66.6	1.1	0.0
R2	V2	65.0	80.0	400	TAR	67.0	68.2	0.0	0.0
				300	PER	73.9	75.2	34.2	0.0
R3	V1	106.6	126.2	400	VIC	108.0	108.9	0.0	0.0
				100	VAL	117.1	118.2	21.9	0.0
R4	V2	132.0	148.7	700	VAL	139.0	140.7	0.0	0.0
R5	V1	180.8	196.0	250	ZAR	187.0	188.8	0.0	0.0
R6	V2	183.0	193.3	350	AND	187.0	188.4	0.0	0.0

are also noticeable when transport orders are prioritized based on the highest amounts rather than the due dates (see schedule *s3* from Table 6.6); although a schedule with the same flowtime value (78.3 h) and a slightly higher lateness value is identified after integration (schedule *i33*), note the improved inventory management and the reduced tardiness measure (nearly 34 % with respect to schedule *s3*). This may be particularly important when customers satisfaction is a critical point. Again, these results show the wide range of decisions that can be drawn depending on the objective function considered.

In the context of the uncertainty, explicit effects of the integration on the robustness and flexibility features of the schedules cannot be perceived in this case study. In this sense, it is important to mention that these properties highly depend on the characteristics and the tightness of the schedules. In the integration algorithm implemented, the production sequence is rearranged with the implicit incorporation of

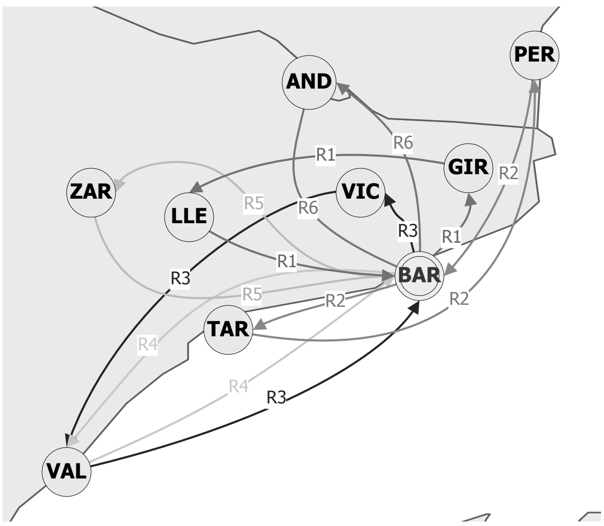


Figure 6.10: Transport routing representation for transport schedule *i11* in Table 6.6.

transport times information, whereas the assignment of vehicles to the associated transport orders remains fixed. Therefore, the routes identified assuming the same set of transport rules are likewise organized.

Rigorous vs. procedure-oriented modeling systems

This example has also been solved rigorously using the MILP formulation presented in Méndez et al. (2006a). Table 6.8 compares the results obtained with both approaches using the multiple cost criterion as objective function. As it can be observed, a poor solution is obtained with the pure MILP model after 10 h CPU time. Instead, the heuristic-based approach proves suitable for the generation of coordinated schedules with acceptable performance. However, using an heuristic algorithm as itself there is no means to know how far the solution is from the optimum one. The development of hybrid techniques coupling the inherent capabilities of MILP models and heuristics could result highly advantageous to efficiently address the simultaneous optimization of production and transport scheduling.

Table 6.8: Comparison between heuristic and rigorous solution algorithms for case study 6.5.2.

	MILP*	Heuristic †
c^{sum}	**8474.9**	**5390.5**
E	16.1	57.1
T	191.5	0.0
F	79.3	90.1
Routes	6	6
CPU [s]	**36000**	240.0
% rel. gap	0.64	-

*MILP formulation presented in Méndez et al. (2006a), implemented in GAMS 20.5, and solved using the MILP solver of CPLEX(7.5) on a AMD Athlon 2000 computer.
†Rules: EDD - BAV - MRT - BD

Due date-based production scheduling

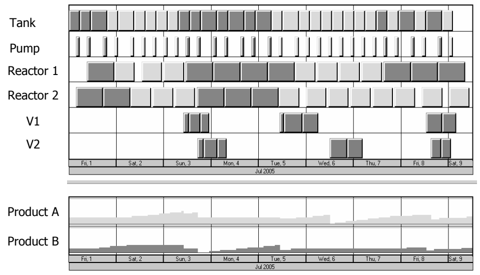
Up to this point, specific due dates of production orders have been neglected in production scheduling, as if all the requests for the same product had been aggregated in a single production order. This perception of the problem is commonly applied in manufacturing plants to derive a production schedule, neglecting the efficiency of the overall SC. The results obtained exemplify that significant improvements can be obtained from the integration of production and transport scheduling, at the expense of slightly suboptimal schedules.

The consideration of specific due dates for production orders when determining the initial production schedule has also been tested using the *Earliest Due Date* rule (EDD) for sequencing. Improvements are also achieved using the integration procedure, as can be observed from the results summarized in Table 6.9.

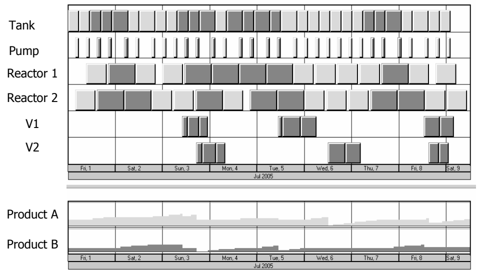
Note that considering the due dates already in the first production scheduling problem, it is difficult to identify better schedules from the multiple cost, lateness,

Table 6.9: Transport schedules based on different combinations of transport rules and determined using sequential and integrated coordination approaches for case study 6.5.2 (due date-based production scheduling).

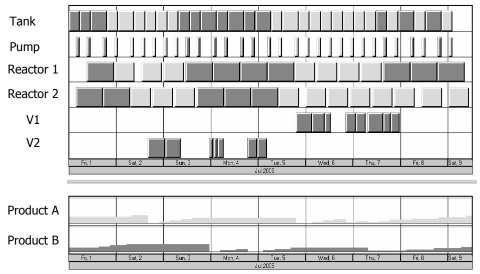
ID	Rules	c^{sum}	c^{tr}	c^{I}	L	T	E	F	E[dev]	E[T]	E[F]	*Routes*
Sequential coordination												
s1	EDD - BAV - BD - MRT	**5390.50**	505.80	38527.22	57.1	0.0	57.1	90.1	13.5	4.2	95.0	6
s2	EDD - BAV - BD - ML	5390.50	505.80	38527.22	**57.1**	0.0	57.1	90.1	13.5	4.2	95.0	6
s3	HD - BAV - FD - DD	9092.30	434.76	28059.39	401.9	171.3	230.6	**78.3**	14.3	174.5	83.2	6
s4	EDD - lUV - FD - MRT	6978.70	505.80	**17870.14**	374.7	0.0	374.7	90.1	14.0	0.04	95.0	6
Integration using minimum multiple cost/lateness criterion												
i11	EDD - BAV - BD - MRT	**5390.50**	505.80	38519.23	57.1	0.0	57.1	90.1	13.5	4.2	95.0	6
i21	EDD - BAV - BD - ML	5390.50	505.80	38519.23	**57.1**	0.0	57.1	90.1	13.5	4.2	95.0	6
i31	HD - BAV - FD - DD	8747.30	434.76	22826.39	415.7	143.7	271.9	**78.3**	14.3	146.9	83.2	6
i41	HD - BFV - FD - MRT	9721.80	526.00	**17067.52**	486.04	123.4	362.6	92.8	12.8	124.6	97.6	8
From integration using minimum flow time criterion												
i13	EDD - BAV - BD - ML	**5441.80**	505.80	39210.46	57.1	3.4	53.7	90.1	13.5	7.6	95.0	6
i23	EDD - BAV - BD - ML	5441.80	505.80	39210.46	**57.1**	3.4	53.7	90.1	13.5	7.6	95.0	6
i33	HD - BAV - FD - DD	8347.80	434.76	20192.39	422.2	115.5	306.7	**78.3**	14.3	117.8	83.3	6
i43	HD - BFV - FD - MRT	9205.30	526.00	**13584.64**	486.5	87.9	398.6	92.8	12.7	88.3	97.5	8



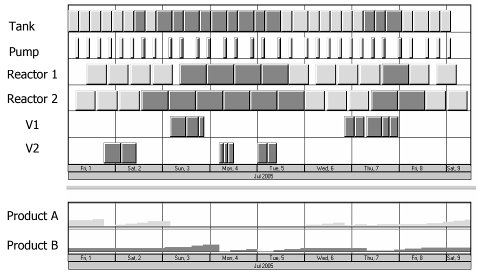
a. s1 (c^I: 38527.22 €).



b. i11 (c^I: 38519.23 €).



c. s3 (c^I: 28059.39 €).



d. i33 (c^I: 20192.39 €).

Figure 6.11: Gantt charts of sequentially (LHS) and integrated (RHS) coordinated schedules for case study 6.5.2 according to selected transport schedules in Table 6.9: a)/b) minimum multiple cost and lateness; c)/d) minimum flow time.

and flow time points of view. However, an improved management of the transport activities and the storage is attained, thus reducing significantly the inventory costs. Gantt charts of some coordinated schedules are depicted in Figure 6.11.

6.6 Concluding remarks

A more general perspective of the operational level of analysis is achieved in this chapter by extending the scope of research from production to distribution scheduling in a multi-site environment.

The coordination of production and transport activities constitutes a challenging problem, difficult, if not impossible, to generalize in terms of a single objective. A SC environment is highly dynamic and uncertain, and multiple priorities can be established when addressing the problem. In view of this situation, a procedure-oriented modeling and resolution framework has been developed, which allows the evaluation of schedules in terms of alternative criteria, and robustness and flexibility features are also addressed considering the uncertainty in the speed of the vehicles as a source of common unpredictable delays eventually arising in transport systems.

A methodology to sequentially coordinate production and distribution tasks has been implemented, coupled with an exhaustive procedure to evaluate different combinations of transport rules and to identify the transport schedules based on the criterion selected. This technique provides useful insight on the performance of the system. An integrated algorithm has also been developed to exploit the flexibility of the plants by updating the production scheduling problem with information about the associated transport orders and times derived from the transport schedule.

The strategy has been successfully applied to two different case studies showing its suitability to coordinate production and transport activities for the operational management of each entity in a multi-site system. The results obtained illustrate different trends and a wide range of decisions that can be made based on the preferences of the decision maker, as well as the benefits of an integration methodology especially in terms of inventory handling.

The framework can be easily embedded in a hierarchical modeling system for the simultaneous optimization of the SC at different levels (Figure 6.12). In a higher level, and as a result of an aggregated planning problem, tactical decisions are made (global production, warehouse and transport needs); these decisions are then used as constraints in the corresponding local sites (inferior level) when solving their detailed production and transport scheduling.

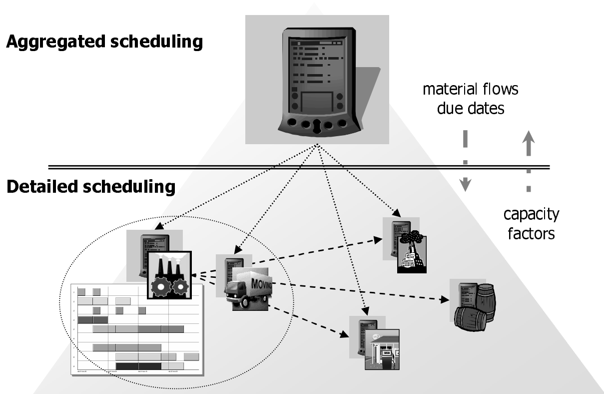


Figure 6.12: Hierarchical modeling system.

Concerning the uncertainty, the effects of variable travel times are merely evaluated, but it is again evidenced that deterministic approaches tend to overvalue the performance of the system, i.e., in terms of time efficiencies, the predicted times are lower than those actually realized during the implementation of the schedules, with the consequent increase of disturbances (see the analysis in Section 3.3.2, Table 3.1).

The recognition of the uncertainty and its incorporation in decision making becomes a step forward on the development of practical decision-support systems. The proactive approach presented in the previous chapter for short-term production scheduling could easily be incorporated in the production scheduling module of the framework developed in this chapter to deal also with uncertain processing times and equipment availability. An interesting proactive modeling approach could be generated, where not only variable travel times would be taken into account in production scheduling, but also the effect that uncertainties in the production process may eventually cause in transport scheduling. However, these operational uncertainties have been excluded from the modeling approach developed in this chapter to focus on the coordination of production and distribution activities, as well as on the transport scheduling problem from an operational perspective, avoiding additional modeling and computational complexities. A contribution is made in this direction, though further research is required to deal with this operational problem as a whole.

7.

Robust scheduling focused on tactical uncertainties: Risk management with uncertain product demands

I wanted a perfect ending. Now I've learned, the hard way, that some poems don't rhyme, and some stories don't have a clear beginning, middle, and end. Life is about not knowing, having to change, taking the moment and making the best of it without knowing what's going to happen next.

Gilda Radner (1946 - 1989)

To complete the development of proactive modeling systems for scheduling under uncertainty, the study in this chapter aims at providing insight on the effect of product demands as a tactical source of uncertainty in the low operational level of analysis. With this purpose, stochastic and robust optimization approaches are developed to address the short-term scheduling problem of batch plants with uncertain product demands. After an introduction and definition of the problem, a *two-stage stochastic programming model* is presented, and then extended to incorporate the availability of option contracts. Next, *management of risk* is explicitly addressed by appending a control measure in the objective function. Three alternative metrics are assessed and compared for this purpose. The suitability of the proactive approach is analyzed in two case studies, to finalize with some concluding remarks.

7.1 Introduction

The problem of product demands uncertainty has been largely considered in strategic and tactical levels of analysis, and different stochastic and robust optimization approaches have been proposed for the design and planning of process systems based on some probabilistic objective function. The main contributions in the field are outlined in Chapter 2.

Proactive scheduling approaches dealing with demand uncertainties and based on stochastic optimization (see Section 2.3) have been proposed. For example, Petkov and Maranas (1997) applied the chance-constrained technique (see Section 2.3.2) to address the multiperiod planning and scheduling problem of multiproduct plants and impose explicit lower bounds on the probabilities of satisfying variable demands; the problem consisted of obtaining the optimal planning policy (production and sales) and a corresponding feasible schedule that maximized the expected profit, while satisfying single or joint product demands with a minimum probability level; the expectation of the objective function, as well as the chance constraints, were expressed in a deterministic equivalent mixed-integer non-linear programming (MINLP) model.

Vin and Ierapetritou (2001) presented a two-stage stochastic programming formulation (see Section 2.3.3) for the short-term scheduling problem of batch plants, where the average makespan over a set of anticipated scenarios was to be minimized; the schedule obtained using nominal demand values and that obtained from the stochastic approach were assessed and compared in terms of different *robustness* measures based on the standard deviation or on one-sided deviations; however, these measures were not incorporated into the decision-making procedure. Another application of two-stage stochastic programming for scheduling a multiproduct batch plant was presented in Engell et al. (2002).

Sand et al. (2000) proposed a two-level hierarchical model involving a long-term planning problem, formulated as a two-stage stochastic linear problem, and a short-term deterministic scheduling problem. This framework was further considered by Engell et al. (2001) to address the same problem with uncertain demands and polymerization yields; it was claimed that scheduling is a real-time problem where only those decisions to be actually implemented have to be made within sufficient short response times based on the information available at decision time; all other coupled decisions should be regarded as a recourse for the effects of realized uncertainties.

With the latter idea, Sand and Engell (2004) proposed the application of two-stage stochastic integer programming techniques within a model predictive scheduling framework to address the real-time scheduling problem of multiproduct batch processes; the model fitted into the framework of multi-stage stochastic integer programming, and was decomposed into a master scheduling problem with demand and plant capacity uncertainties, and a detailed scheduling problem reflecting variable processing times and yields; both problems were approximated by two-stage stochastic integer programs using an scenario-based representation of the uncertainty.

