UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

A contribution to support decision making in energy/water supply chain optimisation

Sergio Armando Medina González

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Decision Making in Energy/Water Supply Chain Optimisation

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A Thesis presented for the degree of
Doctor of Philosophy

Directed by Prof. Dr. Antonio Espuña

Escola Tècnica Superior d'Enginyeria Industrial de Barcelona

Universitat Politècnica de Catalunya

October 2018

*A mi padre y abuelos que están en el cielo, a mi madre y sobre todo a Karen,
con todo mi amor*

“*All truths are easy to understand once they are discovered; the point is to discover them.*”

Galileo Galilei (1564-1642)

Summary

The seeking of process sustainability forces enterprises to change their operations. Additionally, the industrial globalization implies a very dynamic market that, among other issues, promotes the enterprises competition. Therefore, the efficient control and use of their Key Performance Indicators, including profitability, cost reduction, demand satisfaction and environmental impact associated to the development of new products, is a significant challenge. All the above indicators can be efficiently controlled through the Supply Chain Management. Thus, companies work towards the optimization of their individual operations under competitive environments taking advantage of the flexibility provided by the virtually inexistent world market restrictions. This is achieved by the coordination of the resource flows, across all the entities and echelons belonging to the system network. Nevertheless, such coordination is significantly complicated if considering the presence of uncertainty and even more if seeking for a win-win outcome.

The purpose of this Thesis is extending the current decision making strategies to expedite these tasks in industrial processes. Such a contribution is based on the development of efficient mathematical models that allows coordinating large amount of information synchronizing the production and distribution tasks in terms of economic, environmental and social criteria.

This Thesis starts presents an overview of the requirements of sustainable production processes, describing and analyzing the current methods and tools used and identifying the most relevant open issues. All the above is always within the framework of Process System Engineering literature.

The second part of this Thesis is focused in stressing the current Multi-Objective solution strategies. During this part, first explores how the profitability of the Supply Chain can be enhanced by considering simultaneously multiple objectives under demand uncertainties. Particularly, solution frameworks have been proposed in which different multi-criteria decision making strategies have been combined with stochastic approaches. Furthermore, additional performance indicators (including financial and operational ones) have been included in the same solution framework to evaluate its capabilities. This framework was also applied to decentralized supply chains problems in order to explore its capabilities to produce solution that improves the performances of each one of the SC entities simultaneously. Consequently, a new generalized mathematical formulation which integrates many performance indicators in the production process within a supply chain is efficiently solved.

Afterwards, the third part of the Thesis extends the proposed solution framework to address the uncertainty management. Particularly, the consideration of different types and sources of uncertainty (e.g. external and internal ones) where considered, through the implementation of

preventive approaches. This part also explores the use of solution strategies that efficiently selects the number of scenarios that represent the uncertainty conditions. Finally, the importance and effect of each uncertainty source over the process performance is detailed analyzed through the use of surrogate models that promote the sensitivity analysis of these uncertainties.

The third part of this Thesis is focused on the integration of the above multi-objective and uncertainty approaches for the optimization of a sustainable Supply Chain. Besides the integration of different solution approaches, this part also considers the integration of hierarchical decision levels, by the exploitation of mathematical models that assess the consequences of considering simultaneously design and planning decisions under centralized and decentralized Supply Chains.

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

Resumen

La búsqueda de procesos sostenibles fuerza a las corporaciones a cambiar la manera en que operan. Adicionalmente, la globalización industrial implica un ambiente dinámico en los mercados que, entre otras cosas, promueve la competencia entre esas corporaciones. Por lo tanto, el uso eficiente y control de las los indicadores de rendimiento, incluyendo rentabilidad, reducción de costo, satisfacción de la demanda e impacto ambiental asociado al desarrollo de nuevos productos, representa un desafío significativo. Todos esos indicadores pueden ser eficientemente controlados mediante la gestión de cadena de suministro. Por lo tanto, las compañías buscan la sostenibilidad mediante la optimización de sus operaciones individuales dentro de un ambiente competitivo, tomando en cuenta la flexibilidad proveniente de las pocas restricciones en el mercado mundial. Lo anterior puede ser logrado mediante la coordinación de los flujos de recursos a través de todas las entidades y escalones pertenecientes a la red del sistema. Sin embargo, dicha coordinación se complica significativamente si se quiere considerar la presencia de incertidumbre, y se complica aún más, si se busca únicamente una situación de ganar-ganar.

El propósito de esta tesis es extender el alcance de las estrategias actuales de toma de decisiones con el fin de acelerar/facilitar estas tareas dentro de procesos industriales. Estas contribuciones se basan en el desarrollo de modelos matemáticos eficientes que permitan coordinar grandes cantidades de información sincronizando las tareas de producción y distribución en términos económicos, ambientales y sociales.

Esta tesis inicia presentando una visión global de los requerimientos de un proceso de producción sostenible, describiendo y analizando los métodos y herramientas actuales así como identificando las áreas de oportunidad más relevantes. Cabe mencionar que todo lo anterior se centra en el marco de ingeniería de procesos

La segunda parte de esta tesis se enfoca en enfatizar las capacidades de las estrategias de solución multi-objetivo. Durante esta segunda parte, primero se explora el como la rentabilidad de la cadena de suministro puede ser mejorada únicamente considerando múltiples objetivos bajo incertidumbres en la demanda. Particularmente, diferentes marcos de solución han sido propuestos en los que varias estrategias de toma de decisión multi-criterio han sido combinadas con aproximaciones estocásticas. Por otra parte, indicadores de rendimiento (incluyendo financiero y operacional) han sido incluidos en el mismo marco de solución para evaluar sus capacidades. Este marco fue aplicado también a problemas de cadenas de suministro descentralizados con el fin de explorar sus capacidades de producir soluciones que mejoran simultáneamente el rendimiento para cada uno de las entidades

dentro de la cadena de suministro. Consecuentemente, una nueva formulación matemática generalizada que integra muchos indicadores de rendimiento en los procesos de producción dentro de una cadena de suministro es eficientemente solucionado.

Más adelante, la tercera parte de la tesis extiende el marco de solución propuesto para abordar el manejo de incertidumbres. Particularmente, la consideración de diferentes tipos y fuentes de incertidumbre (p.ej. externos e internos) fueron considerados, mediante la implementación de aproximaciones preventivas. Esta parte también explora el uso de estrategias de solución que elige eficientemente el número de escenarios necesario que representan las condiciones inciertas. Finalmente, la importancia y efecto de cada una de las fuentes de incertidumbre sobre el rendimiento del proceso es analizado en detalle mediante el uso de meta modelos que promueven el análisis de sensibilidad de dichas incertidumbres.

La tercera parte de esta tesis se enfoca en la integración de las metodologías de multi-objetivo e incertidumbre anteriormente expuestas para la optimización de cadenas de suministro sostenibles. Además de la integración de diferentes métodos. Esta parte también considera la integración de diferentes niveles jerárquicos de decisión, mediante el aprovechamiento de modelos matemáticos que evalúan las consecuencias de considerar simultáneamente las decisiones de diseño y planeación de una cadena de suministro centralizada y descentralizada.

Por último, la parte final de la tesis detalla las conclusiones finales y el trabajo a futuro necesario sobre esta línea de investigación.

Acknowledgments

I am deeply thanked to my Thesis supervisor, Prof. Antonio Espuña, for giving me the opportunity to do this work, for his guidance, support and encouragement along these last five years. Thank you, for sharing your knowledge with a unique patience. I was delighted to have Prof. Gonzalo Guillén-Gosálbez continuously collaborating in my Thesis. I have nothing else than gratitude to him since he helped me to focus my research and build my character as researcher. His ability to motivating me to question every aspect of my research was the key to deeply understand the strategies that I used. Also, I do owe my gratitude to Prof. Luis Puigjaner and Prof. Fengqi You for their willingness to collaborate and helping me in my research.

I really want to thank my family. They found the way to support me at the distance. Thanks to my dad, that always though me the value of hard work and even in their last days he was dedicated to his family. You have always been an outstanding example to me. Thanks to my mom, Irma, my Brothers, Ramon and Geny, and my niece Airam, because even without knowing it, they support me and reminded me the importance of being close each other. Thanks also to my grandparents, my uncles, my cousins, fathers and brother in law for their support.

Thanks to the CEPIMA crew. Canan Dombyaci, thank you for all the relaxing conversations that we have had. In general, thanks to all my friends (and office mates) during these years of research: Francesca Audino, Ana Somoza, Shabnam Morakabatchiankar, Dr. Hamed Ardakani, Gicela Lupera, Xianwei, Ahmed Shokry and many others. Also to the researchers in CEPIMA, Dr. Moisès Graells and Dr. Montserrat Pérez-Moya

I acknowledge CONACyT that awarded me the scholarship to carry out this Thesis.

Last, but foremost, I am absolutely and sincerely grateful to my fiancée, Karen, who has completely supported and motivated me all these years with her love. Without her, I would not be where I am now. Thank you Karen, I love you and I'll always do.

Agradecimientos

Estoy profundamente agradecido con mi supervisor de tesis, Prof. Antonio Espuña, por brindarme la oportunidad de realizar este trabajo, por su guía, apoyo, y animo en los últimos cinco años. Gracias por compartir su conocimiento con una paciencia única. Fui honrado en tener al Prof. Gonzalo Guillén-Gosálbez colaborando continuamente en mi tesis. No tengo más que gratitud hacia él ya que me ayudo a enfocar mi investigación y construir mi carácter como investigador. Su habilidad para motivarme a cuestionar cada aspecto de mi investigación fue la clave para entender a profundidad las estrategias que utilice. También debo mi gratitud al Prof. Luis Puigjaner y Prof. Fengqi You por su disposición a colaborar y ayudarme en mi investigación.

Realmente quisiera agradecer a mi familia. Ellos encontraron la manera de apoyarme a la distancia. Gracias a mi papa, que siempre me enseno el valor del trabajo duro e incluso en sus últimos días estaba completamente dedicado a su familia. Siempre has sido un ejemplo excepcional para mí. Gracias a mi mama, Irma, a mis hermanos, Ramón y Geny, y a mi sobrina Airam, porque incluso sin saberlo, me han apoyado y me han recordado la importancia de estar siempre unidos. Gracias también a mis abuelos, tíos, primos, suegros y cunados por su apoyo.

Muchas gracias a todo el equipo de CEPIMA. Canan Dombyaci, gracias por todas las pláticas para relajarnos. En general, gracias a todos mis amigos (y compañeros de oficina): Francesca Audino, Ana Somoza, Shabnam Morakabatchiankar Dr. Hamed Ardakani, Gicela Lupera, Xianwei, Ahmed Shokry, y muchos más. También gracias a los investigadores de CEPIMA, Dr. Moisès Graells and Dr. Montserrat Pérez-Moya.

Agradezco a CONACyT que me otorgo la beca con la que se llevó a cabo esta tesis.

Por último, pero ante todo, estoy absoluta y sinceramente agradecido con mi prometida, Karen, quien me ha apoyado y motivado completamente todos estos años con su amor. Sin ella, yo no estaría donde estoy ahora. Gracias Karen, Te amo y siempre lo hare.

Contents

List of figures

Part I

Overview

Chapter 1

Introduction

The purpose of this chapter is to place the reader within the context of this Thesis giving an overview of the main challenges to be addressed in the near future by the global industry in terms of process economics and resources consumption. A brief overview of the current state of the art will be provided (and extended in further chapters) in order to identify the most promising alternatives used to improve the process sustainability. The search for sustainability approaches is focused but not limited to design and supply chain management (SCM) optimization techniques. The chapter finishes with the general objectives and the outline of this Thesis.

1.1. Introductory perspective and global market issues

During the last 30 years, the European Union (EU) has established itself in the top three of the chemical producers worldwide, just below China and EEUU *(European Chemical Industry Council 2017)*. In 2017, world chemical sales were valued at more than €3,000 billion, of which the EU accounts for 15.5% approximately, directly contributing to 1.15 million working opportunities. In particular, Germany, France, Italy, Netherlands, Spain, Belgium and the United Kingdom account for 83% of the total EU chemical sales. Notice that EEUU holds the first place as exporter country in the world (19%), while EU as a community was accounting near to 22% (€136.2 billion) of total global trade in 2017. Although it is remarkable the good performance of the EU due to its well-structured financial oriented network, a 20% decrease in EU chemical exportation has been recorded during the last four years which reflects the effect of market globalization *(Kato and Okubo, 2018)*. Consequently, an intensive work in logistic strategies is needed for worldwide enterprises to recover/maintain market leadership disregarding the chaotic and very competitive environment. For this purpose, the following issues have to be simultaneously addressed:

- Efficient model and control of highly complex networks.
  - A well-balanced policy for the material, energy, money and information flows.

- Reducing and preventing unfavorable environmental and social impacts (e.g. "Green engineering").
- Intensive collaboration in multidisciplinary areas, promoting the development of integrated frameworks.
- Efficient resource occupation (optimal process management)

The Process Systems Engineering (PSE) community is particularly well positioned to address the above needs, combining the concepts of modeling, simulation, optimization, and process control for the analysis, evaluation, optimization for the design and operation of chemical systems. Despite the significant advances in the development of approaches, methodologies and computational procedures to address the above issues, the following particular challenges remain as open issues for PSE researchers *(Grossmann, 2017)*:

- Improving the use and quality of the environmental indicators for the design of eco-friendly processes
- Integrating dynamic and discrete strategies (development of hybrid approaches)
- Real-time scheduling and optimization
- Synthesizing safe operating procedures
- Multi-scale dynamic modeling
- Developing integrated frameworks for the control of complex systems

The majority of these issues have their own limitations and specific application requirements to process problems; however, the design and management of sustainable processes (i.e. integrating dynamic and discrete strategies) are of special interest, since it has to be applied for all the industrial activities worldwide. Thus, this Thesis focuses on the issues associated with sustainability problems.

The accelerated environmental deterioration is one of the main side effects of the growth in both, population and industrial presence/activities worldwide. Therefore, in order to preserve/ensure a high quality in life standards, researchers are currently making an effort to develop approaches that promote sustainable solutions facilitating the efficient management of natural resources (such as water and biomass), reduce emissions (i.e. atmosphere issues), and develop alternative energy production processes (i.e. reduce fossil-fuel dependency *(Matson, 2001)*. In particular, these approaches assist in the evaluation, identification and reduction of the most damaging industrial activities; however, they were not applied in the industrial sector until the appearance of high government subsidies.

In this scenario, an efficient water management strategy is essential to promote the sustainability of any industrial network/process since it is unlikely to find an industry operating under a water-free policy. For instance, pharmaceutical, petrochemical, food and energy production processes typically require large amounts of freshwater (bigger amounts than any other resource). Besides, the water is a non-renewable resource; therefore the alternative sources are very limited. Thus, there is a need for a globally efficient water perseveration strategy.

1.2. Water situation

The overexploitation of water reserves has been intensified in the last three decades, due to the inefficient use of water resources, industrial development, and the unproportioned population growth and life standard enhancement. Fig. 1.1 displays the high correlation between water withdrawal and population growth.

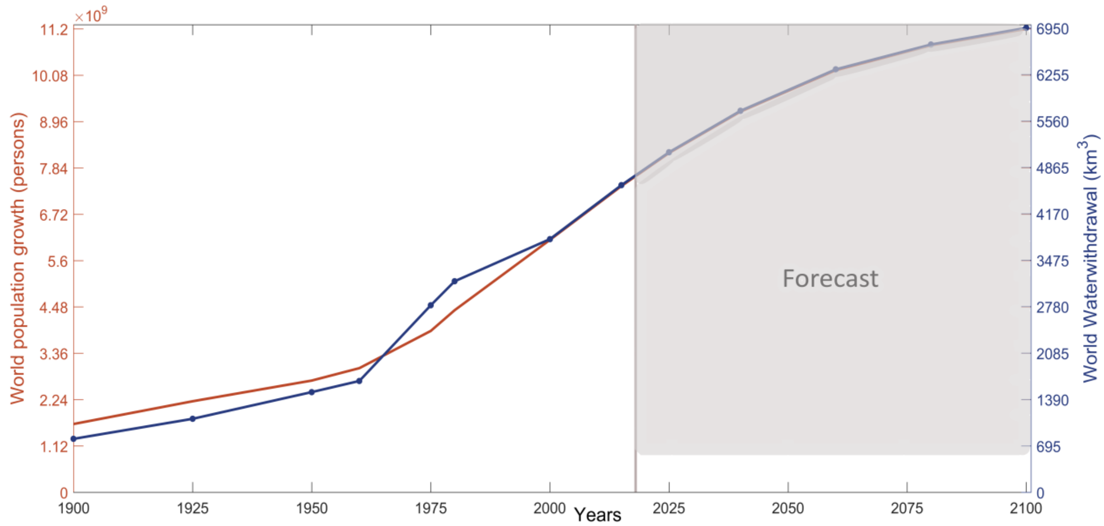

Figure 1.1. Correlation between population and water withdrawal in the last century. *(AQUASTAT, 2016)*.

Recent reports show that agriculture, public supply and industrial activities represent the majority of global freshwater requirements. In particularly, agricultural sector uses 69% of the consumed water worldwide, while industry achieves a 19% *(Shiklomanov, 1999; Mirata and Emtairah, 2010)*. Notice that these values change as a function of the geographical regions. Besides their different water consumptions, agricultural and industrial activities have a global efficiency of 70% and 10%, respectively. These values represent to which extent an activity take profit of freshwater, calculating the ratio between the real exploited water (i.e. water withdrawal minus water losses) and the net water withdrawal. Note that the water losses include evaporation, filtration, and wrong process selection *(Mirata and Emtairah, 2010)*. Fig. 1.2 illustrates the evolution of water efficiency over the last 30 years. Notice that there is a significant opportunity area to improve the performances of agricultural and industrial activities and ultimately reduce the water consumption.

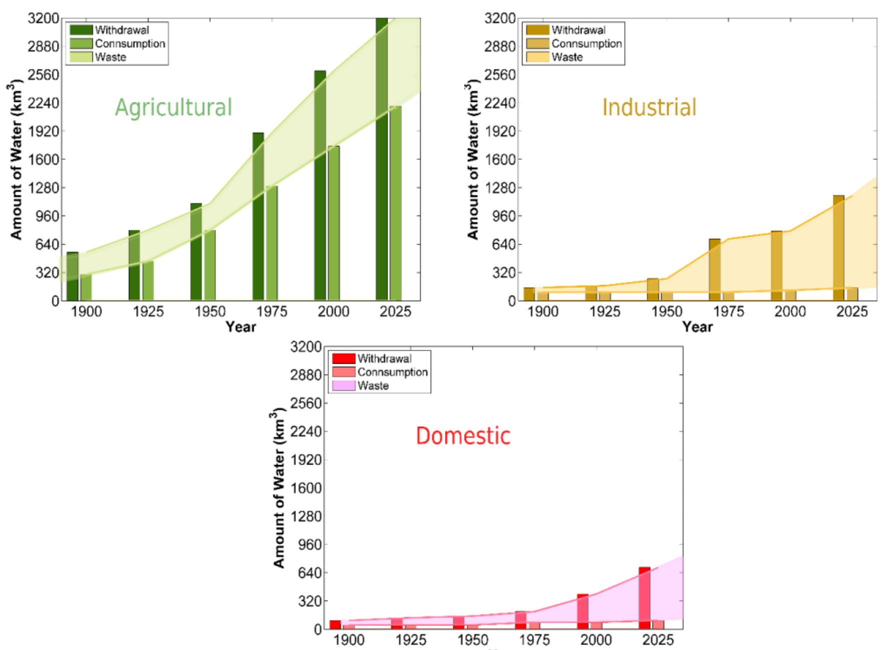

Figure 1.2. Behavior of water consumption in agricultural, industrial and domestic activities around the globe *(AQUASTAT, 2016)*.