A multistage stochastic mixed-integer linear programming (MILP) model for multiproduct batch plants was also presented by Balasubramanian and Grossmann (2004); an approximated resolution strategy was developed based on the solution of a series of two-stage models within a shrinking-horizon approach.

As it can be observed from the literature review, most of the contributions consider the demands uncertainty from a tactical perspective, and optimize only expected performances, thus assuming the decision maker is risk-neutral. In general, however, decision makers tend to be risk-averse, thus implying a major preference for lower variability for a given level of return.

The ability of robust optimization methods to account for different attitudes towards risk is highlighted in Section 2.4. Although the concept of robust optimization has largely been applied in design and planning problems, its extension to the lower level of scheduling is almost void. Within a multiproduct scheduling environment, Sand and Engell (2003, 2004) extended the objective function expressed in terms of expected profit with the concept of *minimum risk criterion* as a measure of the probability to obtain profit values below a certain threshold; nevertheless, demand uncertainties were analyzed in a long-term basis.

This study focuses on the effects of product demands uncertainty in short-term production scheduling, thus considering the interaction of a tactical source of uncertainty in the lower operational level. A proactive scheduling approach based on stochastic programming is first developed, and then extended to manage the risk of performing below a desired level. Alternative measures are evaluated in this robust optimization approach to explicitly control the variability of performances.

7.2 Problem statement

The scheduling problem of multiproduct batch plants with variable product demands is addressed to improve *schedule robustness* and to obtain alternate scheduling policies reflecting different attitudes versus risk in the context of demand uncertainty. Given are the production lines, a set of products to be produced with their given recipes, the time horizon, the economic data, and the probability distributions associated with the uncertain parameters. The decisions involve the number of batches to be produced of each product, the detailed production sequence, and the start and end times of each operation performed.

Schedule robustness is formalized as an expected profit accounting for revenues coming from the sales of products, production costs, changeover costs, inventory costs, and costs for underproduction. According to the general definition for schedule robustness given in Chapter 3 (Section 3.3.2), revenues along with production and changeover costs assess the efficiency of the system, whereas inventory and shortage costs can be regarded as a measure of the effects of uncertain product demands.

The following assumptions are made:

- One production line is considered, with fixed assignment of equipment units to tasks, and fixed batch sizes for each product. This assumption can be easily relaxed with slight modifications in some constraints.

- The zero wait (ZW) transfer policy is adopted. Under this policy, an intermediate product must be immediately transferred to the next processing step just after its production. Neither intermediate storage nor wait times in the processing units are available. This assumption could be easily modified to consider unlimited intermediate storage (UIS) or non-intermediate storage (NIS) transfer policies.

- Scheduling is addressed for a time horizon of one week. It is considered that products have to be delivered at the end of the week in a *just-in-time* (JIT) manner, but scheduling decisions must be made beforehand to start production and be able to meet the expected customer demands.

- Fixed costs for final inventory and shortage are adopted for each product. Costs for product changeovers are also considered to take into account technical difficulties that may arise with the change of products, as well as to avoid excessive shifts between them.

7.3 Modeling approach

The use of an equation-based modeling system is appropriate for describing the features of the underlying problem, and it is again considered for the development of the proactive scheduling application.

A **stochastic programming** approach is first generated based on a **recourse model** with two stages (refer to Section 2.3.3) to optimize an expected performance evaluated in terms of profit. The formulation is further extended with the possibility of selling some amount of products by exercising an **option contract**, thus aiming at introducing flexibility and implicitly reducing the risk of performing below a certain profit level. Both stochastic models assume that the decision maker is risk-neutral. A **robust optimization** modeling system (see Section 2.4) is finally developed for risk management to control the variability of solutions and reduce the risk of low profit values.

The uncertainty associated with product demands can be described indistinctly with discrete or continuous probability distributions, which are then discretized using Monte Carlo sampling (MCS) to generate a finite set of scenarios.

7.3.1 Scheduling model

A *two-stage stochastic MILP* formulation is derived based on a *batch slot* concept. for which the time horizon is viewed as a sequence of batches b, each of which is to be assigned to one particular product i. Decision variables related to the number of batches to be produced of each product and the detailed schedule, that is, the sequence and the start and end operation times of each task j, are considered first-stage decisions since it is assumed that they have to be made at the scheduling stage, before the uncertainty is unveiled. On the second stage, sales (Q^S_{ik}), inventory (Q^I_{ik}), and unsatisfied orders (Q^U_{ik}) are evaluated in each scenario k. A profit value is obtained for each particular realization of demand uncertainty. The model developed (SCHED) accounts for the optimization of schedule robustness, formally stated as the maximization of the expected value of the distribution of profits, and it is detailed below. The notation used is defined throughout the description of the model; however, refer to the Nomenclature chapter in page 153 for an overall reference.

(SCHED)

$$\begin{aligned}\max EPV = & \sum_k \left\{ \omega_k \cdot \left[\sum_i \left(\nu_i \cdot Q^S_{ik} - c^I_i \cdot Q^I_{ik} - c^U \cdot (\nu_i - c^P_i) \cdot Q^U_{ik} \right) \right] \right\} - \\ & - \sum_i c^P_i \cdot Q^P_i - \sum_{b,i,i'} c^c_{ii'} \cdot XM_{bii'} - \lambda \cdot \sum_{j,b} Tin_{jb}\end{aligned} \tag{7.1}$$

$$H \geq Tfn_{jb} \qquad \forall j, b \tag{7.2}$$

$$T_{jb} = \sum_i (X_{bi} \cdot Top_{ij}) \qquad \forall j, b \tag{7.3}$$

$$Tfn_{jb} = Tin_{jb} + T_{jb} \qquad \forall j, b \tag{7.4}$$

$$Tin_{jb'} \geq Tfn_{jb} \qquad \forall j, b < B, b' = b + 1 \tag{7.5}$$

$$Tfn_{jb} = Tin_{j'b} \qquad \forall j, j' = j + 1, b \tag{7.6}$$

$$\sum_{i} X_{bi} \leq 1 \qquad \forall b \tag{7.7}$$

$$\sum_{b} X_{bi} = n_i \qquad \forall i \tag{7.8}$$

$$X_{bi} + X_{b'i'} - 1 \leq XM_{bii'} \qquad \forall b < B, b' = b + 1, i, i' \tag{7.9}$$

$$\sum_{i} n_i \leq B \tag{7.10}$$

$$Q_i^P = n_i \cdot BS_i \qquad \forall i \tag{7.11}$$

$$Q_{ik}^S = \min(\theta_{ik}, Q_i^P) \qquad \forall i, k \tag{7.12}$$

$$Q_{ik}^I = Q_i^P - Q_{ik}^S \qquad \forall i, k \tag{7.13}$$

$$Q_{ik}^U = \theta_{ik} - Q_{ik}^S \qquad \forall i, k \tag{7.14}$$

The maximization of the expected profit value (EPV), equation 7.1, involves an expected second-stage performance, written as a sum of the sales of each product, inventory costs, and a penalty for underproduction in each scenario k weighted by its probability (w_k) of occurrence, and first-stage costs related to variable production costs and costs for product changeovers. Therefore, the maximization of the objective function establishes the most appropriate production policy that balances benefits with the effects of the uncertainty, i.e., inventory costs (which control the overproduction) and the cost for production shortfalls (which measures the loss of profit due to the unavailability of a product, and is modeled with a factor c^U of this profit value; for $c^U = 1$ the underproduction cost equals the profit lost due to the unsatisfied demand, whereas higher or lower values of this parameter impose a stricter or more relaxed safeguard against underproduction, respectively). A product demand satisfaction level is not explicitly imposed. The last term on the right-hand side of the objective function is a timing term, which is incorporated to reduce degeneracy and to assure that the operations will start as soon as possible when some slack time exists. λ is a parameter with a very small value that does not modify the optimality related to the other terms in the objective function.

Equations 7.2 to 7.11 are first-stage constraints that define the sequence and precedence relationships, the timing, and the number of batches to be produced. Equation 7.2 expresses the requirement of all tasks j to end within the time horizon H. Equation 7.3 is incorporated to assign to each batch b the operation times of the product i produced in that batch (Top_{ij}). The binary variable X_{bi} defines the assignment of product i to batch b; it takes the value of 1 if product i is produced in batch b, or 0 otherwise. The connections between the start (Tin_{jb}) and end times (Tfn_{jb}) in each stage j of batch b are provided by equation 7.4. To express the requirement of the initial time of every stage j from batch b to start after the same operation in the previous batch b', the precedence constraint 7.5 is used. In the same way, the sequence constraint 7.6 assures the ZW transfer policy between stages j of the same batch b. According to equation 7.7, at most one product i can be assigned to each batch b. In equation 7.8, the number of batches assigned for each product is constrained to be the number of batches produced of that product (n_i).

Concerning changeovers from product i to product i', the aggregated variable $XM_{bii'}$ is defined to avoid the introduction of non-linearities into the model. With equation 7.9, when a change occurs from product i in batch b to product i' in the following batch b', X_{bi}, $X_{b'i'}$, and consequently $XM_{bii'}$ take the value of 1. Through equation 7.10 the number of batches processed is limited to the maximum number of batches defined B. Finally, equation 7.11 defines the amount produced of each product (Q_i^P) based on the batch size (BS_i).

Second-stage constraints are defined from equations 7.12 to 7.14. They evaluate for each product i in each scenario k the quantity sold (Q_{ik}^S), final inventory requirements (Q_{ik}^I), and production shortfalls (Q_{ik}^U) at the end of the time horizon. Since an amount of product higher than the production can not be delivered, the quantity sold of each product is defined as the minimum between the demand and the amount produced (eq. 7.12 is internally handled in the modeling environment with two inequality constraints as stated in eqs. 7.15 and 7.16).

$$Q_{ik}^S \leq \theta_{ik} \qquad \forall i, k \tag{7.15}$$

$$Q_{ik}^S \leq Q_i^P \qquad \forall i, k \tag{7.16}$$

7.3.2 Scheduling model with option contracts

Options are contracts that give the holder the possibility of purchasing a certain amount of product at an specified price ν_i^{OC}. Since contracts are signed beforehand, the total amount of product that can be sold by exercising the respective *put option* has to be considered independently of the scenario finally realized. However, the amount of products eventually sold allocated to option contracts varies under the different scenarios.

Therefore, in addition to the number of batches and the scheduling decisions, first-stage variables in the new model (SCHEDOC) include the amount of options purchased (Q_i^{OC}). In the second stage, the quantity of product i allocated to option contracts in each scenario k is also assessed (Q_{ik}^{SOC}). The new model is detailed below.

(SCHEDOC)

$$\begin{aligned} \max EPV = & \sum_k \left\{ \omega_k \cdot \left[\sum_i \left(\nu_i \cdot Q_{ik}^S + \nu_i^{OC} \cdot Q_{ik}^{SOC} - c_i^I \cdot Q_{ik}^I - \right.\right.\right. \\ & \left.\left.\left. - c^U \cdot (\nu_i - c_i^P) \cdot Q_{ik}^U \right) \right] \right\} - \sum_i (c_i^{OC} \cdot Q_i^{OC} + c_i^P \cdot Q_i^P) - \\ & - \sum_{b,i,i'} c_{ii'}^c \cdot XM_{bii'} - \lambda \cdot \sum_{j,b} Tin_{jb} \end{aligned} \tag{7.17}$$

subject to:

eqs. 7.2 to 7.11

$$Q_{ik}^S + Q_{ik}^{SOC} = \min(\theta_{ik}, Q_i^P + Q_i^{OC}) \qquad \forall i, k \tag{7.18}$$

$$Q_{ik}^I = Q_i^P + Q_i^{OC} - Q_{ik}^S - Q_{ik}^{SOC} \qquad \forall i, k \tag{7.19}$$

$$Q_{ik}^U = \theta_{ik} - Q_{ik}^S - Q_{ik}^{SOC} \qquad \forall i, k \tag{7.20}$$

$$Q_{ik}^S \leq Q_i^P \qquad \forall i, k \tag{7.21}$$

$$Q_{ik}^{SOC} \leq Q_i^{OC} \qquad \forall i, k \tag{7.22}$$

Equation 7.18 expresses the sales of each product i in each scenario k as the minimum between the demand (θ_{ik}) and the available quantity, which is the product produced (Q_i^P) plus the product available from option contracts (Q_i^{OC}) (as for eq. 7.12, this constraint is handled in the modeling environment with two inequality constraints). Inventory requirements (Q_{ik}^I) and production shortfalls (Q_{ik}^U) are computed in constraints 7.19 and 7.20, respectively. Sales coming from the own production (Q_{ik}^S), can not be higher than the amount produced (Q_i^P); this is expressed by constraint 7.21. On the other hand, the amount of product allocated to an option contract (Q_{ik}^{SOC}) must be lower than the total amount contracted (Q_i^{OC}), as it is stated by inequality 7.22.

7.3.3 Risk management

Different metrics can be considered for robust optimization as a measure of the risk of obtaining poor revenues. As it is reviewed in Chapter 2 (see Section 2.4), the variance is one of the metrics commonly used for quantifying the variability of performances. However, two significant drawbacks of this measure for risk management have been identified. On the one hand, the variance is a symmetric measure of dispersion around the expected value; therefore, in an attempt to reduce the dispersion of values around the mean, some decisions leading to favorable results are discarded. On the other hand, it introduces non-linearities into the formulation, thus increasing the computational requirements of the models.

In view of these limitations, and pursuing the identification of more robust predictive schedules that guarantee an acceptable expected profit value with reduced risk exposures, three alternative measures for risk management are considered and appended as a second criterion to the objective function of the stochastic models presented above: the **financial risk** metric as analyzed by Barbaro and Bagajewicz (2004b), the **downside risk** definition proposed by Eppen et al. (1989), and the **worst-case** performance.

To understand and assess the trade offs between risk and profit, the so called *risk curve* is used, which is the cumulative curve of profit values over all the scenarios, and which indicates the level of incurred risk at each profit value. Depending on the decision-maker attitude towards risk, low risk for some conservative profit aspiration levels or low risk at higher profit aspiration levels (even if risk at lower profit values increases), would be desired. Hypothetical examples of these extremes are depicted in Figure 7.1.

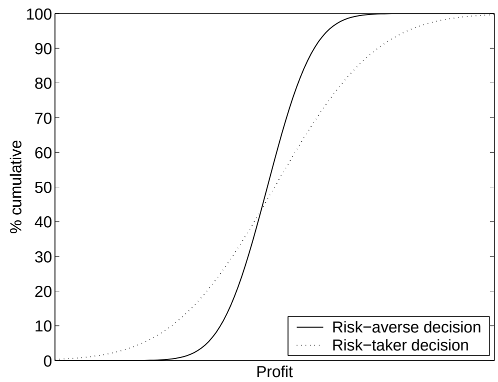


Figure 7.1: Examples of risk curves with different risk preferences.

Financial Risk

Financial risk (FR) is a probabilistic approach for risk management defined as the probability of not meeting a target profit Ω (Barbaro and Bagajewicz, 2004b). It is mathematically expressed as stated in equations 7.23 and 7.24.

$$FR_{\Omega} = \sum_{k} \omega_k \cdot Y_{k\Omega} \tag{7.23}$$

$$Y_{k\Omega} = \begin{cases} 1 & \text{if } PV_k < \Omega, \\ 0 & \text{otherwise} \end{cases} \qquad \forall k \tag{7.24}$$

The risk term is included in the objective function of the stochastic models as expressed in equation 7.25, where the goal programming weight ρ is incorporated to manage the trade off between both criteria. The *EPV* term is defined according to equations 7.1 and 7.17 for the SCHED and SCHEDOC models, respectively.

To enforce the new integer variable $Y_{k\Omega}$ to take the value of 1 if the profit is less than the corresponding target value Ω, constraint 7.26 is required; otherwise, the value of 0 in the optimal solution is assured by the own risk term in the objective function. The PV_k term includes all sales and cost terms defined in the objective function (eqs. 7.1 and 7.17), except for the timing term.

$$max \quad EPV - \rho \cdot \sum_{k} \omega_k \cdot Y_{k\Omega} \tag{7.25}$$

$$PV_k \geq \Omega - M \cdot Y_{k\Omega} \qquad \forall k \tag{7.26}$$

Downside Risk

Downside risk (*DR*) is an alternative measure of risk defined as the expected value of the positive deviation from the target Ω (Eppen et al., 1989). It is mathematically formulated by equations 7.27 and 7.28.

$$DR_{\Omega} = \mathrm{E}[\phi_{k\Omega}] \tag{7.27}$$

$$\phi_{k\Omega} = \begin{cases} \Omega - PV_k & \text{if } PV_k < \Omega, \\ 0 & \text{otherwise} \end{cases} \qquad \forall k \tag{7.28}$$

For robust optimization using the downside risk metric, the stochastic formulations are extended with the incorporation of the downside risk term in the objective function (eq. 7.29), and the additional constraints 7.30 and 7.31. Again, the *EPV* term is defined as in equations 7.1 or 7.17.

$$max \quad EPV - \rho \cdot \sum_{k} \omega_k \cdot \phi_{k\Omega} \tag{7.29}$$

$$\phi_{k\Omega} \geq \Omega - PV_k \qquad \forall k \tag{7.30}$$

$$\phi_{k\Omega} \geq 0 \qquad \forall k \tag{7.31}$$

It is worthwhile to note that financial risk is defined as a probability, whereas downside risk is an expected value. Barbaro and Bagajewicz (2004b) showed the quantitative relationship between financial and downside risk measures stated in equation 7.32. Therefore, downside risk is determined by the area under the risk curve from profit $\xi = -\infty$ to the profit target $\xi = \Omega$. Using downside risk in the framework of two-stage stochastic models leads to modeling strategies similar to the case of financial risk. The advantage of using downside risk is that the spectrum of solutions with different risk preferences can be obtained without the need of introducing binary variables in the model. The only known problem is that downside risk is not monotonic with financial risk, that is, a solution having smaller downside risk than another does not necessarily present an smaller financial risk. This aspect was underlined by Barbaro and Bagajewicz (2004b).

$$DR_{\Omega} = \int_{-\infty}^{\Omega} FR_{\xi} d\xi \tag{7.32}$$

Worst-case risk

The worst profit value (WPV) is also adopted as an alternative metric to control or reduce the probability of meeting unfavorable scenarios. A major difference with respect to the other approaches is that the probability information of the uncertain data is not used. Moreover, both the expected profit and the profit in the worst-case scenario are to be maximized as shown in the modified objective function stated in equation 7.33; as in the previous approaches, the EPV is defined as the objective functions of the stochastic models SCHED (eq. 7.1) and SCHEDOC (eq. 7.17). Constraint 7.34 needs to be also incorporated into the models to assess the worst-case profit value that balances the expected profit with a weight value ρ.

$$max \quad EPV + \rho \cdot WPV \tag{7.33}$$

$$WPV \leq PV_k \qquad \forall k \tag{7.34}$$

The predictive schedule with the best worst profit value attainable (WPV^{max}) can be obtained by applying the following procedure:

STEP 1. Solve the SCHED (SCHEDOC) model maximizing the WPV as a single objective function, instead of equation 7.1 (7.17), and incorporating constraint 7.34.

STEP 2. Solve the SCHED (SCHEDOC) model maximizing the expected profit as defined in equation 7.1 (7.17), and incorporating constraint 7.34 as well as the WPV^{max} value obtained in the previous step as a lower bound (eq. 7.35).

$$WPV \geq WPV^{max} \tag{7.35}$$

7.4 Case Studies

The proactive models developed in the framework of two-stage stochastic programming for risk management in scheduling under demand uncertainty have been tested in the motivating example introduced in Section 1.3, and described in Appendix B.1, as well as in the multiproduct batch plant presented in Appendix B.2.

First, the deterministic formulations with nominal demand values are solved, and the predictive schedules thus obtained are evaluated in front of the different scenarios, i.e., fixing the scheduling decisions, the profit values that would be obtained after the execution of the deterministic predictive schedule in each of the scenarios sampled are computed. Deterministic models derive simply from the stochastic formulations presented above (SCHED and SCHEDOC) considering only one scenario with the nominal demand values. The *pure* two-stage stochastic models are next solved, and the effectiveness of the methodologies developed for risk management are finally investigated.

In both examples, products have to be produced within a time horizon H of one week (168 h), and a value for the production shortfall cost (c^U) of 2 MU has been adopted. Demand uncertainty has been represented with normal probability distributions, which have been discretized in 100 independent and equiprobable scenarios through MCS. The standard deviation of product demands has been assumed to be 50 % of their mean values. Although this deviation is relatively high, it makes sense for the relative short time horizon of operation, during which the required amounts may vary from null orders to some considerable quantities. Besides, the parameter λ for the timing term in the objective function has been fixed at 10^{-6}.

The models have been implemented in GAMS (Brooke et al., 1988), and solved using the MILP solver of CPLEX (7.5) on a AMD Athlon 2000 computer. For information purposes, model sizes and computational requirements for the stochastic and robust formulations of both examples considering options (SCHEDOC) are reported in Table 7.1.

Table 7.1: Model sizes and computational requirements.

	Flow shop (section 7.5.1)	Multiproduct plant (section 7.5.2)
Stochastic model		
Constraints	4849	4948
Binary variables	580	580
Continuous variables	2287	2347
EPV	1732	2192
CPU time*	70.2	645.6
Robust model with FRisk ; DRisk ; WCase		
Constraints	5049 ; 5049 ; 4949	5148 ; 5148 ; 5048
Binary variables	680 ; 580 ; 580	680 ; 580 ; 580
Continuous variables	2287 ; 2387 ; 2288	2347 ; 2447 ; 2348
EPV	1634 ; 1634 ; 1553	2189 ; 1883 ; 1947
$FR_{\Omega=0}; DR_{\Omega=0}; WPV$	0.0 ; 0.0 ; 221	0.2 ; 1.87 ; -108
CPU time*	50.9 ; 67.6 ; 36.9	1956.3 ; 196.4 ; 224.1

*seconds with GAMS 20.5/CPLEX(7.5), on a AMD Athlon 2000 computer.

7.5 Results and discussion

7.5.1 Motivating example

Deterministic vs. stochastic

Detailed results obtained from the resolution of the deterministic and the two-stage stochastic SCHED and SCHEDOC models are reported in Tables 7.2 and 7.3, respectively. The corresponding cumulative distributions of profit values for all the scenarios sampled are plotted in Figure 7.2.

It is important to notice from these results that the solutions predicted with the deterministic formulations poorly represent the uncertain environment, i.e., the schedules obtained assuming nominal product demands (and referred to as *deterministic* predictive schedules) may be critically inefficient when another demand is ordered. Indeed, although the profit values of the deterministic predictive schedules are optimal in the nominal scenario and higher than their stochastic counterparts (see PV_{nom} in Tables 7.2 and 7.3), when the deterministic predictive schedules are executed in the uncertain environment, the expected profit value drops about 65 % from the optimum in the nominal conditions (from 3546 to 1257 MU). The schedules determined using the stochastic models (and referred to as *robust* predictive schedules) perform with a better expected profit over the uncertain space (1596 and 1732 MU), about 21 % and 27 % higher than the deterministic ones (1257 MU). This is also reflected with the shift to the right of the stochastic risk curves (Figure 7.2). Note that the deterministic models do not account for inventory to hedge from adverse scenarios and meet customer requirements, as the stochastic ones do, and hence the deterministic predictive schedules propose fewer batches than the robust ones. Despite the higher inventory costs, the robust predictive schedules show reduced production shortfalls, and hence improved customer satisfaction, thus assuring a much better overall expected profit.

Concerning the availability of option contracts (SCHEDOC model), these are not used in a deterministic context for this case study since no additional benefits are obtained (see Table 7.3). Instead, in the stochastic environment the same number

Table 7.2: Deterministic and stochastic results for case study 7.5.1 with model SCHED (n_i: number of batches for each product; Q_i^P: production amounts; $\mathrm{E}[Q_{ik}^S]$: expected sales; $\mathrm{E}[Q_{ik}^I]$: expected inventory; $\mathrm{E}[Q_{ik}^U]$: expected underproduction; PV_{nom}: profit value in the nominal scenario; EPV: expected profit value).

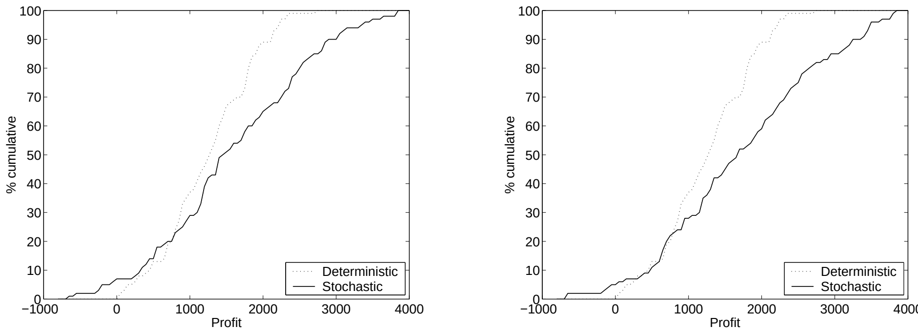
	Deterministic					Stochastic				
Product	i1	i2	i3	i4	i5	i1	i2	i3	i4	i5
n_i	2	1	3	1	1	3	1	4	1	1
Q_i^P	200	100	300	100	100	300	100	400	100	100
$\mathrm{E}[Q_{ik}^S]$	170	83	256	84	84	205	83	295	84	84
$\mathrm{E}[Q_{ik}^I]$	30	17	44	17	16	95	17	105	17	16
$\mathrm{E}[Q_{ik}^U]$	35	13	49	16	15	0	13	10	16	15
PV_{nom}	**3546**					2616				
EPV	1257					**1596**				

Table 7.3: Deterministic and stochastic results for case study 7.5.1with model SCHEDOC (n_i: number of batches for each product; Q_i^P: production amounts; Q_i^{OC}: options purchased; E[Q_{ik}^S]: expected sales from production; E[Q_{ik}^{SOC}]: expected sales from options; E[Q_{ik}^I]: expected inventory; E[Q_{ik}^U]: expected underproduction; PV_{nom}: profit value in the nominal scenario; EPV: expected profit value.).

	Deterministic					Stochastic				
Product	i1	i2	i3	i4	i5	i1	i2	i3	i4	i5
n_i	2	1	3	1	1	3	1	4	1	1
Q_i^P	200	100	300	100	100	300	100	400	100	100
Q_i^{OC}	0	0	0	0	0	0	22	0	28	24
E[Q_{ik}^S]	170	83	256	84	84	205	69	295	66	70
E[Q_{ik}^{SOC}]	0	0	0	0	0	0	22	0	28	24
E[Q_{ik}^I]	30	17	44	17	16	95	31	105	34	30
E[Q_{ik}^U]	35	13	49	16	15	0	5	10	5	5
PV_{nom}			**3546**					2177		
EPV			1257					**1732**		

of batches predicted with the SCHED model is determined, but the use of option contracts introduces some degree of flexibility, which translates into an 8 % higher expected profit (1732 vs. 1596 MU) due to an improved customer satisfaction level.

To assess the value of knowing and using distributions of future outcomes, i.e., to evaluate the advantages of solving the stochastic model, the *Value of Stochastic Solution* (VSS) can be easily computed (Birge and Louveaux, 1997). This value is the difference between the solution obtained from the stochastic formulation and the expected value of the deterministic problem. Without option contracts the VSS is 339 MU (1596 - 1257 MU); with the introduction of option contracts the VSS raises up to 475 MU (1732 - 1257 MU).



a. b.

Figure 7.2: Deterministic and stochastic risk curves for case study 7.5.1 with models: a) SCHED; b) SCHEDOC.

Another metric used in the stochastic domain is the *expected value of perfect information* (EVPI), which measures the value of knowing the future with certainty (see Section 2.3.1). It is evaluated as the difference between the mean value of optimal solutions in each scenario and the solution of the stochastic model. Solving the deterministic SCHED and SCHEDOC models for each scenario, the mean profit value over all the scenarios resulted in 2546 MU and 3448 MU, respectively. Based on these quantities, the EVPI is 950 MU (2546 - 1596 MU) without option contracts, and raises up to 1716 MU (3448 - 1732 MU) when introducing the options.

To further illustrate the suitability of the stochastic formulation developed and the poor adequacy of a deterministic approach in an uncertain context, the performance of the robust and deterministic predictive schedules in the random scenario evaluated in Chapter 1 (see Tables 1.2 and 1.3) is analyzed. As assessed in Chapter 1, the optimum profit of 2723 MU for the random scenario drops about 34 % (to 1790 MU) when the predictive schedule determined assuming nominal demands is executed in the conditions of the random scenario. A better performance is obtained using the robust predictive schedules as a guidance during execution (see the results summarized in Table 7.4). When implementing the predictive schedule derived from the SCHED model, a profit value of 1885 MU is obtained in the random scenario, whereas the benefits are slightly higher (up to 1987 MU) when option contracts are available (SCHEDOC model). These performances represent an increase of 5 % and 10 %, respectively, from the revenues expected if the uncertainty is ignored.

Table 7.4: Results from the execution of the robust predictive schedules in the random scenario defined in Table B.6 for case study 7.5.1.

	SCHED					SCHEDOC				
Product	i1	i2	i3	i4	i5	i1	i2	i3	i4	i5
n_i	3	1	4	1	1	3	1	4	1	1
Q_i^P	300	100	400	100	100	300	100	400	100	100
Q_i^{OC}	0	0	0	0	0	0	22	0	28	24
Q_{ik}^S	250	100	200	100	80	250	130	200	100	80
Q_{ik}^{SOC}	0	0	0	0	0	0	22	0	0	0
Q_{ik}^I	50	0	200	0	20	50	0	200	28	44
Q_{ik}^U	0	30	0	0	0	0	8	0	0	0
PV_{nom}	2616					2177				
PV_{rnd}	1885					1987				
EPV	1596					1732				

Risk analysis

Robustness is next investigated using the robust optimization formulations derived from the appendage of the alternate metrics for risk management presented in Section 7.3.3. Different target profits (Ω) and weight values (ρ) for the risk measures are tested obtaining several alternate predictive schedules. Results related to the profit value in the nominal scenario (PV_{nom}), the expected profit (*EPV*), the worst profit value (*WPV*), and the financial (*FR*) and downside risk (*DR*) values at targets 0 and

500 MU obtained with both SCHED and SCHEDOC models are summarized in Tables 7.5 and 7.6, respectively, for different approaches out of the multiple combinations of target profits and weight risk values. Selected risk curves are depicted in Figure 7.3, where the *pure* stochastic solution is included for comparison purposes.

Table 7.5: Selected results from risk management with financial risk (FRisk), downside risk (DRisk), and worst-case risk (WCase) measures for case study 7.5.1 with model SCHED.

SCHED	PV_{nom}	EPV	WPV	$FR_{\Omega=0}$	$FR_{\Omega=500}$	$DR_{\Omega=0}$	$DR_{\Omega=500}$
Deterministic	**3546**	1257	19	0.00	0.13	0.00	30.43
Stochastic	2616	**1596**	-681	0.07	0.14	20.38	66.58
FRisk$_{(\Omega=500;\rho=10^4)}$	3166	1435	-339	0.05	**0.12**	8.64	46.33
DRisk$_{(\Omega=0;\rho=20)}$	3166	1435	-339	0.05	0.12	**8.64**	46.33
WCase$_{(\rho=0.48)}$	3166	1435	-339	0.05	0.12	8.64	46.33
WCase$_{max}$	3546	1257	**19**	0.00	0.13	0.00	30.43

Table 7.6: Selected results from risk management with financial risk (FRisk), downside risk (DRisk), and worst-case risk (WCase) measures for case study 7.5.1 with model SCHEDOC.