EU agricultural and industrial activities consume 25 and 54% of the total water withdrawals, respectively. Notice that contrary to the global proportion, industrial activities represents a larger proportion if compared with agricultural ones, and the reason is that in average EU economy is based on industry *(Hispagua, 2010)*. Nevertheless, Spain presents a different behavior since it is one of the EU members that based its economy on agricultural activity, consuming for this purpose 55.9 km^3/year against the 25 km^3/year of freshwater used in industry. Thus, the annual waste for Spain is estimated in 39.3 km^3 of freshwater *(AQUASTAT, 2016; UNEP, 2007)*, which can be potentially reduced through the optimal management of the basic water-based tasks in the chemical industry (such as washing, diluting, cooling, or transporting). For this purpose, reuse and recycling strategies have been used for achieving savings up to 50% *(Mirata and Emtairah, 2010)*. In addition, water regeneration strategies have been implemented in the industrial context for the optimal design of water networks *(Foo, 2009)*. Nevertheless, the application of these strategies is sometimes limited to address problems with the following assumptions:

- The regionalized problem in which the variability of water availability and quality are controlled/known beforehand (i.e. Small and/or medium scale problems).
- Single contaminant problems.

Thus, the use of Supply Chain Management (SCM) concepts represents a powerful tool to control the use of resources.

1.3. Supply Chain Management concepts and Integration.

Historically, a set of interconnected entities representing a complete process and distribution network is known as a Supply Chain (SC). The elements/entities within a SC typically play one of the following four roles: supplier, producer, distributor and/or market center as displayed in Fig. 1.3 *(Puigjaner and Guillén-Gosálbez, 2008)*.

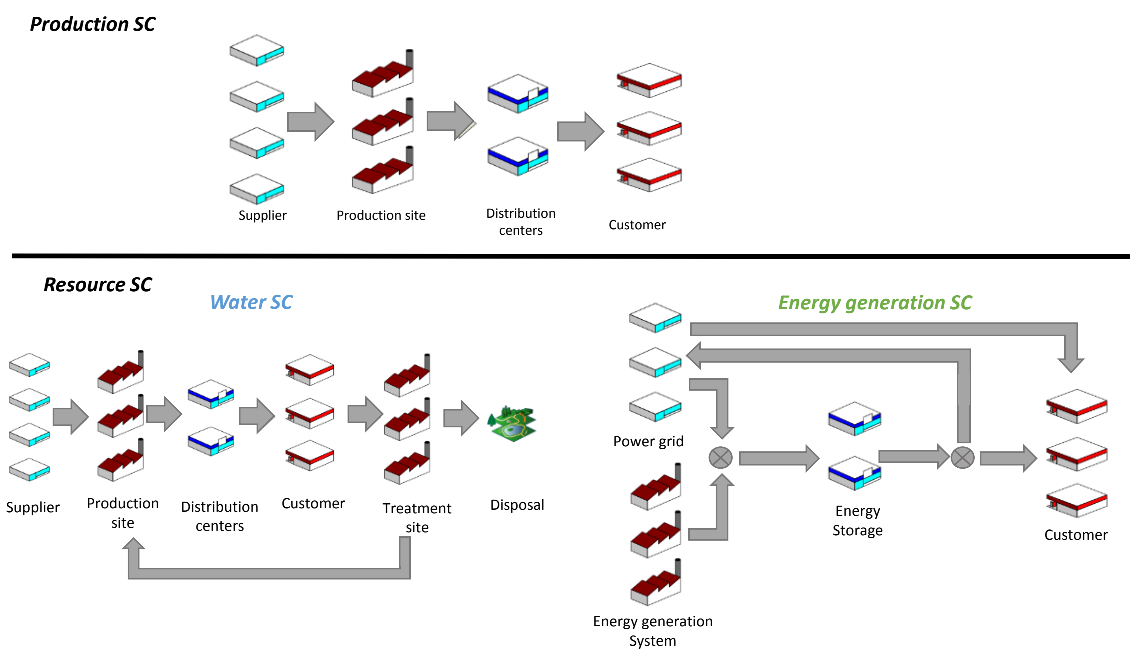

Figure 1.3. Example of different SC's arrangements.

The efficient coordination of the exchangeable resources (i.e. material, energy and information) within the entire SC leads to the concept of SCM *(Beamon, 1998; Tang, 2006)*. The main SCM purpose is to ensure a consumer satisfaction level while maximizing the process performance (typically economic) by synchronizing the following activities:

- Acquiring the required basic supplies (e.g. raw material, water, and electricity).
- Converting raw materials into intermediate and/or specified final products.
- Distributing intermediate and final products across the whole system.

The global concern in environment preservation initially justified the inclusion of waste treatment tasks as a mandatory activity for the SCM to reduce pollutants in residual flows *(Laínez-Aguirre et al., 2007; Tang, 2006)*. Nowadays, this concern has evolved and the concepts of "industrial symbiosis" and "circular economy" play an essential role in the management of a SC *(Zhang et al., 2015)*. Notice that due to the accelerated globalization, the current network includes a huge amount of alternatives for the material suppliers as well as potential customers increasing its complexity and compromising its efficient coordination. Thus, to assist the solution of SCM problems, a classification based on the horizon considered is commonly used.

- *Strategic level (long-term planning)*: This category typically considers a yearly-based discretization, in which the decisions include mainly the number and locations of facilities as well as its capacities. Notice that these decisions have a significant economic impact since large investments is made at this point.
- *Tactical level (medium-term planning)*: This level typically assumes a monthly-based time horizon in which the operations of the process are optimized to satisfy the product demand in the most efficient way. Tactical decisions include the amounts of exchangeable resources (i.e. acquisition and distribution), optimal production targets and inventory levels across the time.
- *Operational level (short-term planning or scheduling)*: Decision at this level includes the detailed equipment operations (startup and shut down), the production quantities, and task sequencing to specific equipment. For this level, a daily time horizon is commonly used and consequently these decisions are constantly adjusted.

Notice that these levels are strongly dependent, therefore, SCM decisions at each level should be coordinated with the decisions made in all the other levels.

1.3.1. Integrated Supply Chain Management.

The general idea behind SCM is to take efficient decisions despite the conceptual barriers produced between the different hierarchical levels and geographical allocations as displayed in Fig. 1.4 *(Varma, et al., 2007)*. Even if there are many works addressing this issue, the original challenge to break down "walls" still remains due to the increasing pressure on respond to the customer requirements with maximum enterprise-wide revenues, efficient facility utilization, minimum inventory, and minimum ecological footprint simultaneously *(Hameed, 2007)*. Such a coordination of multiple SC's at different hierarchical levels represents an Enterprise-Wide Modeling and Optimization (EWMO) problems. Even if EWMO do not add new challenges to the ones associated to SCM, it emphasizes them since many of them have to be addressed together.

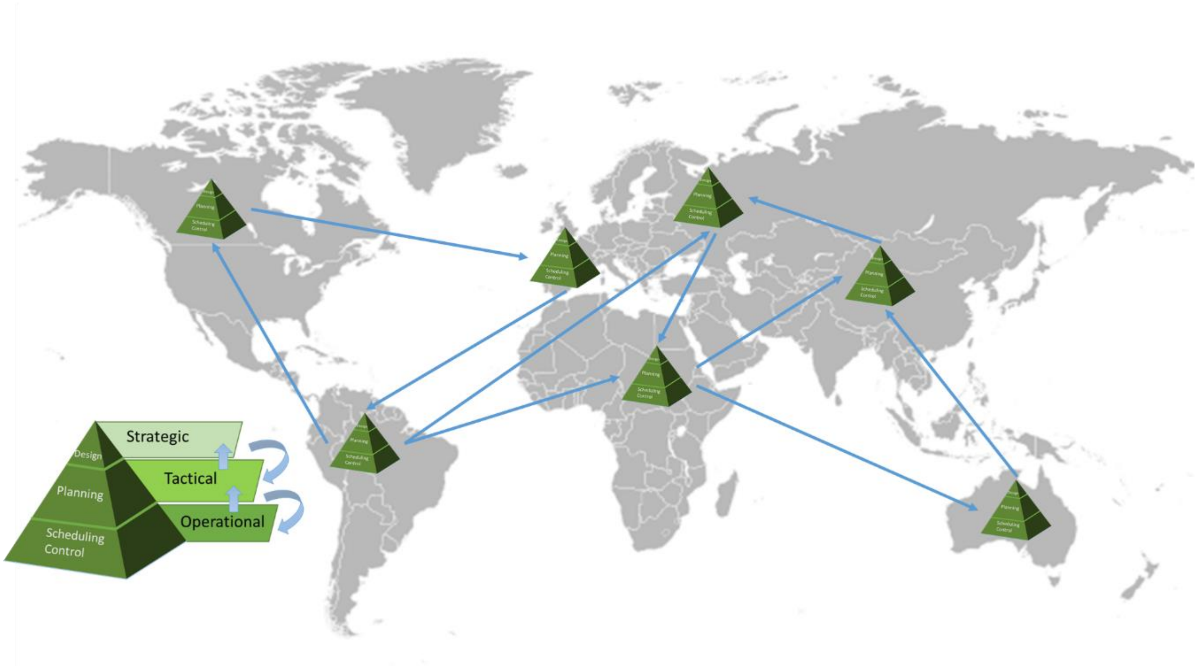

Figure 1.4. Different integration approaches.

The coordination of an enterprise-wide network focuses on taking the planning, scheduling and control, decisions that often requires specific knowledge of process engineering *(Grossmann, 2005)*. In addition, such a management increases in complexity when considering market dynamics, uncertainties, and internal business operations *(Shapiro, 2006; Blanchard, 2004)*. Therefore, an integrated management framework considering uncertainties and SC dynamics is required. Such approach should ensure a flexible, accurate, and robust response to changes in the business environment.

1.3.2. SC Mathematical Modeling

Mathematical modeling aims to represent a defined system as close to the reality as possible through a set of equations. The resulting model is expected to mimic accurately a system's behaviors promoting its control using performance measurements *(Morris, 1967)*. In particular, SC modeling is used for the proper network control and coordination, identifying potential bottlenecks and, ultimately, producing the optimal management.

Structural arrangements

As commented, a SC is a set of different task-oriented entities; moreover, the same set of elements can lead to different organizational problems depending on their particular arrangement. Commonly two categories exist based on the decision-making domain (i.e. the "power"/influence of one decision maker over the different elements of the process).

Centralized. Is the most commonly used scheme in the literature since it significantly eases the network coordination by considering that a single entity has the full control to take all the SC decisions. In particular, such a central entity collects the information describing the whole system and uses it to optimize the performance from a global perspective. The main drawback of such an approach is that the central entity (i.e. decision-maker) assumes a passive attitude for the rest of the SC members and their individual performances are disregarded. Therefore, while addressing dynamic market problems, the use of a centralized scheme is inefficient and very often leads to decisions that are hardly accepted by all the process members (i.e. unbalanced/unfair solutions).

Decentralized. Contrary to the centralized one, this approach is a more accurately representation of the reality considering an active attitude of the entire set of SC members. Thus, they should take their own decisions as a function of their individual performances. Notice that, even if this scheme promotes the generation of a well-balanced solution seeking the highest benefit for all the entities, its application is complex for two main reasons:

(i) The decisions of a SC member affect the system performances and, consequently, condition the other elements decisions *(Vonderembse et al., 2006)*.

(ii) There is a lack of information between SC members regarding performances, preferences and behaviors, compromising the robustness/confidence of the final decisions.

Notice that among these two extreme approaches, an intermediate situation may be considered. This third scheme is named *Semi-centralized;* however this approach has been seldom analyzed in the literature.

1.4.Research Scope and Objectives

The general goal of this Thesis is to apply and extend general PSE methods and tools in order to develop decision support systems assisting the systematic SC's planning and management, focusing on the case of water and energy networks. It is expected to achieve such an objective by the complete fulfilling of the following specific objectives.

- Develop robust mathematical models that better represent the resource SC and the distribution links between members. Here, it is necessary to address the following issues:
  - ➢ Account for the traditional planning decisions and parameters forecasting (i.e. endogenous and exogenous uncertainty).
  - ➢ Develop a multi-objective model considering at least economic, environmental and social aspects.
  - ➢ Evaluate multiple efficiency indexes as decision criteria within a MO problem (risk metrics, water stress, etc.) to, ultimately, provide a robust/confident decision.
  - ➢ Evaluate the effect of uncertainties over a decentralized scheme under a competitive environment.
- Address decision-making issues for sustainability problems under uncertainty by extending the current multi-objective approaches (i.e. optimization and post-optimization strategies).
- Integrate all the available information related to a SC (at different levels) to promote the reuse of resources (i.e. closed-loop problem) for both, centralized and decentralized SC.
- Apply surrogate models as a data-driven decision-making for resource SC problems.

1.5.Thesis outline

The Thesis structure was devised to address the decision-making issues previously discussed (see Fig. 1.5); along it, multi-objective optimization and uncertainty approaches were considered as the two key elements across the different parts of the Thesis.

In addition to the overview of the current sustainability problems, particularly in resource management (Chapter 1), the Part I of this Thesis includes a detailed state of the art for the decision-making applications (Chapter 2) and the description of the advantages and disadvantages of the methods used address sustainable SCM developed until now (Chapter 3). Notice that at the end of Part I, the main trends and challenges are identified. Basically, in Part I the different optimization techniques used throughout this Thesis have been outlined. The main concepts behind each technique have been briefly introduced with the purpose of providing the reader with a general understanding of the theory behind the solution techniques applied in this Thesis. Special emphasis has been made in techniques and algorithms for Multi-objective optimization, stochastic programming and decomposition techniques since their application to sustainability problems requires a solid knowledge of their principles.

Part II evaluates different decision-making approaches aiming to identify the overall better solution for sustainability problems using multi-objective optimization. In particular, Chapter 4 explores the use of Fuzzy-based formulations to address MO problems as a way to expedite the solution identification in terms of quality and time efficiency. Complementarily, Chapter 5 emphasizes on identifying the advantages and limitations of ELECTRE-IV and Fractional approach as decision-making strategies to handle a large number of objectives/criteria as well as the explicit representation of decision maker interests.

In Part III, the main challenges associated with the efficient representation and management of uncertainties within a sustainable energy SC are addressed. Chapter 6 explores the use of a scenario reduction method as a way to narrow down the computational effort required to optimize a problem considering well-represented process uncertainties. In the same way, Chapter 7 proposes a data-driven decision-making strategy capable of considering multiple sources of uncertainty simultaneously within an energy generation SCM problem.

Across the entire Part IV, the above MO and uncertainty management strategies are combined within different integrated decision-making frameworks, which are capable of address multi-objective problems affected by uncertainty conditions. Chapter 8 combines the use of the sample average approximation to relax the two-stage stochastic formulation with the Pareto filter method to identify the overall better solutions, while in Chapter 9 the traditional two-stage stochastic optimization is used within a decentralized water management SC to address the uncertainty condition while identifying the most appealing solution for all the SC partners using the ELECTRE-IV method.

Finally, Part V summarizes the main contribution of this Thesis and draws up concluding remarks for future work.

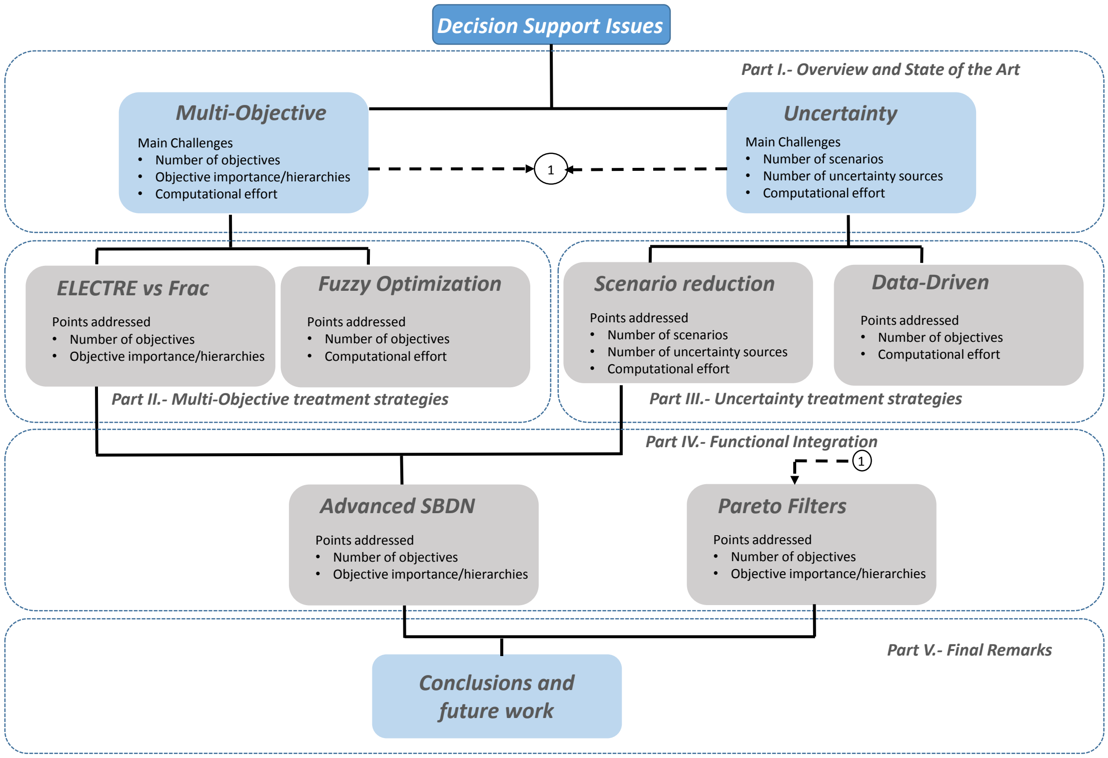

Figure 1.5. Thesis outline.

Chapter 2

STATE OF THE ART

This chapter summarizes the major contributions made so far related to the optimization of SCs. In addition, contributions proposing the combination of decision-support strategies to traditional optimization methods in a single framework for its application to individual and integrated hierarchical optimization problems will be detailed commented. Studies addressing the challenges associated with resource management (including process uncertainties) are also reviewed. Finally, this chapter identifies the most relevant open issues addressed in this Thesis.

2.1.Hierarchical Decision Making for SCM

As described in Chapter 1, since mid-eighties, a hierarchical approach (based on the considered time-horizon has been considered as the most effective way to assist SCM optimization *(Hax and Meal, 1975)*, however, a disconnection between the different hierarchical levels is assumed. Hence, current optimization approaches try to integrate different hierarchical levels using upper-layers results as constraints for the lower-level problems. Such an approach implies handling a large and changing number of constraints that complicates the solution. The above represents a poor approximation, but is still used due to the lack of better analytic and data processing methods that support a holistic integrated optimization approach. Thus, further research improving both, technology and data-based optimization techniques is needed. The following subsections present a detailed literature review on the algorithms and methods used to solve PSE problems at different hierarchical level individually and integrated.

2.1.1. Strategic level

This level provides a general overview of the entire process network by identifying the optimal location and SC's entity type (i.e. supplier, producer, distributor, etc.). Traditionally, any design is optimized based on an economic perspective, which may combine multiple factors, including annual profit, total capital cost, net present value, or financial risk. Particularly, design and allocation problems have been addressed since 1950's, however it was in 1965 when the first mathematically structured model appears by the hand of *Balinski, (1965)*. Later, many mathematical models addressing design and distribution optimization problems were proposed as described in the reviews of *Garcia and You (2015)* and *Govindan et al., (2017)*. These problems include networks of increasing complexity, varying from a simple plant to a simultaneous design/operation of a multi-site SC's. Notice that the investment decisions taken at this level have a significant impact on the global economic performance since design problems are solved for a time horizon ranging between two and seven years. Even if the basic decisions at this level are centered in allocation, process manufacturing and distribution activities are considered from a general perspective employing basic (and very often inaccurate) models. Lower-level decisions provide accurate and detailed information, thus, the development of integrated hierarchical decision frameworks are justified.

These problems are traditionally modeled using a Mixed Integer Linear Program (MILP) formulation that promotes the simplified representation of both, continuous and discrete variables. Actually, the use of MILP formulations to optimize the economic performance of industrial problem has significantly increased, especially after being successfully applied by *Brown et al., (1987)*. The driving force of a SC network design is the constant pursuit of process flexibility, as demonstrated by *Ferrio and Wassick (2008)* which identify the potential production/distribution links and use this information to re-design the existing configuration and increase the process performance. In parallel, *Naraharisetti, et al., (2008)* extend the formulation to consider different investment alternatives describing the increment in equipment capacities. Later, *Li et al., (2016)* use different pricing policies for the design of green supply chains to represent the unpredictable/uncertain behavior of pricing variations. These prices, as well as the changing environmental conditions are represented using a set of scenarios

Before *Li et al., (2016)*, *Guillén and Grossmann, (2009)* stressed that controlling the effect of uncertainties is of great relevance to any process management. The most common uncertainties management technique is the multi-stage stochastic formulation. Many studies use such a formulation in SC design *(Govindan et al., 2017)*, including but not limited to enterprise-wide distribution *(Santoso et al., 2005)*, retrofit problem of a production/distribution network under process uncertainty *(Mele, et al., 2007)* and pharmaceutical industry and resource problems *(Keyvanshokooh et al., 2016; Sadghiani et al., 2015; Vahdani et al., 2012)*. Despite the effective uncertainty management for industrial problems, additional efforts are needed to reduce the solving time required (i.e. computational effort). For this purpose, the contribution by *Laínez-Aguirre et al., (2015)* can be mentioned, in which a framework that combines state-task-network based approach (STN) and Lagrangian decomposition has been proposed. Such a framework addresses the management of a large and detailed amount of information at each node to maximize the economic benefit and network flexibility in a time-effective way. Notice that in addition to Lagrangian decomposition, other decomposition strategies/methods have been considered for the design/re-design of chemical production process and energy networks *(Corsano et al., 2014)*.

Besides the improvements in the optimization strategies for the design of complex networks, another important issue is the simultaneous consideration of multiple objectives and/or key performance indicators. Among these studies, *Laínez-Aguirre et al., (2010)* produce a great contribution in which a Mixed Integer Non-Linear Programming (MINLP) formulation was used to manage the trade-off between marketing and SC design decisions. Similarly, the sustainable SC re-design has been applied to a bioethanol production process considering the global economic performance as well as multiple financial risk metrics as objectives *(Kostin et al., 2012)*. All these contributions consider only economic nature objectives; nevertheless, its combination with another type of objectives (such as environmental ones) is basic for the pursuit of process sustainability. In this line, *Guillén and Grossmann, (2009, 2010)* and *Ruiz-Femenia et al., (2013)* address the sustainable design of chemical production processes, while *Pérez-Fortes et al., (2012)* and *Laínez-Aguirre et al., (2017)* optimized a regional bio-based energy SC and *Gao and You (2015)* the energy-water networks.

Besides the significant advances in optimization strategies combining both, multi-objective consideration and uncertainty management, further studies are still required, especially to address problems under the effect of variable market environments. Therefore, open issues and challenges regarding market behaviors (e.g. industrial cooperation/competition) and computationally limitations (model requirements and technology improvements) must be addressed by the simultaneous development of:

- Efficient multi-objective approaches that consider more than two objectives (or performance indicators).
- New and more efficient numerical algorithms to solve complex non-linear models that provide more accurate problems representation.
- An integrated decision-support strategy (i.e. a combination of multi-objective and uncertainty management methodologies) to promote the identification of reliable solution in terms of financial and environmental performance.

2.1.2. Tactical level

In mid-term planning the most efficient resources acquisition, production, inventory, and distribution levels across the entire network are calculated. Planning problems base their formulation on three main elements:

(i) Material and energy balances between each process equipment/location;
(ii) The detailed information regarding resources availability and demand, distances between SC members, selling/buying prices, raw material availability, production boundaries and distribution/storage capacities.
(iii) Fixed configuration data defined in the upper-level (strategic decisions).

Alike in strategic level, here a MILP model is frequently used not only to include discrete and continuous variables, but also to consider some financial behaviors (including investment cost, price fluctuations, and price policies).

One of the first and outstanding contributions in planning problems is the one presented by *Wilkinson et al., (1996)* in which a continent-wide network consisting of three multipurpose production facilities that supply a vast variety of products across the European market was coordinated. Lately, this kind of mathematical programming has been increasingly used to solve this kind of problems, for instance, *McDonald and Karimi (1997)* extend the Wilkinson formulation to address the optimization of a multi-period SC problem. Similarly, *Jackson and Grossmann, (2003)* enhance even more the multi-period approach to consider a multi-site production/distribution network considering non-linear relations in the production plants. These non-linear behaviors have been modeled through a MINLP formulation and they have been successfully applied to pharmaceutical *(Papageorgiou et al., 2001; Sousa et al., 2011; Susarla et al., 2012)*, agrochemical *(Sousa et al., 2008)*, and refineries planning problems representing, chemical recipes, cost functions, or product/resource properties. More recently, its application to dynamic optimization problems has been considered to address bio-refinery processes by incorporating a Model Predictive Control (MPC) approach *(Santibañez-Aguilar et al., 2015)*. It is worth to mention that these studies improve the quality of the process representation by collecting a large number of details; however, solving a well-represented problem is, most of the times, very difficult (complex) due to a large number of required equations and constraints. Besides the improvements in models development, the reduction of computational effort required to solve them, remains a significant challenge. As well as in the upper-level cases, strategies based on Lagrangean, spatial and temporal decomposition were proposed to address such an issue.

Lagrangean decomposition techniques have been used to address non-linear multi-period production/distribution problems *(Jackson and Grossman, 2003)*. In essence, the large-scale problem is decomposed in different temporal schemes (i.e. smaller instances) that solve it sequentially. Similarly, bi-level decomposition strategies have been used for planning problems, for example, *Ryu and Pistikopoulos (2007)* optimize the operations/distributions of a multi-period SC. In this case, the first level defines the SC demands based on the geographical distribution, while, for the second part, these values are used as parameters for the optimization of the single-site planning problems. Remarkably, decomposition strategies that promotes a time-effective solution to industrial planning problems have been also combined with tailor-made methods such as Vendor Managed Inventory (VMI) formulation *(Al-Ameri et al., 2008)*, Resource-Task Network (RTN) *(Pantelides, 1994)* and Rolling Horizon (RH). Many PSE literature reviews on integrated strategies to address design and planning problems agrees that The treatment of uncertainty requires further research effort to capture aspects such as product prices, resource availabilities etc. In order to ensure that investment decisions are made optimally in terms of both reward and risk, suitable frameworks for the solution of supply chain optimization problems under uncertainty are required *(Papageorgiou, 2009; Mula et al., 2010; Díaz-Madroñero et al., 2014)*.

Multiple PSE authors agree that most of the mentioned approaches, even if computationally efficient, present two main limitations. First, they address the problem considering a unique objective function and secondly, the effect of uncertain/variable conditions on the process behavior is traditionally neglected. Hence, to promote the efficient SC's management and the effective use of resources (such as water and/or energy), it is imperative to address these challenges. In this regard, several studies use a sort of multi-criteria approaches seeking for the process sustainability. For instance, *Fahimnia et al., (2015)* evaluates the trade-off between carbon emissions, energy consumption, and waste generation. In Parallel, *Boukherroub et al., (2015)* proposed a multi-objective model, which considers simultaneously the economic, environmental and social impacts, while *Rojas-Torres et al., (2015)* take into account the water savings and land use as additional objectives to the global economic performance.

As commented, resource SCM has emerged as a seldom explored research field that required not only the consideration of typical MO challenges, but also those associated with their uncontrollable/uncertain conditions. In this regard, several studies have been proposed to promote an environmentally conscious SC design under uncertain parameters/conditions *(Cheng-Liang et al., 2004; Ruiz-Femenia et al., 2013; Luo et al., 2016)*. Mathematical models have been used to represent a wide variety of sustainability problems under uncertainty, including, chemical and pharmaceutical production, food industry and energy/water networks *(Seuring and Müller, 2008; Ahi and Searcy, 2013)*. Despite the significant improvements in uncertainty managements strategies (at single and multiple hierarchical levels), they are limited to single objective problems; thus, there is a need for further studies promoting the development of integrated frameworks combining MO and uncertain management strategies at multiple hierarchical levels.

2.1.3. Operational level

At this level, the equipment allocation and use of resources are calculated for a short-time period, which is critical for both, batch and continuous processes. Even if the basic concepts of this level are similar to those in the upper ones, here the main purpose is to optimize process operation solving the question of what, where, how and when to produce a specific product. In particular, the decisions to be made, include the production dimensions (e.g. lot sizing for batch processes), production allocation, and start-up and shut-down times. Remarkably, in operational models, the main decisions defined in upper hierarchical levels (including, the SC configuration and available/required resources) are generally considered as parameters.

To address scheduling problems, researchers have proposed mathematical models representing different process situations, including short-term scheduling of batch plants *(Pinto and Grossmann, 1995)*, multi-product batch plants *(Méndez and Cerdá, 2007; Marques de Souza Filho et al., 2013; MirHassani and BeheshtiAsl, 2013)* and multi-period optimization models *(Kabra et al., 2013)*. Particularly, MILP models have been used in multi-product, multi-task batch processes for single-stage *(Castro et al., 2008; Castro and Grossmann, 2012)* and multi-stage production plants *(Prasad and Maravelias, 2008)*. Despite the usefulness of the above algorithms for short-term scheduling problems, developing mathematical approaches for the systematic solution of multi-site scheduling problems (i.e. complex enterprises) is a significant opportunity area and needs further efforts. In this line, bi-level decomposition algorithms *(Bok et al., 2000)* and heuristic decomposition algorithm based on variable-length slots *(Jetlund and Karimi, 2004)* appears as a promising alternative.

Alike in upper decision-levels, the effect of uncertain conditions significantly affects the optimization methods. Actually, the use of STN formulation, firstly introduced by *Kondili et al., (1993)*, was used to promote a control of the tasks, raw matter, intermediate and final products at each process node *(Guillén-Gosálbez et al., 2006)*. Furthermore, several authors have used the STN formulation for a discrete *(Maravelias and Grossmann 2003b; 2006)* and continuous time representation *(Maravelias and Grossmann, 2003a)*. Later, *Bose and Bhattacharya (2009)* developed a MILP formulation to optimize the schedule of several continuous processing units using the STN representation. These formulations require the management of a large number of equations/constraints, thus, the use of decomposition strategies is required. Additionally, different approximations techniques can be used including the rolling horizon and graphical approaches (S-graph). Rolling horizon focuses on the management of the uncertain parameters while S-graph seeks to reduce the computational effort comparing with conventional mathematical programming techniques.

Scheduling decisions significantly affect process feasibility and sustainability, thus, in addition to economic performance, environmental and financial robustness criteria must be considered. In fact, many MO strategies assist such a consideration within scheduling problems including goal programming (GP) *(Zhou et al., 2000)*, mixed-integer linear fractional programming (MILFP) *(Yue and You, 2013)*, heuristic approaches *(Lin et al., 2013)*, and Fuzzy programming *(Zakariazadeh et al., 2014)*. Most of have been applied to a wide variety of problems including energy generation, petrochemical industrial processes *(Inamdar et al., 2004)* and discrete scheduling models *(Capón-García et al., 2014)* and its use assist in the generation of a single and well-balanced solution for bi-objective problems. As commented, the solution of any MO problem increase in complexity when considering more than two objectives as well as the effect of uncertainties over the system performance, therefore, strategies addressing both, MO and uncertainty management are presented in sections 3.3 and 3.4.

From this literature review, it is clear that the hierarchical levels share some challenges that can be addressed by developing a solution framework capable of managing MO and uncertainty problems individually and all together. Note that such a framework must be computationally efficient to provide an optimal solution facilitating the decision-maker procedure. Addressing these issues will settle the basis for further contributions regarding hierarchical level integration. Thus, the next sections display the current state of the art on hierarchical level integration, MO and uncertainty.

2.2. Hierarchical levels integration for the decision-making

During SCM, many decisions are taken at each hierarchical level; however, such an issue increases in complexity when considering the interaction between them *(Grossmann, 2004; Shah, 2005; Varma, et al., 2007; Maravelias and Sung, 2009; Papageorgiou, 2009)*. Moreover, hierarchical layers interactions between each pair of are of great relevance for PSE and can be categorized as: (i) Design-planning; (ii) Planning-scheduling and; (iii) Design-scheduling.

To coordinate design and planning decisions, some integrated strategies have been proposed based on decomposition strategies to address a wide variety of problems, including multi-site SCs *(Kallrath, 2002)*, multi-echelon multi-product multi-site SC *(Tsiakis and Papageorgiou, 2008)* and non-linear multi-product SC *(You and Grossmann, 2008)*. Later, *You et al., (2011)* use a multi-period MILP model to optimize a multi-site multi-product large-scale chemical process. Even if using decomposition approaches, they compare Lagrangean and bi-level algorithms to identify the most efficient one in terms of computational effort, being bi-level the one that shows better results. Notice that the increasing interest in developing sustainability process justifies the combination and application of MO strategies within design-planning integration frameworks. A representative example of this kind of problems is the closed-loop SCs (CLSC) in which, in addition to the process performance, the efficient resource exploitation is promoted. In this line, *Lee et al., (2009)* propose a model that manages the system using re-manufacturing activities, while *Zhang et al., (2011)* apply the same reverse logistics to address the management of municipal solid wastes networks. Remarkably, the integrated design-planning of sustainable frameworks also requires to address uncertainty challenges. In this regards, *Kostin et al., (2012)* apply integrated frameworks to the bioethanol and sugar production problem under demand uncertainty, while in the same year, *Zeballos et al., (2012)* use them in a large-size glass industry SC considering quantity and quality uncertainties for the backward flows. Similarly, *Cardoso et al., (2013)* optimize a CLSC model under demand uncertainty, while *Zeballos et al., (2014)* optimize a multi-period multi-stage CLSCs considering the emissions costs of the different logistic modes. More recently, *Ng et al., (2015)* propose a strategy that exploits the concept of industrial symbiosis to integrate design and planning decisions within bioenergy parks.

Within the wide variety of PSE studies addressing the SCM hierarchical levels integration, the ones that deal with planning and scheduling problems have a positive impact on batch processes. In this line, *Maravelias and Sung (2009)* published a very detailed review of the feasible strategies to address these problems focusing on two main approaches:

i) Merge the scheduling decision variables within the tactical model.
ii) Approximating the scheduling decisions by relaxing them.

In such a review, it was concluded that although the use of these approaches would lead to optimal solutions, the problem size and its complexity significantly increases. Hence, several studies were proposed to overcome these challenges. For instance, *Neiro and Pinto (2004)* use an integrated strategy to solve the SCM of a petroleum industry, coordinating multiple refineries, equipment (e.g. distillers), and pipelines networks as multi-period large-scale MINLP problem. Later, *Sung and Maravelias (2007)* model the scheduling decisions as a set of linear surrogate constraints and introduce them into the planning model for a multiproduct process network. In parallel, *Erdirik-Dogan and Grossmann (2007)* use a bi-level decomposition technique combined with a RH approach for the optimization of a single plant while afterward, *Terrazas-Moreno et al., (2011)* extend such a formulation to consider multi-site multi-period SCs combining bi-level with spatial Lagrangean decomposition. Notice that all these studies focuses on promoting the efficient satisfaction of the computational requirements, which, is a challenge becoming more complicated when multiple objectives and/or process uncertainties are considered. Therefore, in recent literature strategies addressing integrated planning and scheduling problems from a sustainability perspective have been presented, including pharmaceutical industry *(Colvin and Maravelias, 2008; Christian and Cremaschi, 2014)*, but also for chemical processes *(Shin and Lee, 2016)* and energy generation problems *(Zhao et al., 2016)*. Commonly, studies in which resource utilization and acquisition are optimized to satisfy the producer requirements under demand/availability uncertainties, uses a decomposition strategy that simply splits the original problem into a planning problem controlling the raw material procurements and a scheduling problem that manage its operations (work orders satisfaction and material utilization). Very recently, *Shang and You, (2018)* propose a distributional robust optimization as a novel approach for the planning and scheduling of a multi-purpose pharmaceutical batch production process under demand uncertainty.

Opposite to the other two interactions, there are significantly low studies regarding complete integration (design-planning-scheduling integration). In this line, the most significant contribution is the one by *Kallrath (2002)* that integrate scheduling and strategic planning in a MILP multi-period model for multi-site real production SCs.

Notice that despite the significant contributions for the integration of hierarchical levels, a large-scale holistic model is required, even if it is likely to result in a very high complex optimization problem. Therefore, in order to integrate different decisions at different time-scales the following issues need more efforts:

- Developing/modifying algorithms to solve multi-objectives integration models.
- Considering new sustainability measures, risk, and resilience.
- Combining planning and scheduling frameworks to promote the systematic decision-making.
- Combining different techniques to manage uncertainty.
- Developing/modifying algorithms to solve stochastic integration models.
- Incorporating different business functionalities and financial issues at different decision levels.
- Considering logistics and inventory management.

Remarkably, the simultaneous consideration of planning and scheduling problems/issues has been briefly addressed. For example, *Gutiérrez-Limón et al., (2016)* propose a mixed integer dynamic model for the optimal planning, scheduling and control of continuous reactors. A heuristic strategy is developed as a reactive approach to tackle the uncertainty of demand, but still, more efforts are required to extend such a holistic approach.

2.3.Multi-objective optimization

Traditionally, industrial processes focus on the optimization of the economic performance by managing the basic operations such as product manufacturing, unit installation, and raw material/product distribution. However, these activities have a negative effect on the environment, hence, the control, as well as the emission reduction and wastes discharge, are the biggest industrial concerns nowadays. Methods used to solve multi-objective optimization problems can be classified into analytical and numerical approaches:

- *Analytical methods* consist of detailed mathematical calculations capable to reach an exact solution. However, this type of methods very often requires a large number of equations to approximate the problem in a realistic way.