SCHEDOC	PV_{nom}	EPV	WPV	$FR_{\Omega=0}$	$FR_{\Omega=500}$	$DR_{\Omega=0}$	$DR_{\Omega=500}$
Deterministic	**3546**	1257	19	0.00	0.13	0.00	30.43
Stochastic	2177	**1732**	-676	0.05	0.10	16.58	52.67
FRisk$_{(\Omega=100;\rho=10^4)}$	2950	1602	100	0.00	0.07	0.00	16.61
FRisk$_{(\Omega=10^3;\rho=10^4)}$	2888	1596	38	0.00	0.08	0.00	17.65
DRisk$_{(\Omega=0;\rho=10)}$	2633	1695	-217	0.02	0.07	4.12	29.57
DRisk$_{(\Omega=500;\rho=100)}$	3198	1475	125	0.00	0.07	0.00	10.10
WCase$_{(\rho=0.3)}$	2891	1623	38	0.00	0.06	0.00	18.94
WCase$_{(\rho=0.4)}$	3002	1584	149	0.00	0.08	0.00	15.62
WCase$_{(\rho=0.5)}$	3074	1553	221	0.00	0.08	0.00	13.87
WCase$_{max}$	3182	1456	**329**	0.00	0.09	0.00	12.41

The results obtained reveal how the risk management methodology tries to restructure the risk curves so as to reduce risk and the dispersion of profits, while maintaining an acceptable expected revenue. Notice that the risk curves obtained lay below the distribution with maximum expected profit (stochastic risk curve) at low profit values and, as expected, they intersect it at some point.

With the SCHED model (see Table 7.5), the same predictive solution is attained with the three alternative risk metrics, and a clear reduction of risk is achieved when compared with the stochastic formulation; however, the realization of some of the scenarios still shows a negative return. Note that the deterministic solution matches the solution with the maximum worst profit, hence any robust solution can be expected with a minimum profit value over all the anticipated scenarios better than 19 MU.

The possibility of using option contracts (SCHEDOC model) translates into a

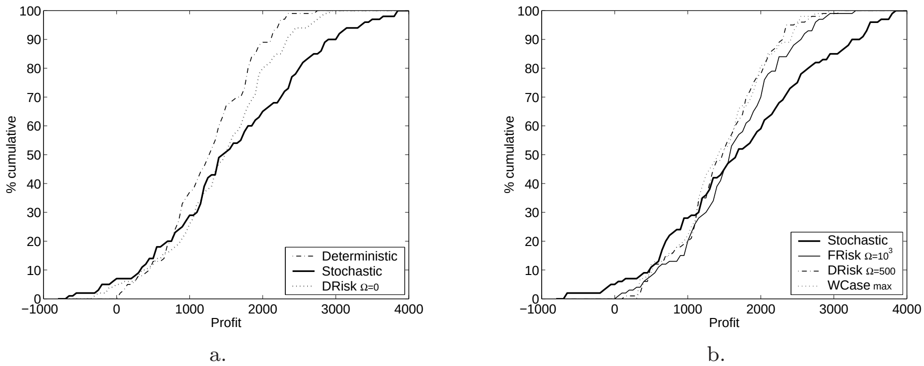


Figure 7.3: Risk curves for case study 7.5.1 with alternative robust formulations with models: a) SCHED; b) SCHEDOC.

larger flexibility and a more effective management of risk, as can be observed from the high number of alternative configurations obtained with the robust optimization methodologies for different weight values (see Table 7.6). In addition, several predictive schedules are obtained with the entire risk curve above a target of 0 MU, i.e., predictive schedules which assure a positive return within the entire uncertain region. The expected profit values of these more robust solutions are slightly lower than the maximum expected profit determined with the pure stochastic model (1732 MU), but they are more than 13 % higher that the expected performance of the deterministic predictive schedule for all the curves identified, with a good revenue also in the nominal scenario.

At this point, the trade off between risk and profit is further investigated by parametrically varying the weight of the risk term in the objective function. Pareto curves obtained managing downside risk at target profits of 0 and 100 MU with the SCHEDOC model are depicted in Figure 7.4 (a). Equivalent curves obtained with the worst-case risk measure are plotted in Figure 7.4 (b).

Each Pareto point corresponds to one risk curve, i.e., an alternative predictive schedule; the decision of which one to implement is up to the decision maker. As it is expected, a reduction of downside risk or a better worst profit value are attained at the expense of a reduction in the expected performance. As the weight value of the risk functions decreases, the expected profit of the solutions converges to the maximum performance obtained with the stochastic model. The latter is also attained by increasing the target profit at fixed weight values.

In general, the results obtained reveal that the three alternative measures implemented in the proactive scheduling approach seem appropriate to deal with the uncertain demands in the decision-making process and provide different risk profiles. Concerning the computational effort, the time required to obtain robust solutions for this case study ranges from 40 to 1000 seconds of CPU time depending on the metric, the target profit, and the weight values (as pointed out previously in Chapter 3, note that the major purpose of the study is to propose a framework for risk management, rather than to developed the most efficient solution algorithm). It is

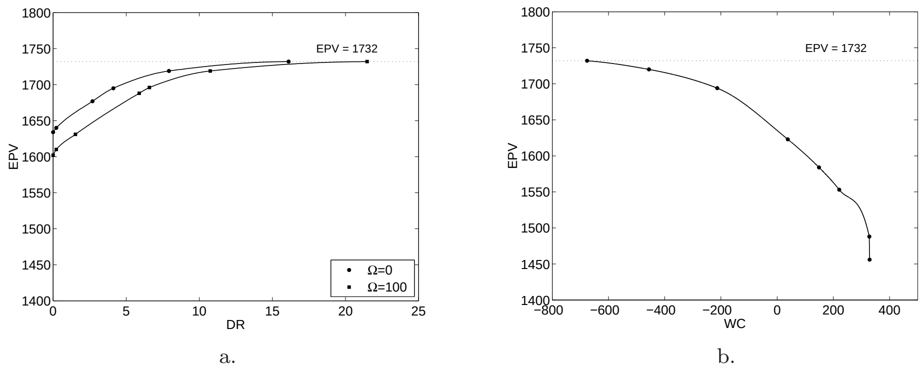


Figure 7.4: Trade off between the expected profit and risk for case study 7.5.1: a) downside risk; b) worst-case risk.

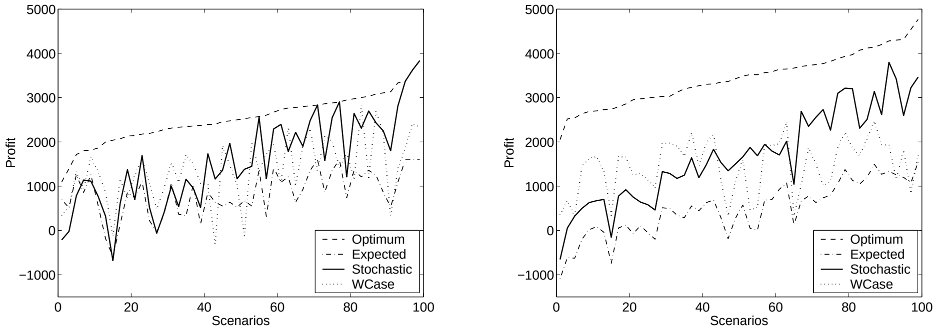
worthwhile to mention the increased combinatorial complexity associated with the financial risk procedure due to the additional binary variables. On the other hand, the simple worst-case risk procedure shows a remarkable efficiency for identifying robust scheduling strategies with a good performance over the uncertain region, with significantly reduced computational requirements.

With the aim to directly compare the robustness of the different methodologies in each scenario, the profit value that would be attained depending on the predictive schedule implemented is depicted for all the anticipated scenarios in Figure 7.5. The optimum performance in each scenario is included, along with the expected profit of each optimal schedule over all the scenarios (optimum and expected values, respectively, in Figure 7.5); these values are obtained by solving the deterministic formulation for each realization of demand uncertainty, and by evaluating each predictive schedule thus determined over all the other scenarios sampled.

The scarce representation of the uncertain environment by the deterministic formulation is also observed in these graphics from the significative difference between the optimum profit value for each scenario and its expectation when the uncertainty is faced. It is important to point out the higher variability of the stochastic solution when compared with solutions attained by controlling risk.

In addition, the pictures in Figure 7.5 clearly illustrate the different performance of the system and the major flexibility when option contracts are available, which leads to larger revenues and a more effective management of risk over all the scenarios. However, the difference between the optimum and the expected profits is stressed, thus emphasizing the need of addressing the uncertainty from a proactive viewpoint to avoid highly unsatisfactory performances. Note that the stochastic modeling systems developed in this study lead to predictive schedules that meet the optimum performance for some scenarios when option contracts are not considered (Figure 7.5 (a)), but they are far from the optimum when options are introduced, although the performance in each scenario is much better than the expected one when adopting a deterministic view of the problem.

On the other hand, it is worthwhile to note that all the predictive schedules ob-



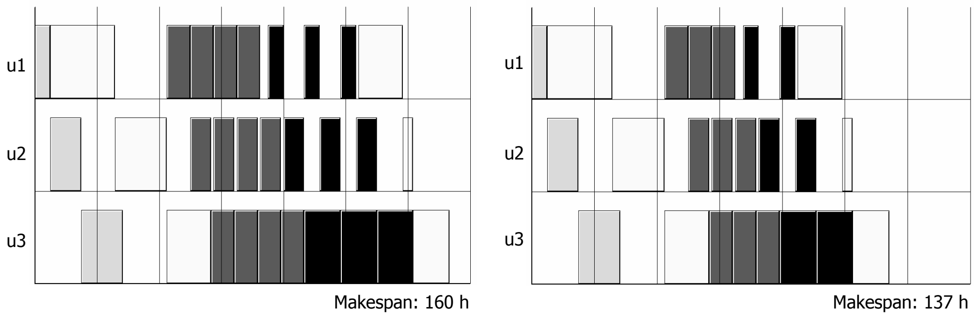
a. b.

Figure 7.5: Optimum and expected profit values in each scenario resulting from the deterministic predictive schedules, and profits obtained when implementing the predictive schedules derived from the stochastic and worst-case approaches for case study 7.5.1 using the models: a) SCHED; b) SCHEDOC.

tained with the different approaches show a coherent performance over the scenarios, which can be considered as an indication of the representability of the scenarios sampled.

Finally, Gantt charts of the predictive schedules with maximum expected profit and maximum worst profit determined with the stochastic and the worst-case risk SCHEDOC formulations are depicted in Figure 7.6.

One important thing to notice for this case study is that the predictive schedule determined with the worst-case risk approach is also identified with the other risk management methods reported in Table 7.6, except for the downside risk with a target profit of 0 MU, and corresponds also to the deterministic predictive schedule. The different revenues and risk values come from the different contracts purchased.



a. b.

Figure 7.6: Gantt charts of predictive schedules for case study 7.5.1 with: a) maximum expected profit; b) maximum worst profit.

7.5.2 Multiproduct plant

Deterministic vs. stochastic

Similar results as those reported for the previous case study are observed in the multiproduct plant example. Tables 7.7 and 7.8 detail the results obtained with the deterministic and two-stage stochastic SCHED and SCHEDOC models, respectively, related to the number of batches for each product, n_i; amounts produced or contracted, Q_i^P and Q_i^{OC}; expected sales, $E[Q_{ik}^S]$ and $E[Q_{ik}^{SOC}]$; expected inventory, $E[Q_{ik}^I]$; expected underproduction, $E[Q_{ik}^U]$; profit value for the nominal scenario, PV_{nom}; and expected profit value, EPV. The corresponding risk curves are plotted in Figure 7.7.

The deficient performance in the uncertain environment of predictive schedules obtained with the deterministic formulations can also be inferred from this example. The expected profit value of the deterministic predictive schedules is about 63 % lower than the optimal performance in the nominal scenario when using the SCHED model, and 66 % lower using the SCHEDOC model (see PV_{nom} and EPV values in Tables 7.7 and 7.8). The robust predictive schedules perform with an expected profit over the uncertain space about 21 % and 27 % higher than the deterministic one. Note also the shift to the right of the risk curves, and the larger variability of the stochastic solution (Figure 7.7). As it is also observed in the previous example, taking into account demands uncertainty in the reasoning procedure leads to the scheduling of a major number of batches, with the consequent increase of inventories to deal with adverse scenarios, and reduced production shortfalls.

Both SCHED and SCHEDOC models show the same trends, but the flexibility obtained with the introduction of option contracts translates into a slightly better expected profit due to the fewer inventory requirements and the somewhat improvement on customer satisfaction.

The VSS for this case study is 454 MU (2140 - 1686 MU) without option contracts, and raises up to 600 MU (2192 - 1686 MU) when the availability of options

Table 7.7: Deterministic and stochastic results for case study 7.5.2 with model SCHED (n_i: number of batches for each product; Q_i^P: production amounts; $E[Q_{ik}^S]$: expected sales; $E[Q_{ik}^I]$: expected inventory; $E[Q_{ik}^U]$: expected underproduction; PV_{nom}: profit value in the nominal scenario; EPV: expected profit value).

	Deterministic					Stochastic				
	i1	i2	i3	i4	i5	i1	i2	i3	i4	i5
n_i	3	2	3	2	3	4	2	4	3	3
Q_i^P	180	160	300	120	180	240	160	400	180	180
$E[Q_{ik}^S]$	153	132	256	100	139	177	132	295	119	139
$E[Q_{ik}^I]$	27	28	44	20	41	63	28	105	61	41
$E[Q_{ik}^U]$	31	21	49	19	9	7	21	10	0	9
PV_{nom}	**4508**					3059				
EPV	1686					**2140**				

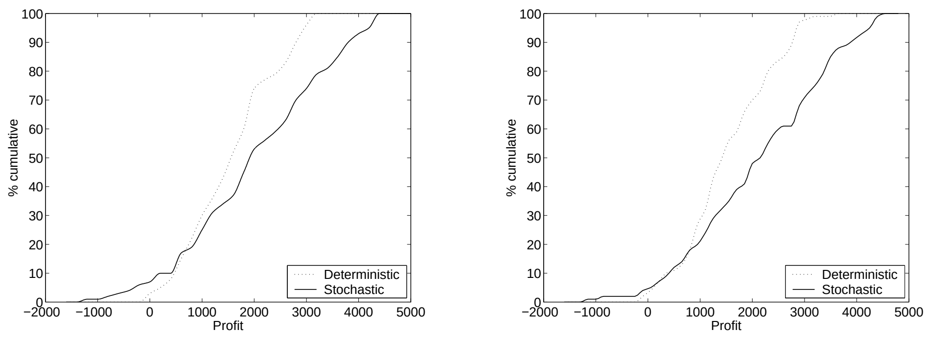
Table 7.8: Deterministic and stochastic results for case study 7.5.2 with model SCHEDOC (n_i: number of batches for each product; Q_i^P: production amounts; Q_i^{OC}: options purchased; E[Q_{ik}^S]: expected sales from production; E[Q_{ik}^{SOC}]: expected sales from options; E[Q_{ik}^I]: expected inventory; E[Q_{ik}^U]: expected underproduction; PV_{nom}: profit value in the nominal scenario; EPV: expected profit value.).