- *Numerical methods* seek to approximate the solution relaxing the complex mathematical formulation and solving the problem iteratively. It has been traditionally preferred to address realistic/complex problems rather than the analytical one.

Analytical methods are extensively used in PSE literature form which ε-constraint can be highlighted as the most widely used since it addresses multi-objective problems *(Bojarski et al., 2009; Guillén-Gosálbez and Grossmann, 2010; Ehrgott, 2005)*. This method systematically solves the MO model at different defined objective constraints producing the well-known Pareto frontier, which collects only dominant solutions (i.e. a solution that cannot improve one objective without deteriorating any other). Even if ε-constraint efficiently identifies the Pareto frontier, the associated solution identification challenge remains unsolved. For this purpose, alternative approaches including Pareto filters *(Pozo et al., 2012; Antipova et al., 2015)*, data envelopment analysis *(Limleamthong et al., 2016)*, ELECTRE methods, and bi-level optimization *(Guarnieri, 2015; Limleamthong et al., 2017)* can be used to narrow down the number of Pareto solutions. Even if these strategies promote the efficient identification of a single overall optimal solution expediting the decision-maker task, their application requires the definition of a set of parameters representing the decision maker preferences. Such a definition (typically arbitrary), introduces subjectivity in the solution identification procedure while compromise the solution optimality. In addition, the evaluation of the feasible solution implies an additional computational effort to the one required to build the Pareto frontier

In order to bypass such an additional time requirement, several approaches have been proposed that promote the generation of a single overall optimal solution directly after solving the model. Those approaches includes, goal programming *(Charnes and Cooper, 1961)*, multiparametric programming *(Pistikopoulos et al., 2007; Oberdieck and Pistikopoulos, 2016)*, analytical hierarchical processes *(Saaty et al., 2008)*, weighted sum approach *(Marler and Arora et al., 2010)*, dictionary ordering *(Cui et al., 2017)*, metaheuristics *(Lin et al., 2013)*, lexicographic minimax *(Liu and Papageorgiou, 2013)*, surrogate modelling *(Beck et al., 2015)*, and fractional programming *(Yue et al., 2013)*. These methods have been extensively used addressing a wide variety of MO problems, including, chemical *(Rodera et al., 2002)*, pharmaceutical, petrochemical *(Zhong and You, 2011)*, automotive, water networks *(Grossmann and Guillén-Gosálbez, 2010; Zhang et al., 2014; Rojas-Torres et al., 2015)*, and power plants *(González-Bravo et al., 2016)* applications. Remarkably, even if these approaches facilitate the solution comparison, they still need a parameters definition. Therefore, the effect of the hierarchies/preferences has to be assessed in further studies.

Recently, the PSE community has intensified the contributions addressing the integration of MOO approaches for the simultaneous management of different hierarchical levels. For example, *Fahiminia et al., (2009)* optimized the production and distribution planning of a two-echelon supply chain network, while *Li et al., (2012)* solved a multi-objective integrated planning and scheduling problem.

Remarkably, all the challenges associated with MO problems increase in complexity when managing uncertain conditions. In this line, several metamodeling-based approaches have been used to map the process performances at different uncertainty values. These approaches include data-driven robust optimization *(Ning and You, 2017)* and meta-multiparametric analysis (M-MP) *(Shokry and Espuña, 2015a; 2015b)*. Particularly, M-MP has been successfully applied to several industrial cases including the sustainable management of a utility plant *(Shokry and Espuña, 2015b)*, energy production process *(Shorky et al., 2017)*, control of batch processes *(Shokry et al. 2016)*, and emission control through systems scheduling *(Lupera et al., 2016)*. Nevertheless, M-MP framework is limited to handle continuous variables; thus, further work is needed to use this framework in Mixed-Integer optimization problems.

From this section, it is clear that solving a pure MO problem is not a challenge anymore; however, there is always an opportunity area to be improved. Actually, the efficient description of the objective function (i.e. obtaining a value that accurately represents the cause-effect of a particular objective) is one of the most relevant gaps. Another open issue is the efficient combination of MO approaches with uncertainty management on which requires additional efforts.

2.3.1. Cause-effect relationships

New tendencies force process managers to take into account many process conditions seeking for a unique and robust solution that simultaneously satisfies multiple objectives. Even if traditional multi-objective approaches have been effectively used, there is an opportunity to improve the objective function formulation, in order to provide detailed information about the process performance as well as the consequences of future operations/decisions. In this regard, the inclusion of different efficiency indexes and performance indicators into the objective function have gain wide popularity. For example, financial metrics, which are the most commonly used, provide information related to the probability of generating winning/loses for a certain solution. Nevertheless, there is another type of indicators, the operational indicators, that provides information about the different environmental/social impact of a process. More information about efficiency indexes is next provided.

Financial indicators

Financial management seeks to reduce the rejection of robust solutions that are commonly discarded for the use of obsolete performance measurements during optimization *(Bonfill et al., 2004)*. The use of risk metrics provides a more accurate and detailed information regarding the economic behavior. Some of the most common financial risk metrics used in the literature is now briefly described:

- *Downside Risk (DR):* provides information related to the potential winnings associated with a particular solution compared to a fixed target (Minimum allowable/desirable revenues). The *DR* mathematical formulation is relatively easy since it avoids the use of binary variables, and thus, it is very computationally efficient. Nevertheless, the lack of linear correlation with the probability of occurrence is the main disadvantage of *DR* application *(Barbaro and Bagajewicz, 2004)*.
- *Financial Risk (FR):* In this case, the probability of not achieving a target value is measured. Contrary to *DR*, the use of *FR* metric within a mathematical model leads to a complex model due to the necessity of several binary variables *(Bonfill et al., 2004)*, and consequently, a large computationally effort is required. Using *FR*, the decision maker forecasts, in some way, the occurrence of favorable solutions and not only maps the economic behavior of a set of solutions. In essence, *FR* describes whether the solution produces winnings but not how much, thus, creating a lack of quantitative knowledge compromising the *FR* metrics usefulness.
- *Value at Risk (VaR)* and *Opportunity Value (OV*): These metrics assess the performance of a solution in a given region of the cumulative probability curve. More precisely, the *VaR* is the difference between the expected profit and the one corresponding to a probability of 5% in the cumulative plot, while the *OV* is conceptually equal to *VaR*, but covers the upper side of the risk curve (typically a percentile of 95%). From a strict point of view, *VaR* and *OV* should be classified as a robustness measurement and not a financial risk metrics *(Aseeri and Bagajewicz, 2004; Aseeri et al., 2004)*, nevertheless, since they have been used in decision support they can be treated indistinctively.
- *Worst Case (WC):* This is the most commonly used alternative to control the probability of meeting unfavorable solutions. Here, the decision maker defines a range of values for which

variations in the process performance are neglected. Traditionally, *WC* has been considered as a risk metric since it correlates the expected profit and worst performance for a set of the solution *(Guillén et al., 2005; Ruiz-Femenia et al., 2013)* while ensuring a low computational effort. Several contributions have proven that *WC* approaches are highly efficient in identifying robust schedules *(Bonfill et al., 2004)*. The main disadvantage of this metric is that in order to be effectively applied it must be analyzed simultaneously with a qualitative objective performance (i.e. profit, cost, etc.) unlike the former risk approaches/metrics.

The use of robust decision support strategies that combines multiple financial metrics has been proposed in the past *(Bonfill et al., 2004)*. Nevertheless, despite the advantages of these integrated strategies, developing a single one that efficiently correlates quantitative and qualitative measurements (probability and potential level of winnings/losses) simultaneously remains an open issue.

Operational indicators

Similarly than the financial metrics, operational indicators seek to reduce the rejection of robust solutions commonly discarded by the use of obsolete performance measurements during optimization. Actually, the use of this kind of indicators is not new, and they are known as Key Performance Indicators (KPI). These indicators may contribute to evaluate the quality of the process performance by using different environmental and social measurements. Despite their proven usefulness, additional efforts are required to extend the use of these indicators within mathematical modeling.

Regarding environmental performance, different resource efficiency indexes (and particularly related to water) have been proposed, including Falkenmark indicator, social water stress, water resources vulnerability, water supply stress and water stress index. The basic element behind these indicators is the relation of the resource consumption with its actual effect on different sectors as briefly described as follows:

- *Falkenmark indicator* represents the fraction of the total annual runoff water available for human use. Thus, this indicator categorizes a region as no stress, stress, scarcity, and absolute scarcity ones. Its main limitation is that it requires the definition of the water conditions in each geographical area.
- *Social water stress index*. This index is an extension of the *Falkenmark indicator* that considers and represents the “adaptive capacity” of a society affected by the consumption of the overall freshwater availability in a region.
- *Water resources vulnerability* is one of the most complete metrics that calculates the ratio of total annual withdrawals to available water resources. Alike *Falkenmark indicator*, this metric allows classifying the level of potential scarcity of a region based on the withdrawals, instead of their runoff. For instance, a country is considered water scarce if annual withdrawals are between 20 and 40% of annual supply, and severely water scarce if withdrawals exceed 40%. The main disadvantage of this method is that it requires a full knowledge of the inputs and outputs of water, which is often difficult to collect or uncertain.
- *Water supply stress*. This metric allows to quantitatively assessing the relative magnitude of water supply and demand.
- *Water stress index*. Alike the above metrics, *WSI* describes and model the impact of water consumption on its local availability. The main advantage of using the WSI as key indicator tool is that the wastewater reduction or water perseveration can be significantly promoted.

Developing a single operational metric that produces useful information for all the potential environmental implications is a hard task to perform. Such an issue increase in complexity when trying to combine multiple efficiency indexes together in order to produce robust solutions, which justifies the study of decision support strategies capable to manage multiple financial and operational metrics.

2.4. Uncertainty management

As commented across this entire chapter, different types of unexpected events affect processes performance and their operating conditions. The most commonly used uncertainty management techniques are presented in Chapter 3 of this Thesis but, in the meanwhile, this section describes the idea behind addressing/managing uncertainty for the different hierarchical SCM levels. In fact, uncertainty management is becoming crucial for the PSE community since they ensure feasible/efficient processes in terms of quality and applicability.

Particularly, the modeling and solving of design, planning or scheduling problems under the effect of uncertain conditions is a challenging task. Historically, product demand is the most commonly studied uncertainty source due to its direct impact on the sales and, consequently, potential revenues, but other sources of uncertainty can be easily identified, and different classifications for them have been proposed. The first one was the defined by *Ho, (1989)* consisting of two groups:

- *(i)* Environmental uncertainties, which mainly refer to market conditions (demand and supply conditions).
- *(ii)* System uncertainties, that take into account the main process variables (i.e. product quality, equipment failure, and changes in the product structure).

Later, *Davis (1993)* proposed a new classification based on the part of the SC affected by the uncertainty:

- *(i)* Supply uncertainties are focused on both, raw material availability and quality;
- *(ii)* Process uncertainties (for example machine breakdowns) and;
- *(iii)* Customer uncertainties (i.e. demand forecast).

More recently, *Pistikopoulos, (1995)* proposed a more detailed classification:

- *(i)* Model-inherit uncertainties (i.e. kinetics factors)
- *(ii)* Process-inherit uncertainties (i.e. flow rate variations)
- *(iii)* External uncertainties (i.e. feed stream availability and product demands)
- *(iv)* Discrete uncertainties (i.e. equipment and distribution link availability).

Nevertheless, due to the increasing number of uncertainty sources considered, the simpler classification proposed by *Jonsbraten, et al., (1998)* has been commonly accepted:

- *(i)* Exogenous sources consider atmospheric and business environments (e.g. demand, supply, raw material quality, weather conditions, etc.)
- *(ii)* Endogenous sources that consider all the variability inherent in the process including yield, capacity, equipment failure, etc.

Originally, the effect of uncertain conditions over a defined process was bypassed considering a "safety factor" that adds a small percentage of the nominal/optimal operational value to the decision variables (i.e. production amounts, inventory levels/capacities, and equipment size) as a way to ensure the operability and, somehow, the robustness of the process. Nevertheless, such an oversizing approach typically leads to inefficient and costly solutions *(You and Grossmann, 2008; Jung et al. 2004)*, thus, there is a need for more sensitive uncertainty approaches. In the last decades many approaches have been proposed addressing such an issue *(Li and Ierapetritou, 2007*)

2.4.1. Reactive approaches

This kind of approaches focuses on developing a deterministic model, which is solved once the uncertainty is unveiled. Consequently, reactive approaches lead to constant plan adjustments, which hinder the use of these approaches for design problems. Within reactive approaches, the most used ones include Model Predictive Control; Multi-Parametric programming; Rolling Horizon approach and Real-Time Optimization, which are following described.

Model Predictive Control (MPC) is typically used to control the behavior of dynamic systems. Particularly, a prediction of the process output (performance) as a function of some control variables (i.e. process measurements such as temperature, flows, etc.,) is generated. Several contributions address different hierarchical SCM industrial problems using *MPC* as described in the extensive review by *Camacho and Bordons, (1995)* and this trend has been maintained. For example, the management of multi-product multi-echelon problems was addressed individually for tactical decisions *(Mestan et al., 2006)* as well as integrating them with operational ones *(Bose and Penky, 2000)*. *MPC* has been efficiently applied to design problems under demand and inventory uncertainties including semiconductor networks *(Braun et al., 2003; Wang et al., 2007)* management of process production *(Niu et al., 2013),* water distribution networks and energy management of micro-grids *(Velarde et al., 2017)*. Despite the use of *MPC* to address resource problems, the evaluation of sustainability metrics requires additional efforts, specifically for the control and optimization of Drinking Water Networks (DWNs) *(Ocampo-Martínez et al., 2010; 2013)*. Even if resource problems are solved for multiple objectives, an oversimplification approach is commonly employed, thus, there is a need to integrate robust and accurate MO approaches with *MPC* strategies. Additional details on the use of *MPC* as a tool for the sustainable development can be found in the literature *(Kouvaritakis et al., 2015)*.

Multi-Parametric optimization (MP) is a strategy commonly used to map the optimized performances (objective function and decision variables) as a function of the varying parameters. Remarkably, *MP* programming results in a set of models (critical regions) that ensures the optimality of the decision variables within the uncertainty space. Using these regions, the required computational effort for future optimizations is significantly diminished *(Pistikopoulos, 2009)*. Since it reduces computational loads, *MP* approach has been widely used for scheduling industrial problems, including multi-stage MILP inventory processes *(Rivotti and Pistikopoulos, 2014)* and utility plants *(Shokry and Espuña, 2015b)*. Additionally, by combining *MPC* and *MP*, online parametric estimation was significantly promoted *(Krieger and Pistikopoulos, 2014)*. Consequently, the *MPC-MP* framework is particularly useful for applications such as control of batch processes *(Shokry et al. 2016)*, and the dynamic optimization of batch processes *(Shokry and Espuña, 2017)*. Besides the use of *MP* to manage multiple sources of uncertainty, its application to sustainability problems has been recently exploited *(Charitopoulos et al., 2016)*. In addition, recent studies successfully combine *MP* approaches within surrogate models to promote the sustainability of the solution of industrial problems *(Lupera et al., 2016)*.

Rolling Horizon approach (RH) consists in an iterative process that solves the problem deterministically for a defined prediction horizon (i.e. a small length of time compared with the complete period) in which the value for the uncertain parameters are defined or can be easily forecasted. Such a prediction is moved forward in every optimization until the whole time span is covered. The application of the *RH* approach implies assuming a full knowledge of the parameters within the prediction horizon, based on the system feedbacks at each iteration. Due to its dynamic nature, *RH* has been applied almost exclusively to scheduling problems, like in the case of the problem associated to the daily energy generation and storage *(Silvente et al., 2015)*. Additionally, *RH* has been successfully combined with *MP* approaches to address reactive scheduling problems for heat and power units *(Kopanos and Pistikopoulos, 2014)*. Even if several authors agree that *RH* has a significant potential to address sustainability problems, further studies are required to justify its application to real industrial processes.

Real-Time Optimization (RTO) focuses almost exclusively on managing the operation of a continuous process seeking to maximize the economic performance. Most *RTO* solution strategies are based on parameter estimation techniques that update some key parameters. Typically, these strategies have been applied to non-linear steady-state processes using the *MPC* to update the set points after optimizing the process management. Remarkably, the application of pure *RTO* to dynamic problems is complicated, thus, dynamic real-time optimization strategies (*DRTO*) have been proposed to address processes in which the bottleneck moves frequently. Later, the use of non-linear *MPC* has been used as an alternative to address non-linear dynamic optimization problems *(Tosukhowong et al., 2004)*. Notice that ultimately, the global optimization of a dynamic complex process may not be achievable with the available computing resources *(De Prada, et al., 2017)* .

2.4.2. Preventive approaches

This type of approaches assumes a complete knowledge of the uncertain parameters behaviors within the problem formulation (a stochastic model). In particular, three approaches can be highlighted, including, stochastic, robust and fuzzy programming.

Stochastic programming is the most used method to handle process uncertainties. In general, stochastic programming estimates the variables as a function of the unpredictable changes through the set of scenarios with an associated probability distribution. The main purpose of scenario-based approaches (such as stochastic programming) is to obtain the optimal decisions producing the best expected performance disregarding the realization of the uncertainty parameters. The well-known two-stage stochastic programming approach is the most common formulation to solve PSE problems. In this line, a MILP and MINLP formulations were used to address the planning of an industrial SC under supply and demand uncertainties *(You and Grossmann, 2011; Grossmann and Guillén-Gosálbez, 2010)*. In the same way, the design and planning of a multi-echelon SC under demand *(Cheng et al., 2003)*, price *(Tsiakis et al., 2001; Gupta and Maranas, 2003)* and raw material availability uncertainties *(Tong et al., 2014)* have been addressed in the literature. Clearly, there is a wide variety of studies using scenario-based approaches to manage problems under uncertainty, which are of an increasing interest due to their potential to promote process sustainability. One of the most remarkable example in this line is the closed-loop SC problem under uncertainty, for which multiple studies can be found *(Baptista et al., 2012; Gupta and Maranas, 2003; You and Grossmann, 2010; Klibi and Martel, 2012)*. Even if stochastic approaches can promote the process sustainability a framework that combines stochastic programming with MO approaches has been proposed to enhance the sustainability in planning SC under demand uncertainty *(Mirzapour Al-e-hashem et al., 2013)*. Remarkably, despite the recent interest in efficient MO stochastic frameworks, a set of feasible solutions are generated, and consequently, there is a need for further studies regarding decision-support strategies.

Robust Optimization (RO) seeks for a solution that remains feasible for the entire uncertainty space by optimizing the problem deterministically for the worst-case scenario *(Ben-Tal et al., 2009)*. This approach is more tractable than the stochastic one *(Li et al., 2011)*, however, due to its proactive nature (i.e. it does not react to the different uncertain events) *RO* is inefficient for short-term problems *(Zhang et al, 2015; Grossmann et al., 2016)*. In fact, this techniques have been effectively applied to some PSE problems, including, SC operation *(Ben-Tal et al., 2011; Verderame and Floudas, 2009)*, process scheduling *(Li and Ierapetritou, 2008; Zhang et al, 2016b)*, and inventory sizing *(Ben-Tal et al., 2004)*. This kind of approaches is useful since it guarantees a minimum performance level; however, its application implies a significantly high computational effort, which represents an issue to be addressed. For this purpose, *RO* and decomposition strategies have been combined in a single framework capable to solve complex process-scheduling problems *(Zhang et al., 2016b)*. The results justify the use of these effective strategies to address multi-objective problems in order to promote process sustainability *(Tong et al., 2014; Bairamzadeh et al., 2018)*. Even if *RO* strategies have the potential to address MO problems, further studies are required to ensure the systematic generation/identification of sustainable and robust solutions.

Fuzzy programming. The idea behind this formulation is the uncertainties representation using a set of fuzzy constraints. Fuzzy-based optimization has been used to address many industrial problems under uncertainty, including automobile SC *(Peidro et al., 2010)*; water and wastewater reuse networks *(Schultmann et al., 2006; Peidro et al., 2010; Aviso et al., 2010)* and design of chemical products *(Ng et al., 2015)*. The use of fuzzy programming has been also explored as an alternative to solve multi-objective problems addressing the sustainable production of crude palm oil *(Kasivisvanathan et al., 2012)* as well as the "green" operation of SC's *(Mirhedayatian et al., 2014)*. In the same line, a strategy was proposed to address the design and management of integrated networks (heating and cooling plants) by minimizing the operating cost and energy requirements altogether *(Sakawa and Matsui, 2013)*. Recently, *Ehsani et al., (2016)* proposed a single nonlinear fuzzy membership function representing multiple objectives simultaneously. Despite all the studies on fuzzy formulations, two main challenges remain unsolved to address sustainability problems under uncertainty. First, the proper definition of membership functions so as to capture the objectives' behavior and the detailed importance/impact of the uncertain conditions over the process performance. The second challenge consists of developing an approach capable to consider the decision-makers' preferences into the fuzzy model.

Remarkably, typed most of the above uncertainty approaches (i.e. the reactive and proactive ones) suffers of at least one of the three main limitations that hinder their application to further and complex problems as stated in and *(Elluru et al., 2017; Moret et al., 2016, 2017)*

(i) The study of uncertainties effect for the hierarchical levels individually;
(ii) The consideration of a single uncertainty source, and;
(iii) They are applied exclusively to a single objective problem.

These limitations, in addition to the increasing concern on sustainability and green engineering from both, industry and academia, emphasize the need of integrated/holistic approaches to handling multiple and unexplored uncertainty sources simultaneously for multi-objective/multi-criteria problems. In particular, this Thesis tries to contribute to such a line, as described in Part IV.

2.5.Trends and challenges

Across the entire chapter, an extensive literature review has been made focusing on practical and integrated solution methods as well as the main decision support strategies for resource SCM (particularly water and energy ones). Such a survey emphasizes the motivation to drive further research efforts in four main topics (i.e. multi-objective decision-support; uncertainty management; market dynamics and sustainability issues) and in the combined/integrated effect of the above challenges.

Multi-Objective decision support

In general, strategies capable of simultaneously considering a large number of objectives/criteria in a unique and systematic framework while identifying the best overall solution are necessary. The above is of significant importance since nowadays, the largest proportion of the optimization models focuses on an economic perspective, even if addressing multiple objectives (i.e. sum-weighted approach and AHP). The above can be acceptable only under two assumptions: First, the economic performance is significantly desirable over the rest of them, and second, the associated economic formulations for the additional criteria successfully represent the system performance. Nevertheless, these assumptions complicate the effective application of the environmental and social regulations/concerns in industrial processes. Thus, so as to facilitate the process competitiveness, the following challenges must be addressed:

- To develop and/or improve the objective and model formulations in order to increase the accuracy with respect to real-life process industries performance, considering non-linear functions.
    - ➢ Most of the economic functions are subject to fixed capital costs and/or a derivation of NPV with a fixed interest rate. A more realistic non-linear cost/revenue function, as well as a set of financial risk metrics that provides detailed information about the system behavior for these non-linear functions, are to be developed.
    - ➢ LCA has been historically used as a systematic environmental analysis method. The effective calculation of LCA implies the knowledge of huge amounts of data as well as process conditions/constraints. Thus, most of the methods used to calculate LCA relaxes the MO problem by combining a linear approach with weighted sum approaches. As a consequence, the individual effect of resources consumption (such as water, biomass, etc.) has been poorly addressed. Particularly, even if the integration of water footprint within LCA enables a comprehensive assessment of the environmental impact, its application over large-scale water supply chains remains as an open issue. Thus, the use of efficiency indexes (such as water stress) appears as a promising alternative to produce detailed information and drive to a better/confident environmental friendly decision.

- Besides the proper formulation of the multi-objective functions, a detailed analysis of individual objectives effect over the entire system (i.e. for each SC echelons) is needed. The above will aim to identify those activities with the highest impacts for each objective.

    - ➢ Ultimately, the objectives can be assessed to establish systematically a hierarchy/importance from the decision maker perspective, which potentially aims to propose effective industrial changes.

- In general, the large majority of problems addressed in PSE literature (including the sustainability ones) seek to improve the accuracy and quality of the obtained solutions. Nevertheless, even with the highest quality of the obtained solutions, the largest number of them represents a huge decision maker issue, which has been poorly addressed. Thus, a multi-objective/multi-criteria framework is needed for the aim of an accurate/sophisticated decision support strategy.

- Finally, and even if it is completely out of the scope of this Thesis it is important to state the need of an assessment of the current environmental regulatory policies that lead to an adequate definition of new ones.

<u>Uncertainty management issues</u>

Historically, one of the major industrial process issues is the management of endogenous and exogenous uncertainties. In general, the major challenge is to develop a framework that allows modeling these uncertainties and, ultimately, obtaining results which are easy to interpret and implement. Nevertheless, even if huge advances in uncertainty management have been achieved, more studies addressing the following challenges are needed for being successfully applied:

- Uncertainty modeling is an active research area and in fact, there are multiple works exploiting individually the effect of demand and prices uncertainty. However, the simultaneous analysis of uncertainty sources has been scarcely addressed. Such a study would represent a huge opportunity area but, still, would lead to one particular and interesting challenge:
    - The detailed information on the effect of the different uncertainty sources/parameters over the system behavior (individually and considering their interactions) has been briefly studied through multi-parametric programming. However, its potential to define the uncertainty “importance/relevance” has been never exploited. The above is of great interest considering that a set of patterns may be identified while generating an accurate prediction.

    - Managing large amounts of information is an important and complex task. The above can be justified since the performance of any industrial process highly depends on the quality of the input data. Considering that current stochastic models generate a large amount of output information, there is also a need for data-driven tools capable of integrating analytical tools with tailor-made databases. Thus, future research efforts should be focused on establishing a strategy that accurately manages a large amount of process information as well as the different data flows. To fill this gap, knowledge management systems such as surrogate models and ontologies appear as promising alternatives.

- Besides the number of uncertainty sources, another important issue is the number of scenarios a multi-stage stochastic programming system (which is the most used approach) is able to manage. Even if the definition of the smallest number of scenarios has been studied before, its application to medium-large scale industrial problems remains as an open issue.

- Finally, there is a need to use performance indexes that represent uncertainties and quantifies the robustness of the proposed solutions. The above will potentially expedite the application of reactive and preventive approaches (as well as its combination) in the framework of Multi-Objective/Multi-criteria problems, which represents a promising research direction.

Market dynamics and sustainability issues

Following the sustainability principles, the resource management problems turn to be of particular interest. The above can be challenging since it requires addressing simultaneously a large number of uncertainties affecting the resources, and results in MO problems due to the intrinsic multi-objective nature of sustainability. Thus, research efforts are required to improve the strategies for reverse logistics and close-loop problems. Even if these strategies have been intensively studied in the past, their application to large-scale problems has not been efficiently achieved yet, and thus the following challenges have to be addressed in further studies.

- The primary issue to be addressed is to contribute to the integration of industrial symbiosis (IS) strategies within a holistic approach. The symbiosis concept within an industrial process framework seeks for the efficient exploitation of resources between companies/processes (material, energy, information, etc.). In particular, IS problems have specific properties if compared with traditional management issues:
    - IS strategies are particularly useful in addressing decentralized scheme problems that consider, at least, two independent companies/actors that manage the operations considering its individual performances/benefits. Consequently, better process performances for all the actors are promoted (i.e. a Win-Win solution). The above differs diametrically from the traditional centralized scheme, in which a “selfish” behavior is assumed from the decision maker which sacrifices the global benefit for the interest of few participants.
    - It is necessary to evaluate the relationship between the network (i.e. supply chain) players coordination/collaboration and to analyze their willingness to collaborate.
    - For the proper application of IS strategies there is a need for an efficient information flow between the different actors, thus the potential links/collaborations may be accurately identified. Nevertheless, in most of the real-life problems, such an information flow is limited, hindering the IS strategies application. Recently, duality principles have been used to optimize the whole system performance without knowledge of every SC member, which is a better representation of the reality.

- In addition to the above technical/conceptual challenges, the difficulties regarding model formulation is another main issue to address. Notice that issues related to solver development and coding efficiency are out of the scope of this Thesis. Thus, besides the coding complexity, in this particular case we are focused on two main challenges:

    - Since the different SC’s players are allowed to take their own decisions, studies are needed to create strategies capable of react to the constant changes in the market conditions within a single model. In this line a Scenario-based dynamic framework was proposed; however, such a framework uses a simplified uncertainty approach compromising its representativeness. Thus, the proper combination of the scenario base dynamic framework with accurate uncertainty approaches remains an open issue. Such a combined framework will potentially evaluate and assess the effect of the partner's decisions over the system behavior taking into account the uncertainties.
    - In addition, metrics, which are able to quantify/represent the objectives/performance of each shareholder (an individual entity in the

decentralized scheme) are worth to explore. Thus, ultimately, improved decision-maker strategies are required.

Combined/Integration issues

- PSE strategies are moving towards an enterprise-wide optimization framework that aims to integrate different functional decisions into a global model. This model should optimize the overall system performance. Therefore, the major challenge is to find a suitable function/objective that simultaneously represents the individual and global system performances as well as the effect of the interactions between different SC decision levels. Thus, a set of particular challenges must be addressed:

    - As already commented, an extension of Multi-criteria techniques in terms of quality of the decisions that accurately represent the decision maker preferences in a systematic and non-subjective way is required.
    - The proper identification of common variables that allows connecting the different hierarchical levels.

- Currently, researchers guide their efforts to manage the coordination of pricing, production and distribution decisions to break the traditional organizational barriers. The trade-offs between the impact of operational decisions over the entire SC should be examined. Thus, a proper framework is needed.
- So far, an efficient single monolithic model that jointly optimizes each actor decisions is unlikely to exist in the near future. Currently, the high computational burden required to solve large size multi-scale optimization problems makes the computational effort reduction a critical issue to be addressed to achieve a monolithic optimization model. In addition, it can be anticipated that further research efforts address the development/improvement of decomposition strategies in order to handle dual information flow (i.e. obtain and react to a "feedback") within a decentralized structure. In this line, knowledge-based algorithms are a good option to expedite the identification of a feasible space for a specific problematic (e.g., Metamodeling).

Ultimately, the key component in integrated SCM is the decision-making coordination and integration. Thus, by addressing the above challenges, the general goal of this Thesis was achieved. Such an objective can be summarized as the proposal of general PSE methods and tools in order to propose an advanced decision support system for the systematic planning and management of sustainable resource supply chains, and in particular water supply chains (WSC's).

Chapter 3

Methods and Tools

In this chapter, the methods and tools used in the development of this Thesis are described. First, the general principles of mathematical programming are identified, since this is the optimization technique employed across the entire Thesis. The most relevant strategies addressing multi-objective optimization and uncertainty management problems, individually and under a common framework, are described in detail. Finally, the basic ideas behind decomposition techniques are presented.

3.1. Mathematical programming principles

The most commonly used tool for assisting decision-making is mathematical programming, since it is capable of combining different system optimization techniques. Its first records are linked to military purposes managing the training schedules and operation logistics (i.e. deployment of soldiers and supply of equipment's/medicines) *(Gill et al., 2008)*. Since early 1950's, an increasing number of contributions using mathematical programs for process systems engineering (PSE) applications appears. Disregarding the field or subfield of application, a mathematical program must define an objective function, decision variables and constraints, as shown in Eq. (3.1):

$$\begin{aligned} &\underset{x}{Maximize} \quad f(x) \\ s.t.& \\ &h(x) = 0 \\ &g(x) \leq 0 \\ &x \in X \subset \mathbb{R}^n \end{aligned} \tag{3.1}$$

In this formulation, *f(x)*, $h(x)$ and $g(x)$ are functions of vector x. The objective function ($f(x)$) typically represents a quantitative measurement of the system performance. The decision variables (components of vector x) can be of a continuous and discrete nature, and their values are determined during the optimization procedure. Finally, the mathematical formulation must include constraints (for this case $h(x)$ and $g(x)$) in order to represent all the inherent restrictions of real process system (such as physical, logical, thermodynamics, etc.). Identifying these components is the core of modeling. However, depending on the properties of the characteristics of the scalar functions the mathematical problem can be classified:

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

3.1.1. Convexity

A set of points X is convex if a straight-line segment connecting every pair of points $(x_i; x_j)$ does not break the boundaries associated to the set X as shown in Fig. 3.1.

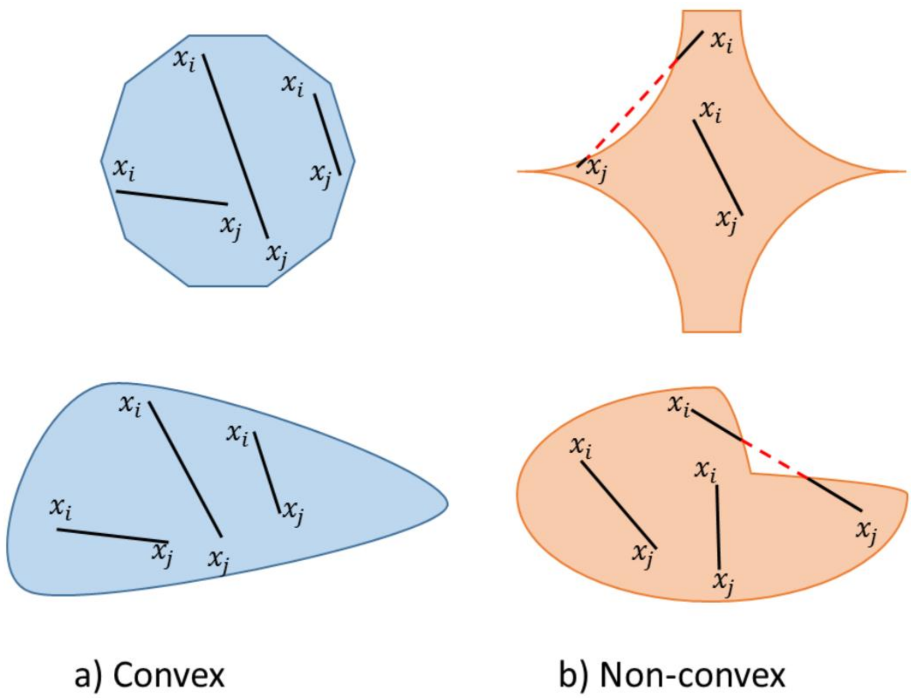

Fig. 3.1. Convex and non-convex graphical representation.

The mathematical representation of convexity is as follows:

$$x \quad is\ convex \quad \Leftrightarrow \quad \forall(x_i; x_j) \in X \wedge \theta \in [1,0]: \left((1-\theta)x_i + \theta x_j\right) \in X$$

Ensuring the convexity of the solution subspace is of significant importance in order to ensure the global optimality in a mathematical formulation. Actually, to handle no-convex problems and, thus, identify the “global” best solution in presence of several local optimums, the global optimization appears as an alternative. The following section describes the most commonly used optimization strategies.

3.2. Optimization techniques

The use of mathematical programming approaches to address decision-making problems implies the development of a framework that combines mathematical representation and optimization algorithms. In particular, mathematical programs are coded considering the main problem characteristics. Remarkably, such a formulation conditions the solution technique used to run the optimization *(Kallrath, 2002; Biegler and Grossmann, 2004; Grossmann and Biegler, 2004; Kallrath, 2005; Méndez et al., 2006; Li and Ierapetritou, 2007; Barbosa-Povoa, 2007)*. In addition to mathematical programming techniques, in this Thesis other optimization methods have been also explored, including logic-based optimization (e.g., constraint programming), heuristics and meta-heuristics. Additionally, multi-criteria and stochastic optimization approaches have been considered to address problems with multiple and conflicting objectives under uncertain conditions. The following subsection describes the idea behind the most relevant mathematical programming techniques.

3.2.1. Linear programming (LP)

Linear programming consists of a mathematical program in which all the functions involved follows a linear behavior. The solution space or feasible region within a LP problem is geometrically defined by the intersection of the hyperplanes representing each constraint (*n*-variables). Thus, any LP problem has an optimal solution, in one of the vertexes of the feasible polytope (See Fig. 3.2).

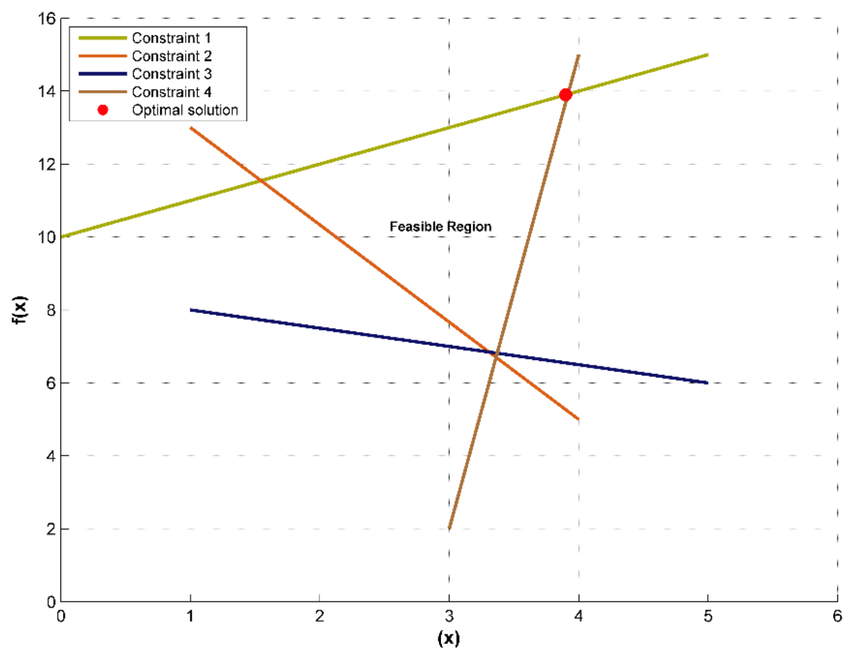

Fig. 3.2. Linear programming scheme and feasible area generation.

Traditionally, two solution methods are widely used to solve this type of problems:

<u>Simplex method</u>

Dantzig, (1963) developed the methodology in which the main idea is to move along the boundaries of the feasible region from one vertex to the next one. More precisely, the algorithm starts with an initial vertex (i.e. feasible solution) in which it is verified if the optimality lies within a defined gap (tolerance value); otherwise, the algorithm moves to an adjacent vertex testing its optimality again. This algorithm is repeated for a finite number of vertexes improving the objective value for each iteration (except in certain pathological cases) until an optimal vertex is finally found (Fig. 3.3(a)).