	Deterministic					Stochastic				
	i1	i2	i3	i4	i5	i1	i2	i3	i4	i5
n_i	3	2	3	2	2	4	2	4	2	3
Q_i^P	180	160	300	120	120	240	160	400	120	180
Q_i^{OC}	0	0	0	0	30	0	31	0	33	4
$E[Q_{ik}^S]$	153	132	256	100	109	177	113	295	80	136
$E[Q_{ik}^{SOC}]$	0	0	0	0	17	0	31	0	33	4
$E[Q_{ik}^I]$	27	28	44	20	24	63	47	105	40	44
$E[Q_{ik}^U]$	31	21	49	19	22	7	10	10	7	8
PV_{nom}			**4631**					3039		
EPV			1592					**2192**		

is considered. To assess the EVPI, the deterministic SCHED and SCHEDOC models have been solved for each scenario resulting in mean profit values over all the scenarios of 3897 MU and 4583 MU, respectively. Therefore, the EVPI is 2301 MU (3897 - 2140 MU) without options, and 2391 MU (4583 - 2192 MU) when considering the options.

Risk analysis

Concerning the robust optimization approaches, results obtained out of the multiple combinations of target profits (Ω) and weight risk values (ρ) tested for each measure of risk are reported in Tables 7.9 and 7.10. Results of the deterministic and



a. b.

Figure 7.7: Deterministic and stochastic risk curves for case study 7.5.2 with models: a) SCHED; b) SCHEDOC.

stochastic formulations are also included for comparison purposes. Detailed are the profit value in the nominal scenario (PV_{nom}), the expected profit (EPV), the worst profit value (WPV), and the financial (FR) and downside risk (DR) values at targets 0 and 500 MU obtained with both SCHED and SCHEDOC models for different approaches. Selected risk curves are represented in Figure 7.8.

Using the SCHED model (see Table 7.9), the same scheduling configuration is identified with the three risk metrics, with a reduction of risk at a target profit of 0 MU above 90 % compared to the stochastic schedule, and better expected performance than with the deterministic approach (1818 vs. 1686 MU). However, the realization of some of the scenarios still presents a negative return. Again, the availability of option contracts translates into a larger flexibility and better management of risk, which allows the identification of predictive schedules with positive returns within the entire uncertain space (Table 7.10). The robust solutions have higher expected profit values than the deterministic schedule, and the revenue in the nominal scenario is only around 7 % lower than the optimum one (4631 MU).

Table 7.9: Selected results obtained from risk management with financial risk (FRisk), downside risk (DRisk), and worst-case risk (WCase) measures for case study 7.5.2 with model SCHED.

	PV_{nom}	EPV	WPV	$FR_{\Omega=0}$	$FR_{\Omega=500}$	$DR_{\Omega=0}$	$DR_{\Omega=500}$
Deterministic	**4508**	1686	-62	0.02	0.07	1.23	19.35
Stochastic	3059	**2140**	-1160	0.06	0.09	33.94	71.67
$\text{FRisk}_{(\Omega=0;\rho=10^4)}$	4190	1818	-29	**0.01**	0.08	0.29	20.72
$\text{FRisk}_{(\Omega=10^3;\rho=10^4)}$	3770	1871	-454	0.04	0.12	7.80	45.18
$\text{DRisk}_{(\Omega=0;\rho=10^3)}$	4190	1818	-29	0.01	0.08	**0.29**	20.72
$\text{DRisk}_{(\Omega=200;\rho=5)}$	3490	2090	-732	0.06	0.12	19.88	64.00
WCase_{max}	4190	1818	**-29**	0.01	0.08	0.29	20.72

Table 7.10: Selected results from risk management with financial risk (FRisk), downside risk (DRisk), and worst-case risk (WCase) measures for case study 7.5.2 with model SCHEDOC.

	PV_{nom}	EPV	WPV	$FR_{\Omega=0}$	$FR_{\Omega=500}$	$DR_{\Omega=0}$	$DR_{\Omega=500}$
Deterministic	**4631**	1592	-49	0.02	0.11	0.96	33.59
Stochastic	3042	**2192**	-1179	0.05	0.11	21.04	54.87
$\text{FRisk}_{(\Omega=0;\rho=10^4)}$	3000	2189	-1222	0.02	0.12	21.00	55.60
$\text{FRisk}_{(\Omega=200;\rho=5\cdot10^4)}$	4075	1949	-144	0.01	0.06	1.44	16.07
$\text{DRisk}_{(\Omega=0;\rho=10^3)}$	4219	1883	0	0.00	0.06	0.00	17.05
$\text{DRisk}_{(\Omega=200;\rho=10^3)}$	3488	2145	-731	0.02	0.07	11.18	29.59
$\text{WCase}_{(\rho=0.3)}$	3738	2090	-481	0.03	0.07	6.79	27.89
$\text{WCase}_{(\rho=0.5)}$	4110	1947	-108	0.02	0.08	1.54	20.52
$\text{WCase}_{(\rho=0.7)}$	4280	1843	61	0.00	0.08	0.00	13.78
WCase_{max}	4400	1750	**181**	0.00	0.17	0.00	13.14

The computational time required for this case study ranged from 200 to 20000 seconds CPU time. As also highlighted in the previous example, the worst-case risk

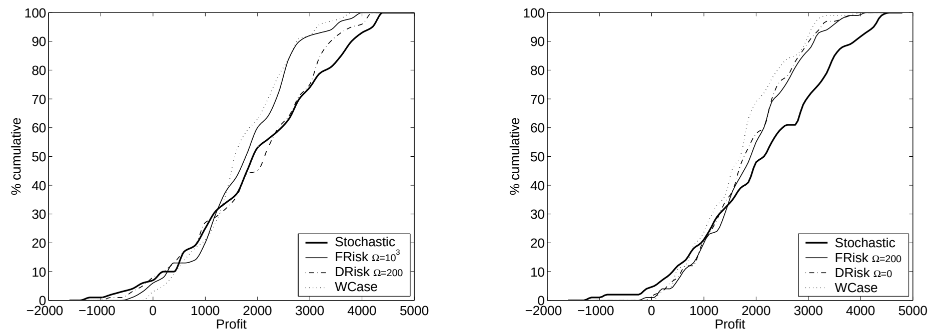


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Figure 7.8: Risk curves for case study 7.5.2 with alternative robust formulations with models: a) SCHED; b) SCHEDOC.

procedure shows the best efficiency for the identification of robust predictive schedules with lower computational requirements.

The trade off between risk and profit is illustrated in the Pareto curves depicted in Figure 7.9. Figure 7.9 (a) shows the Pareto curves obtained managing downside risk at target profits 0 and 200 MU with both SCHED and SCHEDOC models. Pareto curves obtained with the worst-case risk approach are plotted in Figure 7.9 (b). The same trends observed in the previous example apply here. In addition, the advantages of using option contracts are also illustrated in the Pareto graphs, where the curves obtained with the SCHEDOC formulation lie above those obtained without considering option contracts. Therefore, for a given level of risk, higher benefits are expected by holding option contracts.

The profit value that would be attained in each particular scenario depending on

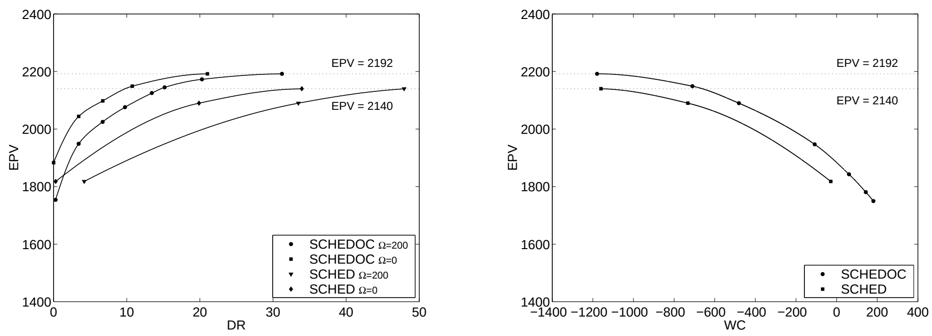

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Figure 7.9: Trade off between the expected profit and risk for case study 7.5.2: a) downside risk; b) worst-case risk.

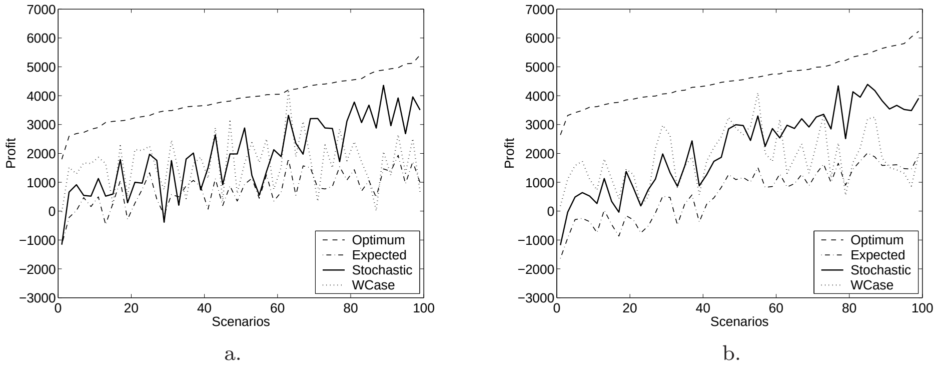

Figure 7.10: Optimum and expected profit values in each scenario resulting from the deterministic predictive schedules, and profits obtained when implementing the predictive schedules derived from the stochastic and worst-case approaches for case study 7.5.2 using the models: a) SCHED; b) SCHEDOC.

the predictive schedule executed is depicted in Figure 7.10, along with the optimum performance in each scenario and the expected profit of each optimal schedule over all the other scenarios.

Note, once again, the higher variability of the pure stochastic solution compared with solutions attained by managing risk, the prevention of negative returns at the expense of relatively lower expected profit values, as well as the considerable gap between optimum revenues for each scenario and its expectation in an uncertain environment, thus denoting the poor robustness of deterministic predictive schedules and the advantages of managing the uncertainty. The different performance of the modeling systems based on the availability of option contracts discussed for the previous case study is also observed.

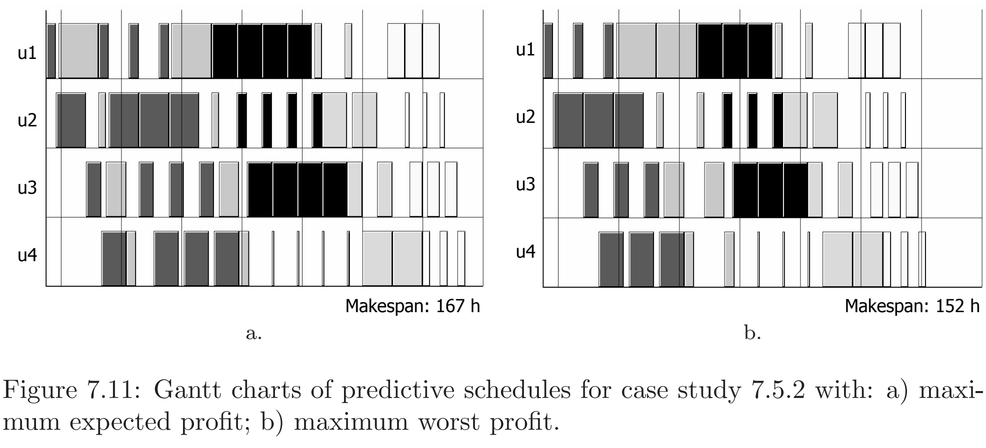

Figure 7.11: Gantt charts of predictive schedules for case study 7.5.2 with: a) maximum expected profit; b) maximum worst profit.

Finally, the Gantt chart of the predictive schedule that maximizes the expected profit, and that for the schedule with the best worst revenue identified with the SCHEDOC model are depicted in Figure 7.11. Notice the different number of batches predicted for each product based on the modeling approach.

7.6 Concluding remarks

The contribution of this thesis to the development of decision-support systems for operational analysis under uncertainty is completed in this chapter with the development of a proactive approach based on robust optimization in the context short-term scheduling of multiproduct batch plants with uncertain product demands. *Schedule robustness* has been evaluated in terms of profit, taking into account sales, production and changeover costs, as well as the effects of the uncertainty in terms of inventory and shortage costs. A two-stage stochastic programming model accounting for the maximization of the expected profit has been first developed, and further extended with the incorporation of the availability of using option contracts to implicitly deal with the effects of the uncertainty. The stochastic formulations have been next extended to explicitly manage the risk of obtaining profit values below a desired level. In this sense, *financial risk*, *downside risk* and *worst-case* risk have been studied as alternative measures for risk management, and have been appended as a second criterion in the objective functions. The suitability of the proactive approach developed has been finally illustrated in two different case studies.

The importance of managing uncertainty features within the modeling systems is shown from a comparison of results obtained between the stochastic model and its deterministic counterpart with nominal demand values. The expected profit of the deterministically generated predictive schedules drops above 60 % from the optimum value when they are implemented in the uncertain environment. On the other hand, stochastic models lead to a significant improvement of the expected performance over all the realizations of product demands. Management of risk is attained with the three alternate measures, and predictive schedules with limited dispersion, reduced risk values, and acceptable expected profits are identified. The three risk measures appear appropriate for the identification of robust predictive schedules, but the worst-case risk approach is shown to be very effective both in terms of robustness and computational effort. Moreover, the availability of option contracts not only provides flexibility to cope with demand uncertainties, but also leads to predictive schedules with higher expected revenues for a fixed level of risk. Therefore, alternative robust scheduling policies in the context of demands uncertainty are easily identified by appropriately managing risk in the decision-making process. The predictive schedule to be finally executed is subject to the decision-maker preferences towards risk.

In general, this final contribution is a step forward on the hierarchical integration of different sources of uncertainty. The study reveals that tactical uncertainties not only have a direct effect on medium to long-term planning analysis, but may also alter production decisions in short-term periods, and clearly shows the benefits of adopting a proactive view of the situation taking them into account in an operational level of reasoning. Globalization and competitive trends may increase the need for JIT deliveries, whereas the exact demands may not be predictable when production is to be scheduled. With the application of the robust optimization methodology, a better management of resources is possible, thus reducing the risk of capital losses while maintaining acceptable expected revenues.

Only uncertainty in product demands has been considered in this study to provide insight on the underlying scheduling problem. The next step would be the incorporation of the model as an upper level within the modeling framework developed in Chapter 5, thus providing a more realistic view of the overall system.

8.

Conclusions

If a man will begin with certainties he shall end in doubts; but if he will be content to begin with doubts he shall end in certainties.

Francis Bacon (1561 - 1626)

The challenge for considering uncertainty issues in modeling process systems undergoes a growing interest due to the increased recognition by most firms of the uncertainties faced in a dynamic and competitive operation environment, as well as to the progress in computer-aided systems, information technology, and optimization capabilities. This thesis contributes to the analysis and development of decision-support systems that take into account the main sources of uncertainty involved in an operational level of analysis. Concluding remarks are discussed throughout the document for the particular issues addressed, but overall conclusions as well as future research directions are outlined in this chapter.

8.1 Research results

Is it worth spending effort to obtain a predictive schedule optimal in economic or temporal terms for nominal conditions that will eventually change at execution time due to disruptions and changes in the operation environment? This thesis outlines an answer to this question by considering the uncertainty not from the traditional reactive perspective, but proactively, that is embedded in the decision-making procedure itself, to deal with the problem before disruptions occur.

The situation is examined in the introduction of the thesis, where an overview of the broad Process Systems Engineering (PSE) area is initially provided to eventually focus on the context of this research work, that is the consideration of uncertainty and robustness features in plant operational analysis. Some motivating issues are presented and a few questions formulated (Section 1.5), which are answered throughout the dissertation.

(1) What do we understand for uncertainty?
(2) How can uncertainty be considered within scheduling modeling systems?

Once established the basis of the problem, the concept of uncertainty is analyzed focused on the occurrence of unexpected events, as well as the presence of ambiguous or incomplete data in the context of PSE. Different sources of uncertainty are extracted and categorized into strategic, tactical and operational uncertainties, similarly to the hierarchical levels of decision. The probabilistic representation of the uncertainty using the scenario or distribution-based approaches is underlined, and stochastic and robust methodologies for decision making under uncertainty are reviewed as the basis of the modeling systems to be developed. The state-of-the-art in the area is also surveyed.

(3) What is understood for schedule robustness and flexibility? Is there any formalism established for these concepts?
(4) Is the problem well solved or deficiencies can be identified?

The analysis reveals the lack of standard and **reliable decision-making systems** able to deal with uncertainty issues, the consequent void of successful commercial Advanced Planning and Scheduling (APS) packages available for the industry addressing the problem proactively, as well as the challenge implied in the area of process operations. The *high computational requirements*, the *multiple sources of uncertainty*, the multiple and *conflicting criteria* involved in a process system, as well as the *lack of a general formalism for the concept of schedule robustness*, are identified as the main **critical issues**.

Although computational issues are relevant in the industrial practice, the main contribution of the thesis is concerned about the appropriate definition of the problem and the management of the uncertainty to improve the robustness features of predictive schedules through the development of **proactive** decision-support systems for operational analysis.

(5) How can schedule robustness be improved? What are the benefits?

This question drives the main contents of the underlying research. The improvement of **schedule robustness** implies a first understanding and definition of the concept. In view of the lack of a common formalism, an attempt is made to establish a general basis to formalize the notion of schedule robustness in the context of operational analysis. Robustness is defined as a **trade off** between scheduling efficiency and the eventual consequences of the uncertainty, both measured either in temporal or economic terms according to the preferences of the decision maker. Notice that with this formalism, and contrary to the measures commonly used so far, critical situations that may arise at execution time are explicitly managed in the reasoning stage, thus providing a more realistic modeling approach for the problem.

The critical issues, as well as the set of specific points involved in the objective pursued (refer to Section 3.2) are covered within three main topics:

I. Robust scheduling focused on operational uncertainties.

A first contribution is the development of proactive modeling systems to account for the main **operational uncertainties in short-term production scheduling** (variable operation times and equipment breakdowns). Schedule robustness is formalized to manage the trade off between the desired efficiency, evaluated in terms of makespan, and the need to avoid the generation of wait times during the execution of a predictive schedule. This new formalism for schedule robustness proves suitable for the identification of more conservative predictive schedules, which not only assure an improved performance with significantly reduced expected wait times when they are executed in an uncertain environment, but also maintain an acceptable efficiency in the nominal scenarios.

Both rigorous and procedure-oriented models are developed and analyzed in this research work. **Stochastic programming** is first used to formulate the problem considering only uncertainty in the processing times. A **simulation-based optimization framework** is finally developed to capture the multiple sources of uncertainty, as well as the rescheduling procedures proactively in the decision stage, thus providing a more complete view of the problem. Instead of formulating a complex mathematical model for the optimization module, the use of meta-heuristics is incorporated to stochastic optimization with the development of a **stochastic GA** (stochGA), which proves to be very promising for the identification of robust predictive schedules.

The results obtained fully validate the convergence properties and suitability of the simulation-based optimization approach. However, the case studies used to test the proactive modeling systems are relatively simple to fully justify their advantages in terms of computational effort.

II. Extension to transport scheduling.

The procedure-oriented modeling system developed in the context of production scheduling is next extended to involve short-term **transport scheduling** in muti-site systems with **uncertain travel times**, thus covering a broader operational perspective. While the integration of production and distribution problems has generally been considered in strategic and tactical levels of analysis, being the presence of uncertainty usually neglected, their coordination in the low operational level is a step forward in this research direction. Though the problem is difficult to generalize because of the multiple features and objectives involved, a better management of inventory profiles and material flows can be easily attained. Concerning the uncertainty, the effects of variable travel times are merely evaluated in this research work, but it is again evidenced that deterministic approaches tend to predict lower times than those realized during the implementation of the schedules, thus contributing to further disturbances.

III. Robust scheduling focused on tactical uncertainties

This research work concludes with the consideration of **product demands variability** as the most common source of **tactical uncertainty** with a direct effect in short-term scheduling decisions. Schedule robustness is formalized in terms of profit, taking into account the inventory and unsatisfied demands as effects of the uncertainty; the problem is analyzed from a **risk management** point of view, using and comparing *financial risk*, *downside risk*, and *worst-case* revenues as alternative control measures. These three metrics prove suitable for identifying predictive schedules with limited dispersion and acceptable expected profits, although the worst-risk approach is shown to be the most effective, both in terms of robustness and computational requirements.

The concept of risk management has largely been used in strategic and tactical levels of decision, mainly in the area of portfolio management. However, its application had not been extended to short-term scheduling. It may be argued that the consideration of demand uncertainty in short-term scheduling is somehow a contradiction, since it is usually related to long-term decisions. Though demand uncertainty has essentially a long-term meaning, its effects may easily propagate to short-term decisions implying changes in production amounts, as it is noticed in this research. It is not uncommon that production scheduling relies on forecast demands to draw a predictive schedule that allows the initialization of production and the delivery of products in a *just-in-time* fashion.

With the research conducted, the objectives devised in view of the situation in the area are successfully achieved. In general, the proactive approaches developed in the thesis prove suitable for the identification of predictive schedules with improved robustness when they are to be executed in uncertain environments, and provide valuable insight and general guidance on the performance of the process system. Instead, it is shown that predictive schedules determined assuming certainty tend to overestimate the performance of the system, leading to suboptimal or even infeasible realizations when they are implemented in practice.

The need to face the uncertainty proactively with the development of modeling systems that incorporate information about the uncertainty at the time of reasoning implies by no means the exclusion of rescheduling at execution time. Multiple sources of uncertainty can be encountered, but some of them may be too minor and it seems not reasonable or even worthy to take all of them into account when modeling the system. Therefore, some reasoning, though simple, will have to be done during execution. However, the proactive view of the uncertainty, with the incorporation of information about not only stochastic parameters, but also rescheduling strategies, is proved to be highly advantageous; on the whole, it provides insight on the performance of the system as well as visibility for future actions, knowledge that can usefully be exploited when planning external activities with customers and suppliers. Besides, the difficulty of rescheduling procedures not only depends on the consequences of a disturbance, but also on the features of the predictive schedule; some predictive schedules may lead to rescheduling problems with lower implementation costs that others.

Therefore, proactive scheduling appears as a promising way to support online scheduling strategies, thus avoiding inefficient or costly reconfigurations and keeping low what is known as schedule nervousness (a schedule is considered nervous if it experiences large and frequent changes). Finally, proactive approaches can be seen as a way to reduce the gap between theory and the industrial practice, and in general, to improve the robustness, flexibility and performance of the overall process system, properties that undergo an increasing interest to remain effective and competitive in current global and dynamic operation environments.

8.2 Future research

The large and multidisciplinary area of PSE, along with the growing trends to operate in global, competitive, dynamic and thus uncertain environments, pose a huge number of directions and challenges for research. Despite the increasing interest in Supply Chain Management (SCM), the impact of flexibility and responsiveness characteristics of every production process and task in the overall supply chain system is highly significant and deserves its own research effort. The contribution of this thesis can be considered as a basis for further improvements on the development of decision-support modeling systems managing uncertainties in operational analysis. Future research and opportunities can be directed, among others, to the following points:

- Optimization under uncertainty, and particularly stochastic optimization, implies large modeling systems quickly affected by the course of dimensionality. Although this subject is the center of significant research, computational issues are still one of the major challenges for the development of applicable and efficient solution algorithms. Effort could be devoted towards the development of decomposition or approximation algorithms for multi-stage stochastic problems, as well as on efficient and uniform sampling techniques. A deeper understanding of the properties and structure of the problem is needed.

- Because of the detailed and complex models required to capture the features of problems under uncertainty, their rigorous resolution is unlikely to reward the computational effort implied. On the other hand, the implementation of purely heuristic-oriented approaches may miss the opportunities for improved solutions. Instead, the combination of heuristic and mathematical programming algorithms should be considered as a promising way to model and solve optimization problems efficiently.

- The notion of robustness has been applied in proactive scheduling approaches to identify predictive schedules. However, it can also be extended to the problem of rescheduling when repairing a predictive schedule, either in an on-line implementation, or in a proactive modeling system as those developed in this thesis. Robustness could be addressed in a rescheduling procedure using only information about the uncertain parameters, without incorporating further rescheduling strategies (otherwise, the modeling approach derives in an endless loop). This new perspective in rescheduling strategies provides also a more realistic and effective reaction.

- Being the interests focused on globalization and SCM, the integration of proactive scheduling methodologies with tactical and/or strategic analysis can be considered so as to provide an improved guidance on the performance of the whole system.

- The formalism of robustness proposed in this thesis could be extended to strategic and tactical levels, and a hierarchical integration of the effects of several sources of uncertainty could be considered. These steps imply the evaluation of the effects of the uncertainties within the different levels of decision, and their incorporation into the performance criteria of the modeling systems.

Nomenclature

The characters and acronyms used in the thesis are defined when are used for the first time. This chapter is a reference of the nomenclature used over the entire document.

Characters

$at\theta$	subscript for associated transport orders
b	subscript for batches
B	upper bound on the number of batches
BS_i	batch size of product i
$c^C_{ii'}$	cost of changeover from product i to i'
c^f_v	fixed cost of vehicle v
c^I, c^I_i	inventory cost (of product i)
c^{OC}_i	cost of option contracts of product i
c^P_i	production cost of product i
c^{sum}	multiple cost
c^{tr}	transport cost
c^U	cost of production shortfall
c^u_v	cost of vehicle v for distance unit
C_l	capacity of location l
C_v	capacity of vehicle v
$dd_{t\theta}$	due date of transport order $t\theta$
dev	deviation criterion
$dist_{ts}$	distance covered in transport stage ts
DR_Ω	downside risk at profit target Ω
E	summed earliness criterion
EPV	expected profit value
$\mathrm{E}[\cdot]$	expected value
F	flow time criterion
FR_Ω	financial risk at profit target Ω

$f^{tr}_{v,l}$	transport factor of vehicle v in location l
H	time horizon
i	subscript for products or processes
j	subscript for stages
J^f_i	set of first stages j of process i
J^l_i	set of last stages j of process i
J_i	set of stages j required for the production of process i
k	subscript for scenarios
l	subscript for location
L	summed lateness criterion
M	large weight value
mk, mk_k	makespan value (of scenario k)
nk	number of scenarios sampled
NK_0	number of initial scenarios in a sampling algorithm
NR	number of replications in a sampling algorithm
n_i	number of batches produced of product i
o	subscript for operations
OF^*_k	optimum objective function value of scenario k
O^f_j	set of first operations o of stage j
O^l_j	set of last operations o of stage j
$O^{seq}_{oo'}$	set of operations o and o' in stages j and j' to be performed sequentially
$O^{sim}_{oo'}$	set of operations o and o' in stages j and j' to be performed simultaneously
$O^{zw}_{oo'}$	set of operations o and o' in stage j to be performed one immediately after the other
O_j	set of operations o in stage j
PV, PV_k	profit value (of scenario k)
Q^I_i, Q^I_{ik}	amount of product i stored (in scenario k)
Q^{OC}_i	amount of product i contracted
Q^P_i	amount of product i produced
Q^{SOC}_{ik}	amount of product i allocated in option contracts in scenario k
Q^S_{ik}	quantity of product i sold in scenario k
Q^U_{ik}	quantity of product i not satisfied in scenario k
Q^d_{ts}	amount of materials discharged in transport stage ts
r	subscript for replications
S^0_i	initial stock of product i
s_v	speed of vehicle v
T	summed tardiness criterion
to	subscript for transport operations
tr	subscript for transport routes

ts	subscript for transport stages
$Tfnr_{oik}$	completion time of operation o of process i in scenario k
Tfn^{p}_{ts}	predicted final time of transport stage ts
Tfn_{jb}	final processing time of stage j in batch b
$Tfn_{tr}, Tfn_{tr\,k}$	final time of transport route tr (in scenario k)
$Tfn_{ts}, Tfn_{ts\,k}$	final time of transport stage ts (in scenario k)
$Tinr_{oik}$	start time of operation o of process i in scenario k
Tin_{i}	start time of process i
Tin_{jb}	initial processing time of stage j in batch b
$Tin_{tr}, Tin_{tr\,k}$	initial time of transport route tr (in scenario k)
Tin_{ts}	initial time of transport stage ts
Top^{break}	duration of a breakdown
Top_{ij}	processing time of product i in stage j
Top^{stop}_{l}	fixed stop time in location l
Top_{oik}	processing time of operation o of order i in scenario k
$Top^{discharge}_{ts}$	discharge operation time of transport stage ts
Top^{travel}_{ts}	travel operation time of transport stage ts
$t\theta$	subscript for transport orders
t^{I}_{i}	period of time of product i in storage
T_{jb}	processing time of stage j in batch b
u	subscript for units
U_{ij}	set of units u available to process stage j of process i
v	subscript for vehicles
wt	wait times
wt^{0}_{ik}	start wait time or delay of process i in scenario k
wt^{s}_{oik}	wait time between stages (after operation o of process i in scenario k)
WPV	worst profit value
$XM_{bii'}$	variable indicating the change from product i to i' in batch b
X_{bi}	binary variable denoting the assignment of product i to batch b
$X_{iji'j'}$	binary variable denoting that stage j of process i is processed before stage j' of process i'
Y_{iju}	binary variable denoting the assignment of stage j of process i to unit u
$Y_{k\Omega}$	binary variable denoting that the PV_k is lower than the target profit Ω
Z_{AR}	absolute robustness criterion
Z_{DR}	robust deviation criterion
Z_{RR}	relative robustness criterion
$\bar{t}^{break}$	mean time point at which a breakdown occurs

Greek characters

α	confidence level
$\delta_{nk,\alpha}$	half-length confidence interval for nk samples and confidence level α
γ	relative error of an estimate of a mean value
λ	low weight value
ν_i^{OC}	sales price of option contracts of product i
ν_i	sales price of product i
Ω	target profit
ω_k	probability of occurrence of scenario k
$\overline{\mu}$	mean value of performance measure μ
$\phi_{k\Omega}$	positive deviation of the profit value from target Ω in scenario k
ρ, ρ_i	weight value (of criterion i) in a multi-objective function
σ	standard deviation value
θ_i^{tr}	transport request of product i
θ_i, θ_{ik}	production request of product i (in scenario k)

Acronyms and abbreviations

APS	advanced planning and scheduling
CPI	chemical process industry
CRP	capacity requirements planning
DARP	dial-a-ride problem
DRP	distribution requirements planning
EON	Event Operation Network
ERP	enterprise resource planning
EVPI	expected value of perfect information
GA	genetic algorithm
GSL	GNU scientific library
HSS	Hammersley sequence sampling
IT	information technology
JIT	just-in-time
LHS	left-hand side
LP	linear programming
MCS	Monte Carlo sampling
MES	manufacturing execution systems
MILP	mixed-integer linear programming

MINLP	mixed-integer non-linear programming
MRP	materials requirements planning
MU	monetary units
NIS	non-intermediate storage
NLP	non-linear programming
nom	nominal value
OC	option contract
PDP	pickup and delivery problem
PDPTW	pickup and delivery problem with time windows
PMX	partially mapped crossover
PSE	Process Systems Engineering
PV	profit value
RHS	right hand side
rnd	random value
ROI	return of investment
SA	simulated annealing
SC	supply chain
SCM	Supply Chain Management
TSP	traveling salesman problem
TU	time units
UIS	unlimited intermediate storage
UML	unified modeling language
VRP	vehicle routing problem
VRPTW	vehicle routing problem with time windows
VSS	value of the stochastic solution
WU	weight units
ZW	zero wait

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A.

Publications

The research work developed in the scope of this thesis has resulted in several publications either articles in scientific journals, articles in conference proceedings, and communications in congresses. Besides, there has been the opportunity to participate in different research projects. All these contributions are detailed in this appendix.

A.1 Journal articles

Bonfill, A., Espuña, A., Puigjaner, L., 2006. Decision support framework for coordinated production and transport scheduling in SCM. Computers and Chemical Engineering (submitted for publication).