Interior-point methods

Contrary to the simplex method, the interior-point method search through the interior of the feasible region without touching the border. An initial feasible point is assumed, and then the search for the optimal solution (vertex) is started from the interior moving iteratively through the possible feasible region (Fig. 3.3(b)). Further details can be found in *Gonzaga, (1992)* and *Marriot and Hallo,(1998)*.

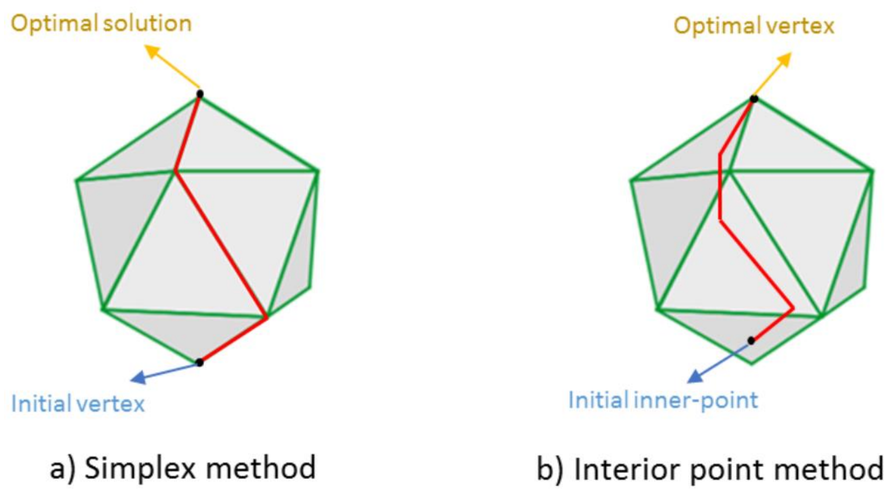

Fig. 3.3. Graphical representation of LP solution algorithms. a) Simplex method; b) Interior point method.

There is still no valid way to classify the problems and identify the algorithm that produces better results, thus, the commercial software incorporates both algorithms (and sometimes a hybrid one). For a more detailed explanation regarding LP algorithms the reader is referred to *(Dantzig and Thapa, 1997a; 1997b)*.

3.2.2. Non-linear programming (NLP)

NLP corresponds to mathematical models in which all variables are defined as continuous but, unlike LP the problem contains nonlinearities in either the objective function and/or the constraints. The presence of nonlinearities is very common in real-life problems, and PSE problems are not an exception. These nonlinearities may include kinetics associated with chemical reactions, pricing policies, process characteristics, among others. The main complexity associated with solving NLP problems is the presence and discarding unfeasible local optimal solutions.

There are many algorithms assisting solving NLP optimization problems with large amounts of inequality constraints, including generalized reduced optimization algorithm *(Abadie and Carpenter, 1969; Abadie, 1978)*, sequential quadratic programming (SQP) *(Fletcher, 1987)*, and interior point methods (IPM) *(Wright, 1996)*. These methods can be classified as unconstrained and constrained optimization methods as described in the following section.

Unconstrained optimization

Unconstrained optimization algorithms are divided into two groups, nevertheless, for both of them, there is required to define an initial feasible solution (x_0) of the problem. These groups include:

- *(i)* *Line search methods*. To apply this method, a direction (vector) is defined using the steepest-decent direction, Newton direction, or Quasi-Newton search direction methods. Once the direction has been selected, the algorithm searches along this vector for an adequate step length (a_k), so that it moves from the current "position" (x_k) to a new one (x_{k+1}) with a better objective value. The selection of an adequate step length is the main issue. Since there is a need for an effective mapping to guarantee an objective improvement, the smallest step length is preferred. In this line, methods such as the interpolation method, the golden section method and the Fibonacci method assist in the definition of a sufficiently small step length. Notice that, Even if by reducing such a step the time required to solve the problem increases, the accuracy of the obtained solution justifies the use of these methods.
- *(ii)* *Trust region methods*. For this method, a step-based direction approach is also used to approximate the optimal solution. Unlike in the line search method, this one identifies the trust region (feasible area) during the first step, while the further solution search uses the same approach. The most commonly used strategy to identify the feasible region for this method is the Taylor series expansion that has been explained in detail in *(Laínez-Aguirre, 2009)*.

Constrained optimization

This kind of methods seeks an approximate solution by replacing the original constrained problem by a sequence of unconstrained sub-problems. Hence, the underlying idea is to construct a closely related unconstrained problem and apply the algorithms proposed for the unconstrained optimization problems. There are many methods addressing this kind of problems that based their solution strategy in either Lagrange or Karush-Kuhn-Tucker approaches *(Kuhn and Tucker, 1951)*.

3.2.3. Mixed-integer programming

Typically, real-life processes need to take yes/no decisions as well as enforcing logical conditions, modeling fixed costs or piecewise linear functions, thus, the use of binary variables turns out to be necessary. Mathematical formulations including both, continuous and integer variables are called mixed-integer programs, thus, LP and NLP models that also contain integer variables lead to:

- *Mixed-Integer Linear Programming (MILP)* is one of the most extensively explored formulations due to its flexibility and extensive modeling capability. The methods to solve MILP problems are enumerative algorithms that discard the less efficient alternatives. Among the algorithms used to solve MILP problems both, Branch and Bound (B&B) algorithm, and Branch & Cut (B&C) algorithm can be highlighted.

- *Mixed-Integer Non-Linear Programming (MINLP)* has been mainly applied to synthesis and design problems, and in less proportion to planning and scheduling ones. The complexity of the MINLP problems is subject to the non-convexity of the feasible region. Thus, different methods are used to solve MINLP problems, including Branch and Bound (B&B), Generalized Benders Decomposition (GBD), and Outer-Approximation (OA).

The algorithms used to address both, MILP and MINLP problems are following described.

Branch and Bound (B&B)

This is the basic method for solving integer programming problems. B&B was introduced by *Land and Doig (1960)*, and it operates following a tree-search approach splitting the original problem into continuous sub-problems and solving them sequentially. The optimal solution is obtained by analyzing the associated results and comparing them to each other. Notice that the root node corresponds to the original problem (in its relaxed version), and each subsequent nodes represents a sub-problem.

As implied by its name, B&B algorithm consists of two strategies; first, the branching part divides the solution space creating nodes with additional constraints on lower and upper bounds. On the other hand, the bounding part consists in discarding a node when is infeasible or when its objective function is not improved (see Fig. 3.4). The main limitation regarding B&B is the exponential generation of nodes creating a large number of solutions, thus, challenges such as data management and large computational effort are promoted. It is important to comment that, B&B method only grows the most promising nodes (i.e., partial solutions), which are identified by estimating a bound on the best value of the objective function for further stages in each node.

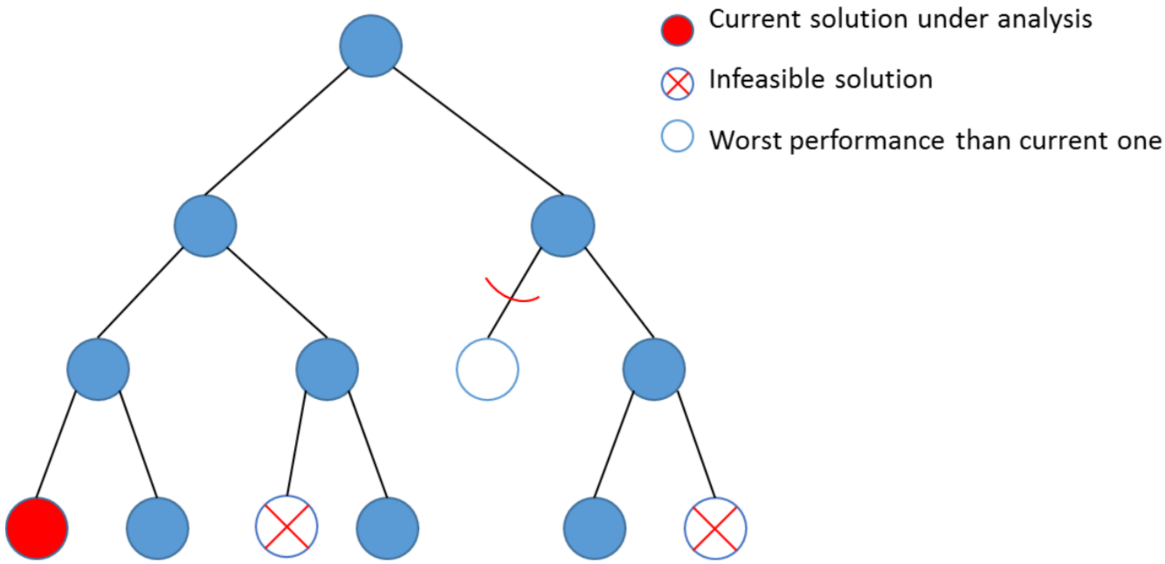

Fig. 3.4. Graphical representation of the Branch-and-Bound method.

The reduction of branches can be achieved by following these steps:

- If a branch contains no integer feasible solutions with a better value than the incumbent solution, such a branch can be directly eliminated.
- A lower bound of the final integer solution can be determined for any intermediate node. In the worst case, the relaxed LP can be always used as lower bound.

Cutting-plane methods

As commented, B&B expedites the narrow down of nodes that are the most critical challenges of the tree-search approaches; however, there is an additional alternative for this purpose using the so-called cutting planes. The main idea behind the cutting-plane method is to introduce additional constraints (called cutting planes) to a program until the optimal solution satisfies integrality constraints. The cuts reduce the solution space (i.e. convex set) for a fractional solution as displayed in Fig. 3.5.

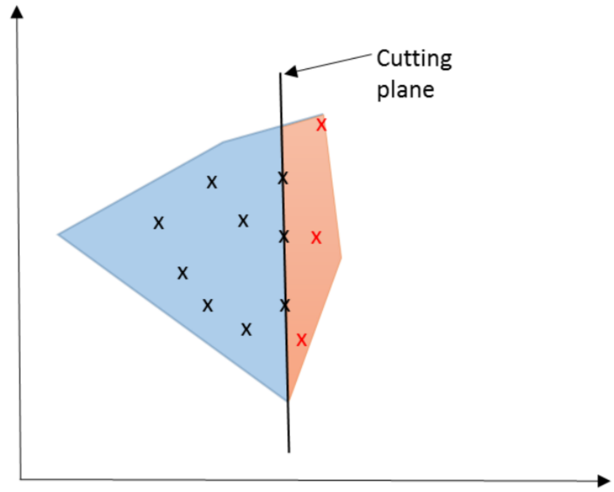

Fig. 3.5. Graphical representation of cutting-plane approach.

Some of the most known techniques to generate these cuts are the Gomory's cuts, the Kelley's, and the Kelley-Cheney-Goldstein methods. Although initially this methodology was considered unstable and ineffective, it can be effective in combination with branch and bound methods. In fact, nowadays, all commercial MIP solvers use Gomory cuts in one way or another.

Generalized Benders Decomposition (GBD)

GBD algorithm was extensively studied in *(Geoffrion, 1972)* and since then, it has been widely applied to MINLP. This algorithm assumes that the variables in the MINLP non-convex problems can be divided into two categories: complicating and non-complicating variables, where the binary variables are the complicating variables. By fixing the binary variables, the problem is divided into a sequence of NLP sub-problems, and MILP master problems. Particularly, the NLP sub-problems generate the upper bounds of the problem, and the MILP master problems generate a combination of discrete variables to be used as lower bounds for the NLP sub-problems. The optimal solution then can be found when the upper and lower bounds converge.

Outer-Approximation (OA)

Similarly than GBD, the OA algorithm splits the MINLP non-convex problem into NLP sub-problems and a MILP master problem *(Duran and Grossmann, 1986)*. Nevertheless, in OA a feasible region is defined by solving the NLP sub-problems, while, the master problem is generated by approximating the non-linear constraints of the feasible region (NLP sub-problems results).

Although the last two methods aim to solve MINLP problems, the identification of global optimum solutions for non-convex MINLP problems remains as an open issue. For this purpose, different solvers are used as displayed in *Section 3.7*.

3.3.Multi-Objective Optimization

Multi-objective optimization (MOO) addresses the optimization of a problem in which multiple objectives should be considered simultaneously. These objectives result from modeling particular impacts (such as social and/or environmental ones) as part of the optimization in addition to the traditional economic performance. MOO assists the decision-making challenge and, in particular, plays an important role in engineering design and management. The MO mathematical representation adopts the following form.

$$\max_{x} \; \{f_1(x), \dots, f_{ob}(x), \dots, f_{|OB|}(x)\}$$
$$s.t. \tag{3.2}$$
$$h(x) = 0$$
$$g(x) \leq 0$$
$$x \in \mathrm{X} \subset \mathbb{R}^n$$

Mathematically, a large amount of combinations (solutions) satisfies the conditions in Eq. (3.2), thus, there is a need to define the "dominance" of each of these. Notice that the dominance concept follows the following theorem:

- ***Theorem 3.1:*** A solution is said to be dominant if there is no other solution showing a better performance in any of the possible k-elements (ob).

Remarkably, the set of feasible solutions includes both, dominated and dominant solutions. The dominant ones are commonly called efficient or Pareto solutions and as a group they form the well-known Pareto frontier (See Fig. 3.6).

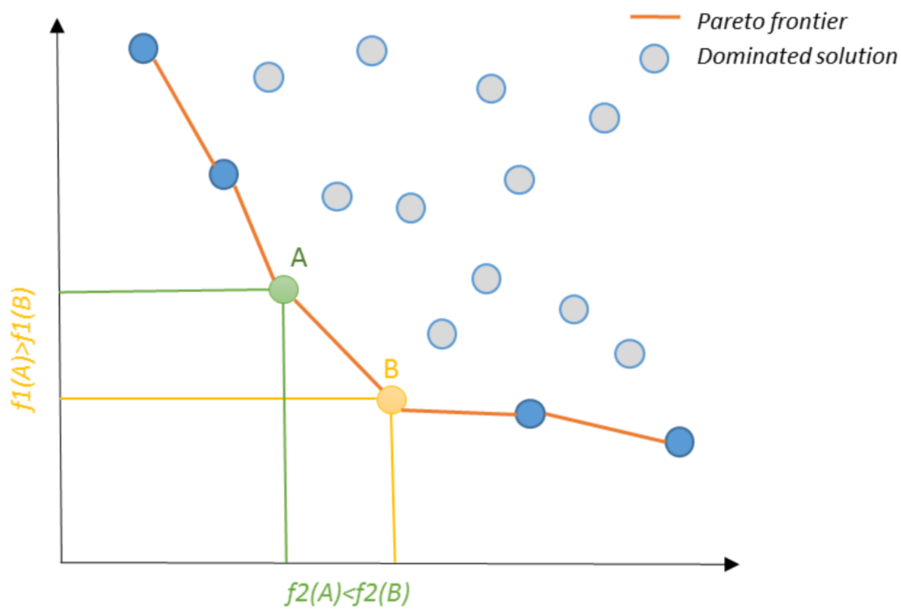

Fig. 3.6. Pareto frontier and dominated solutions.

The most commonly used approach for the systematic generation of the Pareto frontier is the well-known ε-constraint method. Despite its utility, it has been used together with other strategies that identify one solution within the Pareto frontier that better satisfies all the decision maker criteria. In general, these strategies can be categorized into two groups:

(i) <u>*During optimization strategies*</u>, are approaches that produce a feasible and optimal solution directly after running the optimization procedure. These strategies include, analytical hierarchical processes *(Saaty, 2008)*, weighted sum approach *(Marler and Arora, 2010)*, dictionary ordering *(Cui et. al., 2017)*, fuzzy programming and fractional approach;

(ii) *Post-optimization strategies*. Unlike the former category, these strategies require an additional analysis to sort the whole set of solution and identify the best one. These strategies include ELECTRE method, Pareto filter and data envelopment analysis.

The next section focuses on to describe the core strategies of this Thesis, being the ε-constraint, and a set of identification methods.

3.3.1. The ε-constraint method

The ε-constraint method was introduced by Haimes et al., (1971), and its main purpose is to generate the Pareto frontier by sequentially producing several dominant Pareto solutions. Each solution is produced using a single objective (SO) optimization that is performed by constraining all the additional objectives by some allowable levels ε_0. Notice that the optimization should be repeated as many times as ε_0 levels considered. The overall algorithm for the methodology is as follows.

1. Solve a SO problem for each one of the objectives under analysis ($ob \in OB$).
2. Let LB_{ob} and UB_{ob}be the lower and upper bounds for the objectives under analysis (limitation of the feasible area).
3. Chose the objective to be optimized and to let the rest of them be constraints.
4. Let e represent the number of points to generate the Pareto frontier.
   4.1. For $e = 1:1:|E|$.
   4.2. Define the value for the constrained objective (ε_0) as: $\varepsilon_0 = LB_{ob} + e * \left(\frac{UB_{ob}-LB_{ob}}{|E|+1}\right)$
   4.3. Solve model MO problem subject to the constraint ε_0. Let solution $x^*_{e,ob}$ be the optimal solution, for point e at constrained objective ob.
5. Obtain the corresponding Pareto frontier.

Ultimately, this method leads to a set of feasible solutions that represents an appealing option for the decision maker. It is important to mention that even if this algorithm is typically applied to bi-objective problems, it can be easily extended to more objectives at the expense of increasing the effort required to complete the loop. In addition to the Pareto frontier, there are three points that must be identified to evaluate the desirability of the dominant solutions. Those points are the utopia, nadir and p-anchor points (see Fig 3.7).

- *Utopia point*: This point represents that situation in which every individual objective achieves its optimal value found by solving the SO problem for each objective individually. Logically, this solution lies out of the feasible area.

- *Nadir point*: Opposite to utopia, nadir point consist on the worst performance for each individual objective found using the same optimized values found during utopia point, but this time identifying the worst values. Even if this solution may lie within the feasible area, it Does not belong to the Pareto set since it represents the worst possible combination.

- *The p-anchor points*: These points are the extremes of the Pareto frontier.

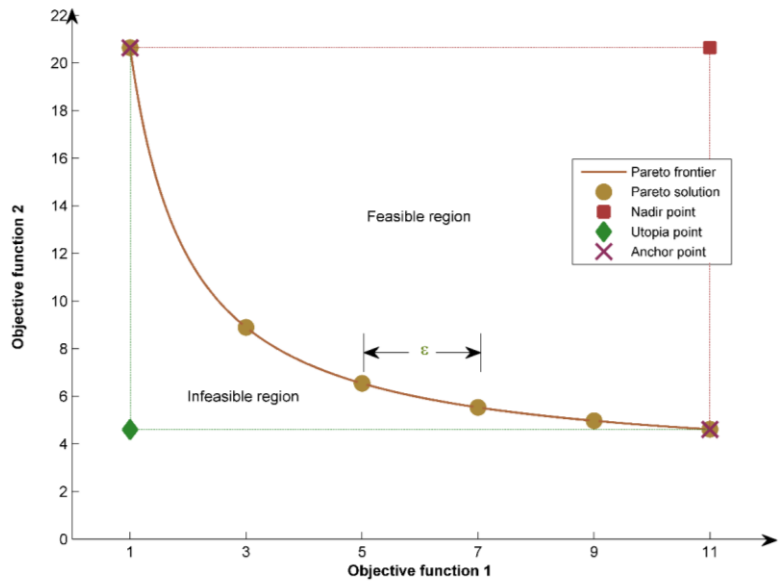

Fig. 3.7. Pareto frontier construction and its most significant points for a minimizing bi-objective situation.