Bonfill, A., Espuña, A., Puigjaner, L., 2006. Proactive approach to address the uncertainty in short-term scheduling. Computers and Chemical Engineering (submitted for publication).

Arbiza, M., **Bonfill, A.**, Guillén, G., Mele, F., Espuña, A., Puigjaner, L., 2006. Metaheuristic multiobjective optimisation approach for the scheduling of multiproduct batch chemical plants. Journal of Cleaner Production (accepted for publication).

Bonfill, A., Espuña, A., Puigjaner, L., 2005. Addressing robustness in scheduling batch processes with uncertain operation times. Industrial and Engineering Chemistry Research 44, 1524 – 1534.

Bonfill, A., Bagajewicz, M., Espuña, A., Puigjaner, L., 2004. Risk management in scheduling of batch plants under uncertain market demand. Industrial and Engineering Chemistry Research 43, 741 – 750.

A.2 Articles in conference proceedings

Méndez, C., **Bonfill, A.**, Espuña, A., Puigjaner, L., 2006. A rigorous approach to coordinate production and transport scheduling in a multi-site system. Accepted in European Symposium on Computer-Aided Process Engineering - 16, Garmisch-Partenkirchen, Germany.

Musulin, E., Arbiza, M., **Bonfill, A.**, Espuña, A., Puigjaner, L., Olsson, R., Arzen, K., 2005. Closing the information loop in recipe-based batch production. In: Puigjaner, L., Espuña, A. (Eds.), European Symposium on Computer-Aided Process Engineering - 15. Elsevier, Barcelona, Spain, 1381 – 1386, ISBN: 0-444-51987-4.

Bonfill, A., Espuña, A., Puigjaner, L., 2005b. Proactive approach to address robust batch process scheduling under short-term uncertainties. In: Puigjaner, L., Espuña, A. (Eds.), European Symposium on Computer-Aided Process Engineering - 15. Elsevier, Barcelona, Spain, 1057 – 1062, ISBN: 0-444-51987-4.

Bonfill, A., Arbiza, M., Cantón, J., Guillén, G., Mele, F., Espuña, A., Puigjaner, L., 2004. Metaheuristic multiobjective optimization approach for the scheduling of multiproduct plants. In: 16th International Congress of Chemical and Process Engineering (CHISA 2004). Process Engineering, Praha, Czech Republic, 1416, ISBN: 80-86059-40-5.

Guillén, G., **Bonfill, A.**, Espuña, A., Puigjaner, L., 2004. Integrating production and transport scheduling for supply chain management under market uncertainty. In: Barbosa-Póvoa, A., Matos, H. (Eds.), European Symposium on Computer-Aided Process Engineering - 14. Elsevier, Lisboa, Portugal, 919 – 924, ISBN: 0-444-51694-8.

Bonfill, A., Arbiza, M., Musulin, E., Espuña, A., Puigjaner, L., 2004. Integrating robustness and fault diagnosis in on-line scheduling of batch chemical plants. In: Taisch, M., Filos, E., Garello, P., Lewis, K., Montorio, M. (Eds.), IMS International Forum 2004, Global Challenges in Manufacturing. Vol. Part 1. Grafica Sovico srl - Biassono (Milano), Villa Erba - Cernobbio - Italy, 515 – 522, ISBN: 88-901168-9-7.

Bonfill, A., Cantón, J., Bagajewicz, M., Espuña, A., Puigjaner, L., 2003. Managing financial risk in scheduling of batch plants. In: Kraslawski, A., Turunen, I. (Eds.), European Symposium on Computer-Aided Process Engineering - 13. Elsevier, Finland, 41 – 46, ISBN: 0-444-51368-X.

A.3 Communications in congresses

Méndez, C., **Bonfill, A.**, Espuña, A., Puigjaner, L., 2005. A MILP-based formulation to integrate production and transport scheduling in a multi-site system. 10th Mediterranean Congress of Chemical Engineering, Barcelona.

Bonfill, A., Espuña, A., Puigjaner, L., 2005c. Proactive scheduling approach for batch processes under uncertainty. 10th Mediterranean Congress of Chemical Engineering, Barcelona.

Bonfill, A., Méndez, C., Espuña, A., Puigjaner, L., November 2005. Coordinating production and transport scheduling in SCM through rigorous and heuristic-based methods. AIChE Annual Meeting, Cincinnati, OH, USA.

Bonfill, A., Espuña, A., Puigjaner, L., November 2004. Stochastic genetic algorithm to address short-term uncertainties in robust scheduling of batch plants. AIChE Annual Meeting, Austin, Texas.

Arbiza, M., **Bonfill, A.**, Espuña, A., Puigjaner, L., November 2004. Integrated framework for the production and transport scheduling in SCM. AIChE Annual Meeting, Austin, Texas.

Bonfill, A., Espuña, A., Puigjaner, L., 2003b. Extension of the s-graph representation to manage demand in due-date driven batch production scheduling. AIChE Annual Meeting, San Francisco, USA.

Bonfill, A., Espuña, A., Puigjaner, L., November 2003. Robustness and risk assessment in scheduling batch processes with uncertain operation times. AIChE Annual Meeting, San Francisco, USA.

Bonfill, A., Cantón, J., Bagajewicz, M., Espuña, A., Puigjaner, L., 2002. Risk controlled scheduling of batch plants under uncertainty. 9th Mediterranean Congress of Chemical Engineering, Barcelona.

Bonfill, A., Mele, F., Sequeira, S., Puigjaner, L., 2002. Metaheuristic - multiobjective optimization approach for the scheduling of multiproduct plants. 9th Mediterranean Congress of Chemical Engineering, Barcelona.

Bonfill, A., Espuña, A., Puigjaner, L., November 2002. Improving robustness and validating strategies in scheduling batch processes under uncertainty. AIChE Annual Meeting, Indianapolis, Indiana, USA.

Mele, F., Guillén, G., **Bonfill, A.**, Espuña, A., Puigjaner, L., November 2002. Integration of batch plant design into a supply chain network under uncertainty. AIChE Annual Meeting, Indianapolis, Indiana, USA.

A.4 Participation in research projects

GICASA-D, 2002 - 2005. Gestió Integral de la Cadena de Subministraments Ampliada i Distribuïda (Generalitat de Catalunya, I0353).

OCCASION, 2003 - 2005. Desarrollo e Implementación de un Sistema de Gestión y Optimización de Cadena de Suministro Global en Tiempo Real (Ministerio de Educación y Ciencia, DPI 2002-00856).

CHEM, 2001 - 2003. Advanced Decision Support System for Chemical / Petrochemical Manufacturing Processes (European Community, G1RDT-CT-2001-00466).

VIP-NET, 2001 - 2003. Virtual Plant-wide Management and Optimisation of Responsive Manufacturing Networks (European Community, G1RDT-CT-2000-00318).

B.

Case studies - Problem data

The processes used as case studies to assess the suitability of the modeling approaches developed in this thesis are described in this appendix. Their configurations and problem data are also reported.

B.1 Motivating example

The motivating case study is a comprehensive example that consists of a five-product three-stage flow shop plant studied first by Balasubramanian and Grossmann (2002). A scheme of this plant is shown in Figure B.1. Each stage involves one single operation, and only one unit is available for its processing (Table B.1).

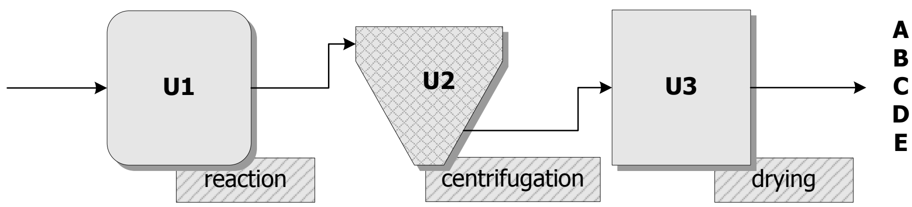

Figure B.1: Scheme of the flow shop plant of the motivating example.

The operation times are considered uncertain, and are represented by discrete probability distributions with three possible time realizations for each product operation in each stage. The example is extended with information related to uncertainty

Table B.1: Recipe data for the motivating example.

Stage	Unit	Operation	ID
j1	u1	reaction	o1
j2	u2	centrifugation	o2
j3	u3	drying	o3

in the availability of unit *u2*, as well as with production and economic data. Concerning the uncertain equipment availability, an exponential distribution function is used to describe the breakdown time, whereas the downtime is represented using a uniform probability distribution. Production and time data are provided in Section B.1.1, whereas economic data is given in Section B.1.2.

B.1.1 Operational data

A common batch size of **100 kg** is assumed for all the products; nominal product demands are detailed in Table B.2. The characterization of the uncertain equipment availability, that is, the mean breakdown time ($\overline{\theta}_i^{nom}$) and the minimum and maximum breakdown durations (Top^{break}), are given in Table B.3. Concerning the time data, Table B.4 reports the mean operation times. These values have been calculated based on the discrete probability distributions reported in Table B.5, which describe the uncertain processing times for each product operation. A scenario with product demands different than the nominal ones is evaluated in Sections 1.3 and 7.5.1; this particular scenario is reported in Table B.6. Finally, a specific scenario with random operation times used for validation purposes in Sections 1.3 and 4.4 is detailed in Table B.7.

Demands are defined in **kg**, whereas times are given in arbitrary time units, **TU**.

Table B.2: Nominal demands ($\overline{\theta}_i^{nom}$) for the motivating example.

Product	$\overline{\theta}_i^{nom}$
i1	200
i2	100
i3	300
i4	100
i5	100

Table B.3: Characterization of the uncertain equipment availability for the motivating example.

Unit	$\overline{t}^{break}$	Top^{break} (min - max)
u2	75	12 - 24

Table B.4: Mean operation times for the motivating example.

Operation	A	B	C	D	E
reaction	6	6	9	25	17
centrifugation	8	12	8	20	4
drying	14	16	9	17	14

Table B.5: Characterization of the operation times uncertainty for the motivating example.

Orders	Operation	k_1		k_2		k_3	
		t	ω	t	ω	t	ω
A	o1	2	0.15	4	0.25	8	0.60
A	o2	6	0.50	10	0.15	12	0.35
A	o3	12	0.125	14	0.775	16	0.10
B	o1	3	0.30	5	0.30	8	0.40
B	o2	4	0.50	15	0.25	25	0.25
B	o3	8	0.40	15	0.20	25	0.40
C	o1	5	0.10	7	0.40	12	0.50
C	o2	6	0.20	8	0.50	10	0.30
C	o3	8	0.80	10	0.10	14	0.10
D	o1	12	0.15	24	0.25	28	0.60
D	o2	16	0.50	20	0.15	25	0.35
D	o3	11	0.125	17	0.775	23	0.10
E	o1	15	0.30	18	0.40	19	0.30
E	o2	2	0.25	4	0.50	5	0.25
E	o3	8	0.40	14	0.20	19	0.40

Table B.6: Random product demands scenario ($\overline{\theta}_i^{rnd}$) for the motivating example.

Product	$\overline{\theta}_i^{rnd}$
i1	250
i2	130
i3	200
i4	100
i5	80

Table B.7: Random operation times scenario for the motivating example.

Operation	A	B	C	D	E
reaction	2	5	7	28	15
centrifugation	6	4	10	25	4
drying	16	15	8	17	8

B.1.2 Economic data

Concerning the economic information for the motivating example, data related to sales prices (ν_i, ν_i^{OC}), production costs (c_i^P), costs for option contracts (c_i^{OC}), inventory costs (c_i^I), and costs for product changeovers ($c_{ii'}^C$) is reported in Tables B.8 and B.9. This data is used in Sections 1.3 and 7.5.1. Prices and cost parameters are assumed to be in monetary units, **MU**.

Table B.8: Sales prices (ν_i, ν_i^{OC}), production costs (c_i^P), costs for option contracts (c_i^{OC}), and inventory costs (c_i^I) for the motivating example.

Product i	ν_i	ν_i^{OC}	c_i^P	c_i^{OC}	c_i^I
A	10	10	5	5.5	0.5
B	12	12	6	6.5	0.6
C	7	7	3.5	4	0.3
D	10	10	5	5.5	0.5
E	8	8	4	4.5	0.3

Table B.9: Costs for product changeovers ($c_{ii'}^C$) for the motivating example.

	A	B	C	D	E
A	0	3	1	2	1
B	1	0	1	1	2
C	1	3	0	2	1
D	1	2	1	0	1
E	2	3	1	2	0

B.2 Multiproduct plant

The multiproduct plant case study is an adaptation of the example presented in Petkov and Maranas (1997), which consists of a multiproduct batch plant with 4 production stages and 5 different products. Only one production line is considered, and a scheme of the plant is depicted in Figure B.2.

Operational data related to product demands, batch sizes and processing times for each product is given in Section B.2.1. Section B.2.2 details the economic in-

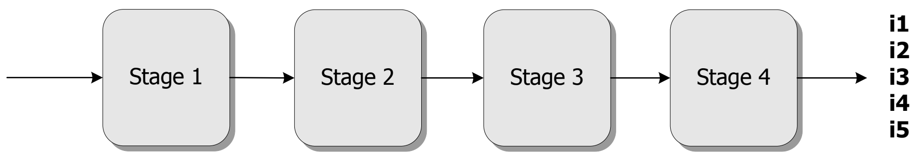

Figure B.2: Scheme of the multiproduct plant of case study B.2.

formation. Operation times, sales prices, and production costs are taken from the example in Petkov and Maranas (1997). Different product demands and batch sizes are considered because of the distinct time horizon and requirements of the modeling systems developed in this thesis. Additional data for inventory costs, costs for option contracts, and changeover costs is specified.

B.2.1 Operational data

Data concerning nominal product demands ($\overline{\theta}_i^{nom}$) is reported in Table B.10. Batch sizes (BS_i) and operation times are assumed known with certainty for each product, and are given in Tables B.11 and B.12, respectively.

Times are specified in hours **h**, whereas demands and batch sizes are given in **kg**.

Table B.10: Nominal demands ($\overline{\theta}_i^{nom}$) for the multiproduct plant example.

Product	$\overline{\theta}_i^{nom}$
i1	180
i2	160
i3	300
i4	120
i5	150

Table B.11: Batch sizes (BS_i) for the multiproduct plant example.

Product	BS_i
i1	60
i2	80
i3	100
i4	60
i5	60

Table B.12: Processing times for the multiproduct plant example.

Product	stage 1	stage 2	stage 3	stage 4
i1	10	4	10	1
i2	3	10	6	12
i3	4	12	6	10
i4	16	3	8	4
i5	7	2	5	3

B.2.2 Economic data

Economic data related to sales prices (ν_i, ν_i^{OC}), production costs (c_i^P), costs for option contracts (c_i^{OC}), inventory costs (c_i^I), and costs for product changeovers ($c_{ii'}^C$) is defined in Tables B.13 and B.14. This information is assumed to be in monetary units, **MU**.

Table B.13: Sales prices (ν_i, ν_i^{OC}), production costs (c_i^P), costs for option contracts (c_i^{OC}), and inventory costs (c_i^I) for the multiproduct plant example.

Product	ν_i	ν_i^{OC}	c_i^P	c_i^{OC}	c_i^I
i1	9	9	4.5	5	0.8
i2	9	9	4.5	5	0.8
i3	12	12	6	6.5	1
i4	12	12	6	6.5	1
i5	8	8	4	4.5	0.6

Table B.14: Costs for product changeovers ($c_{ii'}^C$) for the multiproduct plant example.

	i1	i2	i3	i4	i5
i1	0	1	5	3	2
i2	2	0	4	5	1
i3	1	1	0	1	2
i4	1	2	2	0	3
i5	3	2	5	4	0

B.3 Procel

Procel is a batch production pilot plant located in the laboratory facilities of the chemical engineering department in the Universitat Politècnica de Catalunya. It consists of three tank reactors, three heat exchangers, and the necessary pumps and valves to allow configuration changes. The production recipes used in this facility involve 3 production stages and 8 operations to manufacture two different products. A scheme of this process is presented in Figure B.3. Uncertainty has been introduced in the processing times for the operations of loading, heating and discharging, as well as on the availability of *Reactor1* used in the third procedure.