Remarkably, even if many contributions address the systematic identification of a single solution within the Pareto frontier, additional efforts are still required. In this line, many Multi-Criteria Decision Making (MCDM) strategies have been proposed as described in the following subsections.

3.3.2. Multi-Criteria and Multi-Objective Decision Making

Multi-Objective Decision Making (MODM) along with MCDM are the two main categories that cover a wide branch of decision-making strategies *(Gal and Hanne, 1999)*. These categories include methods based on both, outranking and distance normalization methods. Their main purpose is to identify the most efficient solution considering multiple objectives/criteria/attributes. A view of MCDM and MODM methods is shown in Fig. 3.8, while the basic ideas behind the most relevant ones are briefly described in the following subsection.

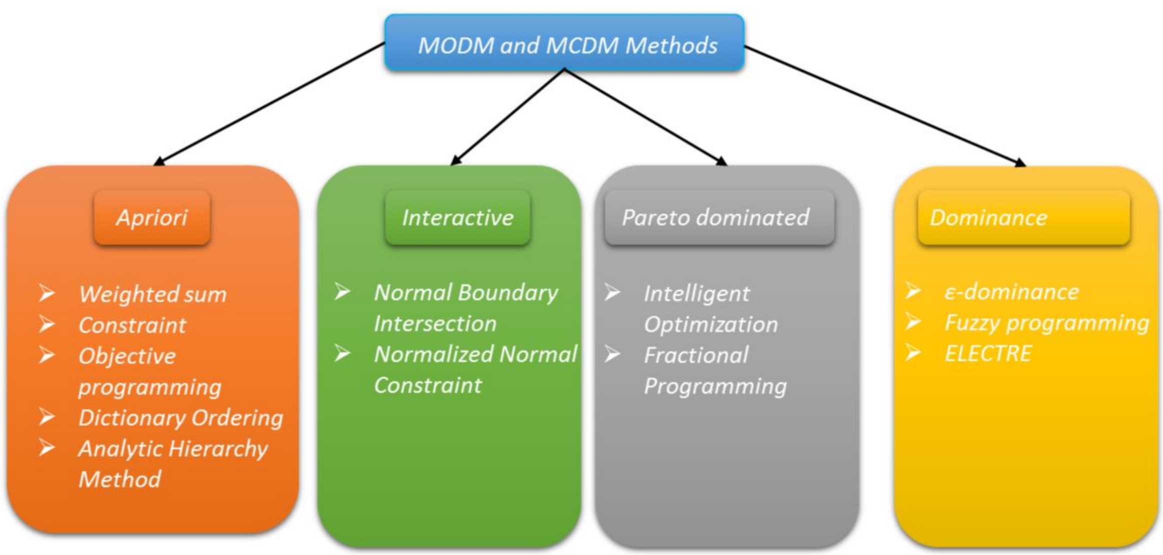

Fig. 3.8. Multi-Criteria and Multi-Objective decision-making.

Predefined/Apriori methods

These methods are basically parametric linear programming techniques that measure the efficiency of a set of entities by transforming all the objectives into single vector value.

Analytical Hierarchical Processes (AHP)

Analytical Hierarchy Processes (AHP) were developed by *Saaty (1980)* and later applied to PSE problems *(Zamarripa et al., 2012; Balinski, 1965)*. AHP decompose the problem into a multi-level hierarchy structure as described in the following four steps general algorithm *(Vaidya and Kumar, 2006)*:

1. Generate the mathematical model for the problem identifying the main objective as well as the additional criteria.
2. Construct the hierarchy structure by decomposing the problem and correlating the different levels. Such a structure must contain all essential elements relevant to the problem.
3. Introduce comparison judgments (typically using a matrix) that reflect the preferences of each pair-wise of elements in each level of the hierarchy.
4. Using these preferences matrices, the priority of each solution is calculated and ultimately the best solution can be identified.

Within these steps, the most critical one is the pair-wise comparison, in which a numerical representation of the relationship between two elements is determined and, ultimately, one of them is identified as the most important. The Saaty's fundamental scale *(Saaty, 1980)* is most widely used one to assess the intensity of preference between two elements as displayed in Table 3.1.

Using such a numerical representation, the method computes and aggregates the objectives eigenvectors until the composite final vector of weight coefficients for alternatives is obtained. One of the major advantages of AHP is that it calculates the inconsistency index as a ratio of the decision maker's inconsistency and randomly generated index. This index is important for the decision maker since it guarantees the consistency in his/her judgments. On the contrary, the main challenge of this approach is that the performance of the final solution is significantly affected by the structure assumed at the very beginning.

Table. 3.1. Typical AHP numerical equivalences/preferences.

Importance Scale	Definition of the importance scale
1	Equally preferred
2	Equally to moderately preferred
3	Moderately preferred
4	Moderately to strongly preferred
5	Strongly preferred
6	Strongly to very strongly preferred
7	Very strongly preferred
8	Very strongly to extremely preferred
9	Extremely preferred

Weighted Sum Approach (WSA)

This is the most commonly used approach to ease the identification of an overall optimal solution for its mathematical representation and calculation. Such an approach allows identifying the best alternative by optimizing and satisfying Eq. (3.3) in which multiple objectives are transformed into a single objective:

$$F(x) = min \sum_{i=1}^{m} f_i(x) w_i \tag{3.3}$$

Eq. (3.3) converts the multi-objective problem into a scalar optimization one creating a convex combination of the different objectives. In particular, *m* weights (w_i) such that w_i > 0, i = 1, . . . , *m* and $\sum_{i=1}^{m} w_i = 1$ are usually employed. Notice that the weights have a significant effect over the final solution; nevertheless, they are generated beforehand based on the decision maker experience, which compromises the robustness of the final solution. Despite WSA structure is very easy to understand and apply; the commented limitations represent the main disadvantage and restrict its use in many PSE applications.

Constraint/Objective programming method

Unlike in the previous methods, here, the decision maker defines a set of target values for each objective $(do = [do_1, do_2, \ldots, do_m]^T)$ which are included into the optimization objectives as constraints.

$$\begin{aligned} & \min\ f(x) \Rightarrow \min \sum_{i=1}^{m} |f_i(x) - do_i| \\ s.t \\ & x \in \Theta \end{aligned} \tag{3.4}$$

Since the desired values shall be set within the feasible region, the final solution is significantly conditioned beforehand. Consequently, this method is effective addressing simply linear programming problems but less effective in solving nonlinear complex problems. Alike WSA, this method is simple to use and it is based on a prior experience, thus, the limitation regarding robustness remains unsolved.

Lexicographic minimax method

All the above methods assume that the decision maker has a clear idea regarding its preferences for any objective; however, very often this is not the case. When all the objectives are equally important, the solution identification process is challenging. Then, a sensible solution can be obtained after solving the minimax problem (Eq. 3.5).

$$\begin{aligned} & min\{max\, f_{ob}(x)\} \\ s.t \\ & x \in \Theta; ob = 1, \ldots, OB \end{aligned} \tag{3.5}$$

This method seeks to generate a fair solution in which all normalized objective function values are as much close to each other as possible *(Lui and Papageorgiou, 2013)* where all the *ob* objectives are first normalized to the same scale. However, the disadvantage of the minimax problem is that the solution is not unique, and some of them may not be Pareto-optimal.

Data Envelope methods

Data Envelope Analysis (DEA) is a non-parametric linear programming technique that measures the efficiency of a set of entities, known as decision-making units, each transforming multiple inputs into multiple outputs *(Charnes et al., 1978)*. In addition to calculating the efficiency scores, DEA provides specific guidelines, expressed as quantitative targets, which can be used to improve the efficiency level, for instance the level of sustainability. Within these kinds of methods, Fractional Programming is the most widely used.

Mixed-Integer Fractional Programming (MIFP)

MIFP is a class of nonconvex MINLP that includes both, continuous and discrete variables seeking to optimize an objective function that is formulated to represent the ratio of two linear functions subject to linear constraints as displayed in Eq. (3.7).

$$\max\left\{Q(x) = \frac{N(x)}{D(x)}\right\}$$
$$s.t \qquad (3.7)$$
$$x \in S$$

Due to the non-convexities/nonlinearities associated with the objective function and the combinatorial nature given by the existence of binary variables, large-scale MILFP problems are hard to optimize with general solution methods. Three main characteristics can be highlighted for the MIFP objective function (Yue et al., 2013):

(i) It is either pseudo-convex or pseudo-concave;
(ii) It is strictly quasi-convex and quasi-concave, and;
(iii) Every local optimum is also its global solution.

Even if all the above MOO methods are simple to use, they cannot guarantee a globally optimal solution for non-convex optimization problems. Thus, even if ensuring an optimal solution, the complete Pareto frontier is not properly explored and consequently these methods do not reach all the feasible solutions while considering non-convex problems as displayed in Fig. 3.10 (Pohekar and Ramachandran, 2004).

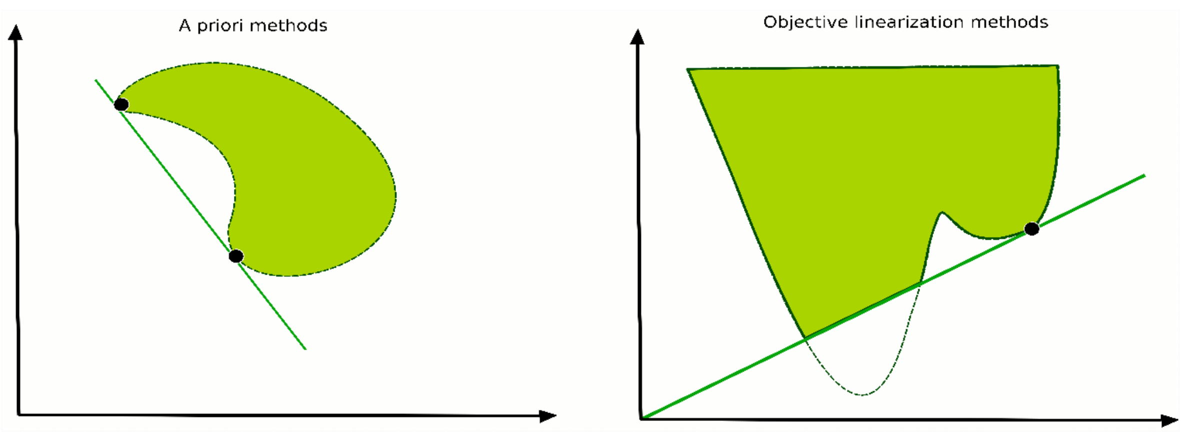

Fig. 3.10. Behavior of some MCDM approaches for non-convex problems.

The above is important since the main purpose of these formulations is the identification of a well-balanced solution rather than building the Pareto frontier. In this sense, the following additional methods represent promising alternatives.

Dominance methods

Fuzzy Programming

Fuzzy-based strategies are based on reformulating the original MO model defining a membership function for each objective. Typically, a linear relation is used following general expression (Zimmermann, 1978) (Eq. 3.6).

$$\lambda_{ob}(x_{ob}) = \begin{cases} 1 & if\ x_{ob} \geq \bar{b}_{ob} \\ 1 - (\bar{b}_{ob} - x_{ob})/(\bar{b}_{ob} - \underline{b}_{ob}) & if\ \underline{b}_{ob} < x_{ob} < \bar{b}_{ob} \\ 0 & if\ x_{ob} \leq \underline{b}_{ob} \end{cases} \tag{3.6}$$

Where x_{ob} represents the objective performance, while $\lambda_{ob}(x_{ob})$ can be interpreted as the degree of x_{ob} for the specific objective ($ob \in \{1,\ 2, \dots OB\}$). Moreover, $\bar{b}_{ob}$ and $\underline{b}_{ob}$ represent the objective boundaries (maximum and minimum value, respectively). The value of $\lambda_{ob}(x_{ob})$ is expressed in the range zero to one, where zero corresponds to the minimum value and one to the maximum one. Notice that different "shapes" may be used to represent the cause-effect relationships as displayed in Fig. 3.9.

Notice that, when compared with other transforming MO approaches (such as WS or AHP), the capacity of the proposed fuzzy formulation to relax the non-linear objectives behaviour while still clearly representing the cause-effect relationship behind the different objectives, lead to clear advantages, especially in terms of quality of the final solution. More details regarding the mathematical analysis that justifies the final solution optimality using fuzzy programming can be found in the work of *Li and Lai, (2000)*.

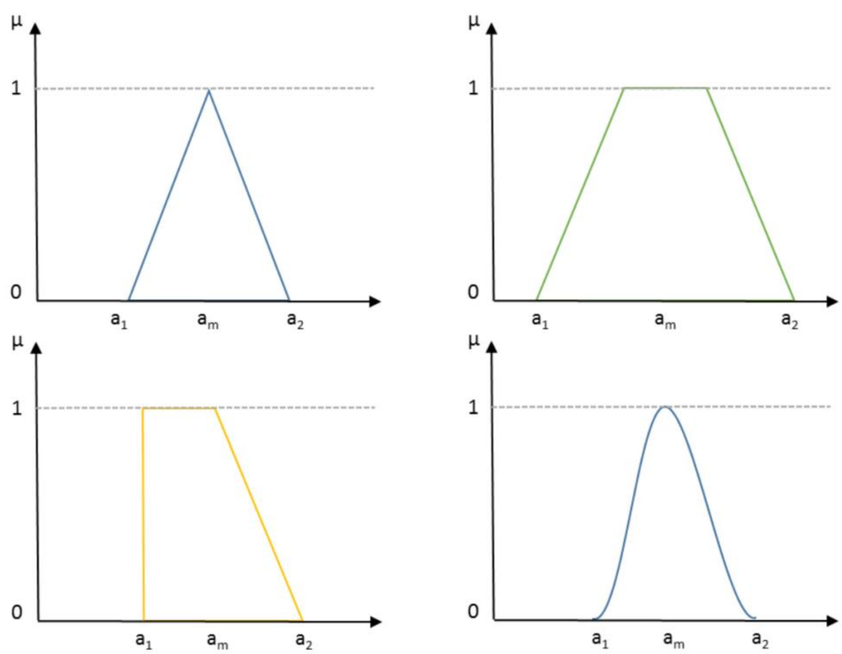

Fig. 3.9. Membership function shapes.

ELECTRE methods

ELECTRE methods were first introduced in the mid-1960's by and became widely known after the work of Roy *(Roy, 1991)*. These methods evaluate every possible pair of solution combinations within a set of multiple options (solutions) for a set of criteria that quantify the level at which each option outranks all others. Nevertheless, since an outranking relation must be constructed beforehand, a strong source of subjectivity is assumed and, consequently, the reliability in the final solution is not guaranteed *(Figueira et al., 2013; Rogers et al., 2010)*. Moreover, the ELECTRE-IV method has been used as a decision support system for multiple criteria problems and proposes an alternative/derivation of the original ELECTRE method. ELECTRE-IV is an attractive one due to its capabilities to obtain a solution that guarantees the decision maker satisfaction while avoids subjectivity sources using a systematical construction of fuzzy outranking relationships defining three “preference” parameters as displayed in Fig. 3.11 *(Hokkanen and Salminen, 1997; Shanian and Savadogo, 2006,Greco et al., 2016).*

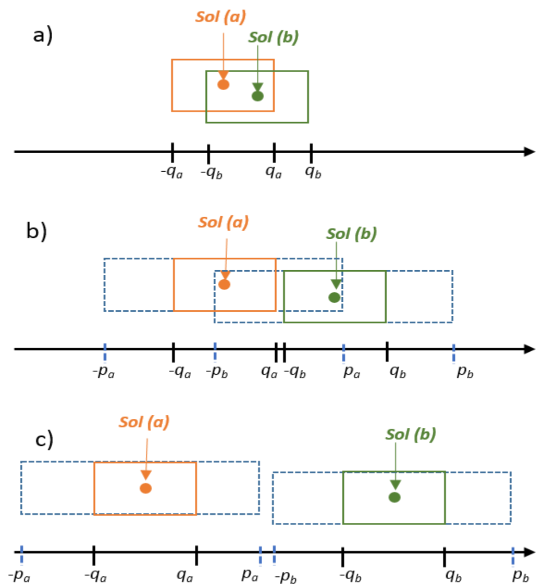

Fig. 3.11. Comparison of two solutions using the preference, indifference and veto thresholds.

These parameters express the thresholds at which one option will be considered preferred, indifferent or undesirable for each criterion. Using the thresholds, a pairwise comparison is performed and a classification is made as follows:

- $m_p(Sol_a, Sol_b)$ is the number of criteria for which Sol_a is strictly preferred to Sol_b,
- $m_p(Sol_b, Sol_a)$ is the number of criteria for which Sol_b is strictly preferred to Sol_a,
- $m_q(Sol_a, Sol_b)$ is the number of criteria for which Sol_a is weakly preferred to Sol_b,
- $m_q(Sol_b, Sol_a)$ is the number of criteria for which Sol_b is weakly preferred to Sol_a,
- $m_i(Sol_a, Sol_b)$ is the number of criteria for which Sol_a is considered indifferent to Sol_b but such that Sol_a has a better criterion value than Sol_b,
- $m_i(Sol_b, Sol_a)$ is the number of criteria for which Sol_b is considered indifferent to Sol_a but such that Sol_b has a better criterion value than Sol_a and,
- $m_o(Sol_a, Sol_b)$= $m_o(Sol_b, Sol_a)$ is the number of equal criterion values of Sol_a and Sol_b.

The above classification expresses the strongest domination relations between solutions for each criterion; however, a second step of the classification procedure is required in order to rank the candidate solutions accounting the entire set of criteria. Such a classification is made by defining the outranking relationships constructed as follows:

- Quasi-dominance S_q

$$aS_qb \Leftrightarrow m_p(b,a) + m_q(b,a) = 0 \quad and$$
$$m_i(b,a) \leq 1 + m_q(a,b) + m_p(a,b)$$

- Canonic-dominance S_c

$$aS_cb \Leftrightarrow m_p(b,a) = 0 \qquad and$$
$$m_q(b,a) \leq 1 + m_p(a,b) \qquad and$$
$$m_q(b,a) + m_i(b,a) \leq 1 + m_i(a,b) + m_q(a,b) + m_p(a,b)$$

- Pseudo-dominance S_p

$$aS_pb \Leftrightarrow m_p(b,a) = 0 \qquad and$$
$$m_q(b,a) \leq m_q(a,b) + m_p(a,b)$$

- Veto-dominance S_v

$$aS_vb \Leftrightarrow if\ m_p(b,a) = 0$$

The above hierarchical outranking relationships are transformed into a numerical value, using the following assumption:$S_q = 1$, $S_c = 0.8$, $S_p = 0.6$, $S_v = 0.4$. Therefore, a new normalized matrix is obtained and a ranking procedure is applied. The exploitation procedure is as follows:

- Construct a partial pre-order KO_1 and KO_2
- Construct the complete pre-order KO =$\text{KO}_1 \cap \text{KO}_2$ as the result.