Recipe data related to the production stages, operations in each stage, available equipment units, and processing times for each product is given in Table B.15. For the operations with variable processing times, this uncertainty is described with a uniform distribution function, and the minimum and maximum values are reported.

The parameters related to the availability of *Reactor1*, i.e., the nominal breakdown time ($\bar{t}^{break}$) characterizing an exponential distribution function, and minimum

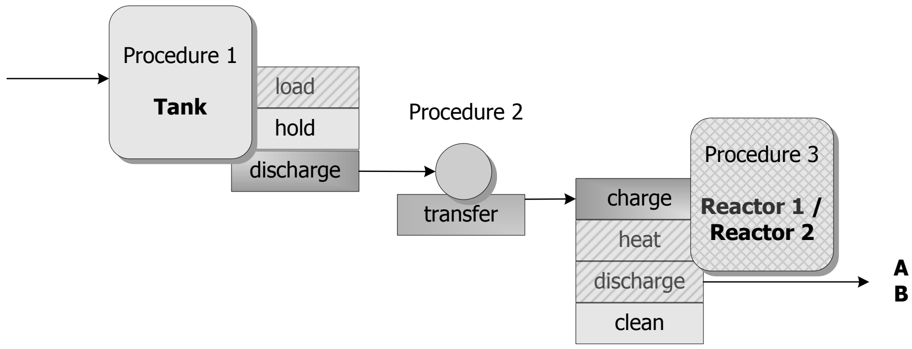

Figure B.3: Production process of Procel.

and maximum breakdown durations (Top^{break}) defining the boundaries of a uniform distribution, are reported in Table B.16. Time data is given in hours, **h**.

Table B.15: Recipe data for Procel.

Recipe	Stage	Unit	Operation	Top_A (min - max)	Top_B (min - max)
A/B	Procedure 1	Tank	load tank	2.3 - 3.0	2.3 - 3.0
			hold	1.0	1.0
			discharge tank	2.0	2.0
	Procedure 2	Pump	transfer	2.0	2.0
	Procedure 3	Reactor 1/2	charge	2.0	2.0
			heat	2.1 - 2.8	4.0 - 4.7
			discharge	4.0 - 4.8	5.2 - 5.9
			clean	1.5	2.0

Table B.16: Characterization of the uncertain equipment availability for Procel.

Unit	$\bar{t}^{break}$	Top^{break} (min - max)
Reactor 1	15	9 - 15

B.4 Washing subprocess

The washing subprocess case study is an industrial-based example that consists of the scheduling of a washing subprocess of a more complex single product production process. A scheme of this subprocess is shown in Figure B.4.

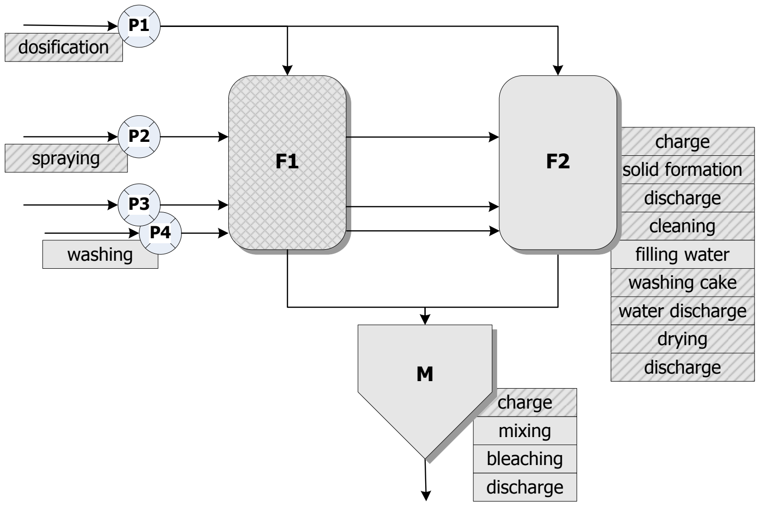

Figure B.4: Washing subprocess scheme.

The processing environment is essentially of batch nature, and involves 6 production stages with 18 different activities, either batch operations in filters or semi-continuous auxiliary operations. The importance of addressing the operation times uncertainty comes from the desire to achieve high and uniform product quality.

Table B.17: Recipe data for the washing subprocess.

Stage	Unit	Operation	ID	Top (min - max)
Filtration	F1	charge	o1	10.6 - 22.4
	F2	solid formation	o2	30.0 - 34.0
		discharge	o3	8.3 - 16.6
		cleaning	o4	2.0 - 3.6
		filling water	o5	8.0
		washing cakes	o6	50.0 - 70.0
		water discharge	o7	10.0 - 12.0
		drying	o8	6.6 - 11.0
		discharge	o9	5.0 - 5.6
Mixing	M	charge	o10	simultaneous with o9
		mixing	o11	10.0
		bleaching	o12	30.0
		discharge	o13	5.0
Dosification	P1	pumping	o14	simultaneous with o1
Spraying I	P2	spraying I	o15	simultaneous with o4
Spraying II	P2	spraying II	o16	simultaneous with o9
Washing	P3	washing I	o17	simultaneous with o5
	P4	washing II	o18	simultaneous with o6

Recipe data concerning the stages, operations in each stage, available equipment units, and processing times information is given in Table B.17. The uncertain processing times are described with uniform probability distributions between the minimum and maximum values given in the table. The availability of unit *F1* is also subject to uncertainty; the nominal breakdown time ($\bar{t}^{break}$) characterizing an exponential distribution of failure times, as well as minimum and maximum values of a uniform distribution for the breakdown duration (Top^{break}), are reported in Table B.18. Times are assumed to be in arbitrary time units, **TU**.

Particular scenarios with random values for the uncertain parameters have been defined to assess the suitability of the proactive approaches developed in the thesis. In Chapter 4 (Section 4.5.2) only uncertainty in the processing times is addressed, and the random scenario tested is detailed in Table B.19. For the proactive approach developed in Chapter 5 (Section 5.5.3) managing both uncertain processing times and equipment availability, the scenario with definite breakdown time ($\bar{t}^{break}$), breakdown duration(Top^{break}), and operation times is reported in Tables B.20 and B.21.

Table B.18: Characterization of the uncertain equipment availability for the washing subprocess.

Unit	$\bar{t}^{break}$	Top^{break} (min - max)
F1	240	72 - 96

Table B.19: Operation times for the washing subprocess in a particular scenario analyzed in Section 4.5.2.

ID	Order 1	Order 2	Order 3	Order 4
o1	17.7	18.6	12.0	13.0
o2	32.9	31.8	33.2	31.2
o3	16.4	12.9	14.3	9.4
o4	2.7	2.3	2.3	2.7
o6	53.8	56.8	69.6	57.1
o7	10.7	10.9	10.4	10.3
o8	10.2	6.8	6.9	10.5
o9	5.6	5.3	5.5	5.2

Table B.20: Equipment availability for the washing subprocess in a particular scenario analyzed in Section 5.5.3.

Unit	t^{break}	Top^{break}
F1	112.8	81

Table B.21: Operation times for the washing subprocess in a particular scenario analyzed in Section 5.5.3.

ID	Order 1	Order 2	Order 3	Order 4
o1	15.0	20.9	15.0	12.1
o2	32.5	32.5	33.5	32.5
o3	9.3	9.3	13.5	11.4
o4	2.8	2.8	2.8	2.8
o6	45.2	60	60	60
o7	*	10.8	10.3	10.8
o8	*	9.4	10.5	8.3
o9	*	5.1	5.1	5.2

*rejected operations because of the breakdown.

B.5 Production & transport: single product facility

A multi-site environment involving the production and distribution of a single product is adopted as case study to test the approach developed for integrating production and transport scheduling. It is based on the example proposed in Dondo et al. (2003). A product manufactured in a processing plant P is to be distributed in 10 different locations. The production recipe involves a single production stage with one operation, and a fleet of 2 vehicles is available in the plant.

Production data concerning the recipe, production orders, and inventory conditions is reported in Section B.5.1. Problem data related to the transport problem is detailed in Section B.5.2. Capacities and demands are assumed to be in weight units **WU**, time data is given in hours **h**, distances are in **km**, and costs are supposed to be in **€**, or **€/WU** if they are unitary costs.

B.5.1 Production data

Recipe data related to the process stage, operation, available equipment unit, batch size, and operation time is detailed in Table B.22. Table B.23 reports the initial level of stock in the plant (S_i^0), production orders (θ_i), and unitary inventory costs (c_i^I).

Table B.22: Production recipe data for case study B.5.

Recipe	Stage	Unit$_{(BS=2000)}$	Operation	Top
A	Procedure 1	Reactor	Reaction	0.5

Table B.23: Initial stock level (S_i^0), production orders (θ_i), and unitary inventory cost (c_i^I) for case study B.5.

Material	S_i^0	θ_i	c_i^I
Product A	4000	10000	0.3

B.5.2 Transport data

Transport data for the vehicles, locations, the distances matrix, and transport orders established in the sites is reported in Tables B.24 - B.27, respectively.

In addition, the transport factor ($f^{tr}_{v,l}$) used as unloading rate to evaluate the operation time of a discharge operation is assumed to be **0.000083 (**12000^{-1} **h/WU)** for all vehicles in all the locations; the weight values for the flow time (F), *Routes*, earliness (E) and tardiness (T) measures in the multi-objective criterion are fixed at ρ_1=**50**, ρ_2=**100**, ρ_3=**5**, and ρ_4=**20**, respectively; and the schedule start time is set at time **12:00 h**.

Table B.24: Vehicles data for case study B.5 (C_v: capacity; s_v: mean speed; c^u_v:unitary cost; c^f_v: fixed cost).

Vehicle	C_v	s_v	c^u_v	c^f_v
V1	7500	30	0.5	30
V2	7500	30	0.5	30

Table B.25: Locations data for case study B.5 (C_l: capacity; Top^{stop}_l: fixed stop time).

Location	C_l	Top^{stop}_l
P	15000	0.30
T1	1000	0.15
T2	1000	0.15
T3	2000	0.15
T4	1000	0.15
T5	3000	0.15
T6	1000	0.15
T7	1000	0.15
T8	2000	0.15
T9	3000	0.15
T10	2500	0.15

Table B.26: Distances matrix for case study B.5.

	P	T1	T2	T3	T4	T5	T6	T7	T8	T9	T10
P	-	6.2	9.5	8.2	9.7	14.8	12.7	9.6	8.6	12	10.7
T1	6.2	-	3.4	6.7	9.2	7.6	6.4	3.4	4.6	8.3	5.5
T2	9.5	3.4	-	3.3	4.8	4.2	4.7	4.0	6.2	9.5	8.0
T3	8.2	6.7	3.3	-	1.5	6.3	8.4	7.3	9.6	13.2	12.3
T4	9.7	9.2	4.8	1.5	-	5.5	8.6	8.8	11.1	14.8	13.8
T5	14.8	7.6	4.2	6.3	5.5	-	3.4	6.5	8.7	9.4	11.5
T6	12.7	6.4	4.7	8.4	8.6	3.4	-	3.1	5.3	6.0	8.1
T7	9.6	3.4	4.0	7.3	8.8	6.5	3.1	-	2.3	5.9	5.0
T8	8.6	4.6	6.2	9.6	11.1	8.7	5.3	2.3	-	3.7	2.9
T9	12	8.3	9.5	13.2	14.8	9.4	6.0	5.9	3.7	-	3.2
T10	10.7	5.5	8.0	12.3	13.8	11.5	8.1	5.0	2.9	3.2	-

Table B.27: Transport orders (θ_i^{tr}) and related due dates for case study B.5.

Order	Location	Material	θ_i^{tr}	Due date
1	T1	A	440	13:00
2	T2	A	580	13:00
3	T3	A	1370	13:00
4	T4	A	820	13:00
5	T5	A	2850	14:00
6	T6	A	750	14:00
7	T7	A	520	14:00
8	T8	A	1480	15:00
9	T9	A	2500	15:00
10	T10	A	1940	15:00

B.6 Production & transport: Procel

A multi-site environment based on Procel pilot plant described in Section B.3 is considered as a case study for production and transport scheduling. It involves two final products that have to be distributed in 8 retail outlets geographically spread around 200 km from the production site. Two vehicles with different features are available. A scheme of this example is represented in Figure B.5.

Figure B.5: Scheme of case study B.6.

Production data is reported in Section B.6.1, whereas Section B.6.2 details the input information for transport scheduling. Capacities and demands are specified in weight units **WU**, times are given in hours **h**, distances in **km**, and costs are assumed to be in **€**, or **€/WU** if they are unitary costs.

B.6.1 Production data

Recipe data related to process stages, operations in each stage, available equipment units, batch sizes, and operation times for each product is detailed Section B.3 above (Table B.15). Nominal operation times are adopted for the uncertain operations. Table B.28 reports the initial level of stock in the plant (S_i^0), production orders (θ_i), and unitary inventory cost (c_i^I).

Table B.28: Initial stock level (S_i^0), production orders (θ_i), and unitary inventory cost (c_i^I) for case study B.5.

Material	S_i^0	θ_i	c_i^I
A	500	1750	0.20
B	300	1250	0.25

B.6.2 Transport data

Data characterizing the vehicles, locations, the distances matrix, and transport orders established in the sites is reported in Tables B.29 - B.32, respectively.

The transport factor ($f_{v,l}^{tr}$) used as unloading rate to evaluate the operation time of a discharge operation is assumed to be **0.001 h/WU** for all vehicles in all the locations; the weight values for the flow time (F), *Routes*, earliness (E) and tardiness (T) measures in the multi-objective criterion are also fixed at ρ_1=**50**, ρ_2=**100**, ρ_3=**5**, and ρ_4=**20**, respectively; and the schedule start time is set at time **day 1 - 00:00 h**.

Table B.29: Vehicles data for case study B.6 (C_v: capacity; s_v: mean speed; c_v^u:unitary cost; c_v^f: fixed cost).

Vehicle	C_v	s_v	c_v^u	c_v^f
V1	500	50	0.12	10
V2	700	50	0.12	12

Table B.30: Locations data for case study B.6 (C_l: capacity; Top_l^{stop}: fixed stop time).

Location	C_l	Top_l^{stop}
BAR	5000	1.0
GIR	2000	0.5
LLE	1500	0.5
TAR	2000	0.8
VIC	1500	0.5
VAL	2500	1.0
ZAR	2500	1.5
PER	2000	1.0
AND	1500	1.0

Table B.31: Distances matrix for case study B.6.

	BAR	GIR	LLE	TAR	VIC	VAL	ZAR	PER	AND
BAR	-	103	178	101	70	351	311	192	198
GIR	103	-	256	194	68	444	389	96	215
LLE	178	256	-	107	158	348	149	346	153
TAR	101	194	107	-	162	260	240	283	273
VIC	70	68	158	162	-	411	356	158	151
VAL	351	444	348	260	411	-	328	535	534
ZAR	311	389	149	240	356	328	-	479	302
PER	192	96	346	283	158	535	479	-	163
AND	198	215	153	273	151	534	302	163	-

Table B.32: Transport orders (θ_i^{tr}) and related due dates for case study B.6.

Order	Location	Material	θ_i^{tr}	Due date
1	GIR	B	300	day 3 - 12:00
2	LLE	A	200	day 3 - 19:00
3	TAR	A	400	day 3 - 19:00
4	VIC	B	400	day 5 - 12:00
5	VAL	A	800	day 6 - 19:00
6	ZAR	B	250	day 8 - 19:00
7	PER	B	300	day 5 - 12:00
8	AND	A	350	day 8 - 19:00

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