KO_1 and KO_2 are constructed through a descending and ascending discrimination procedure respectively *(Rogers et al., 2010)*. The combination of these two partial preorder alternatives provides a unique and robust descending desirability hierarchically ordered list. From such a list, a single feasible alternative (or a reduced set of them) is obtained. For more details regarding the ELECTRE methodologies (including ELECTRE-IV) and its application, the reader should refer to *(Figueira et al., 2013; Rogers et al., 2010)*.

Pareto filters

Pareto filters are used to expedite the solution identification from the infinite number of solution that composes the Pareto frontier. The overall strategy consists of a sequential application of different methods to narrow down the number of Pareto solutions and retain for further inspection solutions showing better overall performance (discarding in turn the rest). In this Thesis, 2 types of Pareto filters will be used

Smart Pareto filter.
This filter uses a defined tolerance value (Δt) to discard solutions that are potentially repeated or redundant as described in *Mattson et al., (2004)*. The method selects one solution and scans the tolerance area in order to find and discard points falling within it, thereby removing dominated solutions considering such a tolerance. The tolerance value is defined by the user and has a strong impact on the outcome of the algorithm. If it is too large, the final set of alternatives will be very small, but appealing solutions may be lost, whereas if it is too small the opposite situation will occur.

Fig. 3.12 illustrates the idea behind the smart Pareto filter. Given the set of solutions $\text{Sol}_{s,}$ Sol_1 is taken as core solution and compared with the rest. The dominated solutions and the ones inside the tolerance area (shaded region) are removed from the pool. Afterward, the nearest Pareto solution will be selected as core and the operation will be performed again until no Pareto solutions remain unexplored. In this example, solutions Sol_7, Sol_8 and Sol_9 are dominated solutions and they were removed from the pool of solutions when solutions Sol_2 and Sol_3 are evaluated, respectively. Additionally, even if solution Sol_{10} is Pareto optimal, it lies in the tolerance area of solution $\text{Sol}_{3,}$ so it is considered indistinguishable from it and thus eliminated.

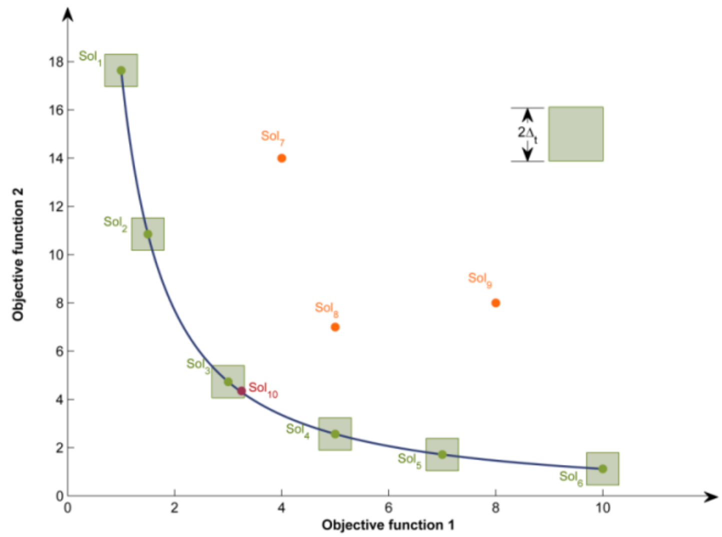

Fig. 3.12. Representation of the Smart Pareto filter algorithm. A solution is considered indistinguishable from another one if the first (red point) falls into the tolerance area (shaded gray zone) of the solution under analysis (green points). Dominated solutions (orange points) are also identified and eliminated.

Order of efficiency filter.

A solution is said to be efficient of order k if it is not dominated by any other solution in any of the possible k-elements subsets of objectives. This filter makes use of this concept, which assesses the "level of optimality" of a solution, and ranks the Pareto points according to their order of efficiency, k. The order of efficiency was originally introduced by *Das (1999)*, and has been recently applied to metabolic engineering *(Pozo et al., 2012)* and desalination plants *(Antipova et al., 2015)*.

From this definition, it follows that if xx^* is efficient of order k, it is also efficient of any order greater than k. Note that lower orders of efficiency reflect a better balance among objectives in the solution and, in some way, the more appealing for decision-makers.

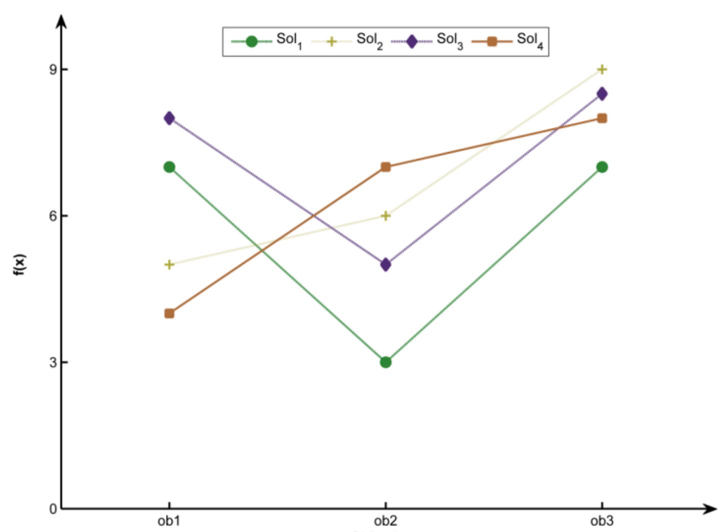

Fig. 3.13. Illustration of the order of efficiency filter. There are 4 solutions that have to be minimized for all the 3 objectives considered. Sol_1 is efficient of order 2 whereas Sol_2 and Sol_4 are efficient of order 3, and Sol_3 is inefficient (i.e., not Pareto optimal).

The concept of Pareto efficiency of order k is illustrated in Fig. 3.13, which shows the parallel coordinates plot where each line represents one of the solutions retained in the previous example (i.e., Sol_1, Sol_2, Sol_3 and Sol_4). Note that 4 solutions are used for clarity purposes. As can be seen, solutions Sol_1, Sol_2 and Sol_4 are Pareto optimal, that is, they are at least efficient of order three (recall that due to the normalization step, values equal to 0 is the best objective performance). On the contrary, Sol_3 is an inefficient solution because Sol_1 dominates it. The next step is to check whether solutions Sol_1, Sol_2 and Sol_4 are also efficient of a lower order, for which all the possible subsets of $k<3$ objectives must be considered. For instance, Sol_1 dominates solutions Sol_2, and Sol_4 in a subset $\{ob_2, ob_3\}$, so they are no longer candidates to be efficient of order two. Conversely, Sol_1 is not dominated neither in subset $\{ob_1, ob_3\}$ nor in $\{ob_1, ob_2\}$ and is therefore efficient of order two. An inspection of subsets of one objective reveals that both, Sol_2 and Sol_4 dominate Sol_1 in $\{ob_1\}$, and thus Sol_1 is not efficient of order one. As a result, the minimum order of efficiency for Sol_1, Sol_2 and Sol_4 is 2, 3, 3, while Sol_3 is inefficient. Hence, solution S_1 would be the most appealing, since it shows better average performance when considering all of the objectives simultaneously.

Pareto filters application.
Based on these 2 filters, an overall application algorithm can be described as follows. We first define the objectives to be analyzed $ob \in OB$ and set a tolerance value for the Smart Filter (Δt). Let *NOO* be the number of objectives considered. The algorithm starts by applying the smart filter for a given tolerance. Then, the order of efficiency filter is applied until further reductions in the Pareto set cannot be attained.

1. Apply **Smart filter** to solutions *NSS* considering objectives $ob \mid ob \in OB$ using tolerance Δt. Let M’ be the set of solutions retained after the application of the filter.
2. If $M' = \emptyset$, stop, further reduction is not possible. Else:
    2.1. For $k = NOO$:1:1
        2.1.1. Apply **Order of efficiency filter** to solutions M' for k. Let V_k be the set of solutions, which are efficient of order k.
        2.1.2. Make $M' = V_k$.
    2.2. End for
3. End if.

Note that the use of Pareto filters implies stronger conditions than the conventional Pareto optimality criterion. This concept avoids the use of any arbitrary ‘‘criterion of merit’’ or visualization technique, thereby making the approach suitable for high-dimensionality problems *(Pozo et al., 2012; Das, 1999)*.

3.4. Optimization under uncertainty.

Stochastic programming.

The efficiency of all the previously presented solution strategies and methodologies highly depends on the consideration of deterministic problems (i.e. all the data required is assumed to be known in advance). In this section, stochastic programs in which some data may be considered uncertain are described. In particular, the most commonly used formulation to address problems under uncertainty is the well-known two-Stage stochastic one, for which two sets of decisions variables have to be identified:

- *First stage decisions*. This set of decisions are taken before unveil any uncertain parameter. They are also known as "here and now" decisions.
- *Second stage decisions*. They are determined after most of the uncertain data is unveiled. These decisions are also known as "wait and see" decisions.

In order to simplify the problem representation, the function $Q(x, \theta)$ is introduced next.

$$\begin{aligned} & Q(x) = \max_{x,y} f(x, y, \theta) \\ s.t \qquad & h(x, y, \theta) = 0 \\ & g(x, y, \theta) \leq 0 \\ & x \in X; y \in Y;\ \theta \epsilon \Theta \end{aligned} \tag{3.8}$$

Here, x and y are the first and second-stage decision variables, respectively, whereas θ denotes the uncertain parameters values that belong to the space Θ of uncertain parameters. First-stage decisions may contain integers due to allocation requirements. $f(x, y, \theta)$ represents the objective function; $h(x, y, \theta)$ and $g(x, y, \theta)$ are vectors of equality and inequality constraints. Notice that the efficiency of the above formulation highly depends on the representation of the uncertainty parameters (θ). For such a reason, the use of scenario-based approaches has been used.

<u>The scenario-based approach</u>

Traditionally, uncertain parameters (θ) are represented using a discrete number of possible scenarios (i.e., a finite discrete distribution), thus, a deterministic equivalent program can be formulated for a stochastic program as displayed in Eq. (3.9):

$$\begin{aligned} & \max_{x,y_s}\ f_{ob} = \sum_{s}^{S} prob_s\, f(x, y_s, \theta_s) \\ & h(x, y_s, \theta_s) = 0 \qquad \forall s\ \in\ \mathrm{S} \\ & g(x, y_s, \theta_s) \leq 0 \qquad \forall s\ \in\ \mathrm{S} \\ & x \in \mathrm{X}\,, y_s \in \mathrm{Y}, \theta_s \in \Theta \end{aligned} \tag{3.9}$$

Here, θ_s is the vector of values taken by the uncertain parameters in the scenarios *s* and $prob_s$ is the probability of occurrence of scenario s belonging to the set S. To approximate a feasible global solution by using two-stage model (Eq. (3.9)) a set of scenarios that represent the problem variability can be used by using a scenario tree representation (Fig. 3.14).

Note that, the better the representation of the scenarios used, the better the approximation to the robust solution. In this line, the most used strategy is the Monte-Carlo sampling. Such a method is based on a random generation of uncertain parameters considering a mean value as well as a standard deviation. Without loss of generality, in this Thesis, Monte-Carlo sampling has been used as unique sampling technique, however, there are additional sampling techniques that may be used, such as Sobol sampling, polynomial-based methods (cubature formula) and methods based on low-discrepancy samples (also known as quasi-Monte Carlo methods).

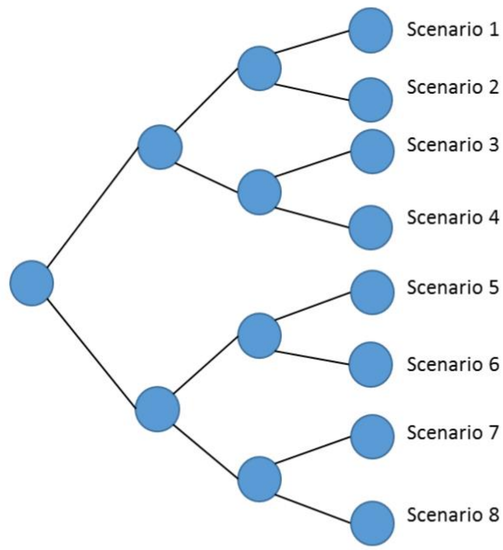

Fig. 3.14. Scenario tree representation for a stochastic programming.

Besides the representativeness of the set of scenarios, its size significantly affects the computational effort (i.e. optimization time). In this line, scenario reduction methods have been proposed. These methods promote the selection of a small and representative set of scenarios as displayed in Fig. 3.15.

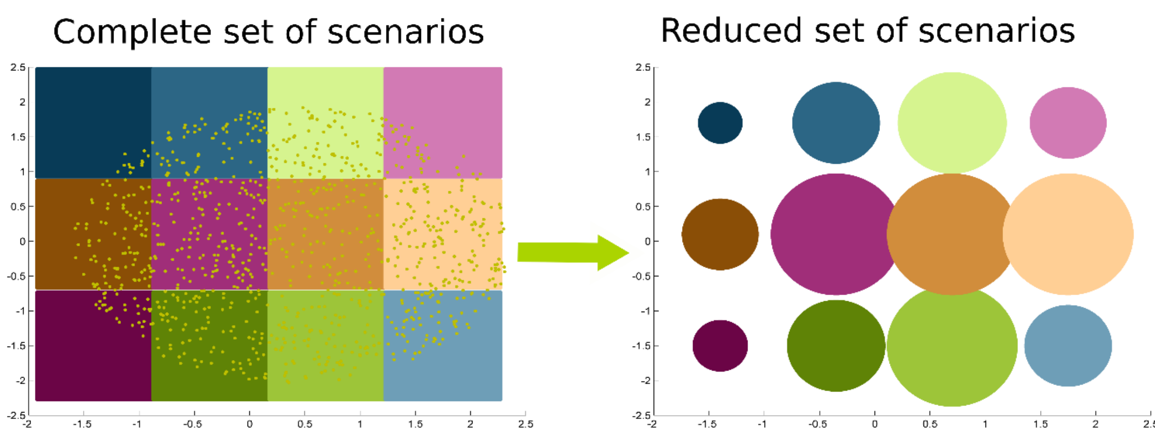

Fig. 3.15. Graphical representation of the clustering technique for scenario reduction method.

Currently, the most effective method for scenario reduction is the transportation distance-based scenario reduction initially proposed by *Heitsch and Römisch, (2003)* and later extended by *Li and Floudas (2014a)*. Such a method, systematically minimizes the distance (i.e. Kantorovich distance) among scenarios, finding the optimal subset representing the original set of scenarios.

3.5. Relaxation strategies.

The accurate modeling of real-life problems typically requires the combination of many of the above problems leading to a highly complex problem. For this purpose, decomposition techniques have been proposed in order to produce an efficient computationally exploitation of the mathematical programs.

The idea behind decomposition techniques is to solve the problem in different steps (typically sequential). In other words, instead of solving the entire problem in a monolithic manner, independent sub-problems are solved iteratively while approximating the global optimal solution. It is important to comment that, in some mathematical models there are constraints that hinder the application of decomposition approach (i.e. a set of common equations also known as complicating constraints). The problem can be directly optimized by solving each of the n-sub-problems only if disregarding the complicating constraints. The most common decomposition strategies are following described.

3.5.1. Sample Average Approximation (SAA).

The Sample Average Approximation (SAA) algorithm has its roots in the so-called stochastic counterpart and the sample path optimization methods *(Plambeck et al., 1996)*. To apply the SAA, the problem has to be solved in its deterministic form considering only one scenario. Then, the values obtained are fixed for the first-stage variables and the model is optimized again for the stochastic problem considering the complete set scenarios. This process is repeated recursively for each of the remaining scenarios, by replacing the corresponding scenario parameters. Note that the standard SAA approximates the solution by solving a series of stochastic sub-problems, each of them with fewer scenarios than the original full space stochastic model *(Verweij et al., 2002; Santoso et al., 2005)*. The overall algorithm is as follows.

1. Define the set of scenarios S and initialize the raw set of solutions *RSS* = Ø
2. For *e* = *1:1:* $|S|$
   2.1. Solve Model P considering only the scenario with index *e* (say scenario s_e). Let solution $\bar{x}^*$ be the value of the first stage variables in this problem.
   2.2. Fix first stage variables as in $\bar{x}^*$.
   2.3. Solve Model P including all the $|S|$ scenarios. Let $\bar{x}^*, \bar{y}^*_s$ be the values of the first and second stage variables in the full optimal solution (the solution with optimal second-stage variables for the first-stage values generated in step 2.1).
   2.4. Make *RSS* = *RSS* ∪ $\bar{x}^*$ and free the first-stage variables,
3. End for.

It is important to highlight that the problem with first and second-stage variables is not rigorously solved and, consequently, the proposed methodology cannot guarantee global optimality for the solutions obtained. However, the proposed approach is indeed an approximation method (i.e., heuristic) to solve the full space multi-objective stochastic model. Consequently, the resulting SAA solution is proved as feasible, even other solutions may dominate them.

3.5.2. Bi-level programming.

The bi-level optimization splits the optimization problem into two problems: an upper-level problem and a lower-level problem. The idea behind bi-level formulation is that the upper-level optimization model is solved taking into consideration the optimal solution of the lower-level problem, as both are solved simultaneously (the lower-level problem is embedded as constraints in the upper-level problem). The general form of the bi-level formulation is displayed in Eq. (3.10)

$$
\begin{aligned}
& \min_{x \epsilon X, y} \; f_u(x,y) \\
s.t \quad & h(x,y) \leq 0 \\
& \quad y \; solves \quad \min_{y} \; g_l(x,y) \\
& \qquad\qquad s.t \quad k(x,y) \leq 0
\end{aligned}
\tag{3.10}
$$

Where $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$ represents the upper and lower-level variables. Similarly, $f_u, g_l: \mathbb{R}^{n_u} \times \mathbb{R}^{n_l} \longrightarrow \mathbb{R}$ are the upper-level and lower-level objective functions respectively and $h: \mathbb{R}^n \times \mathbb{R}^m \longrightarrow \mathbb{R}^u$ define the upper-level constraints while $k: \mathbb{R}^n \times \mathbb{R}^m \longrightarrow \mathbb{R}^l$ the lower-level ones. Notice, that the constraints of the upper-level problem depend on both the upper-level and the lower levels decision variables (x and y). The application of Bi-level optimization is limited to small-size problems up to date. Solving large-scale non-convex MINLP bi-level models is still a challenging research topic.

3.6.Game Theory.

All the strategies described until now are oriented to centralized problems. However, since industrial problems very often require decisions under a decentralized environment, the interaction between different decision-makers has to be considered. For this purpose, Game Theory (GT) has been proposed as a way to solve problems with different enterprises sharing interests *(Cachon, 2003; Cachon and Netessine, 2004; Wang, 2015; Hennet and Arda, 2008; Leng and Parlar, 2010; Zhao et al., 2010; Li et al., 2013; Yue and You, 2014; Chu et al., 2015; Ramos et al., 2016)*. In general, GT allows considering stakeholders (as game players) with individual and conflicting objectives within the same problem framework. The combination of the potential decisions of each stakeholder represents a game strategy. Additionally, depending on the interaction and flow of information among the different game players, the problem is classified as a cooperative or non-cooperative game. In particular, cooperative games represent the situation in which a coalition is assumed and the objective function is a common (shared) one. Contrary, non-cooperative (or competitive) situation assumes an independent objective function for each player. For cooperative and competitive situations, a zero-sum and non-zero sum situation is obtained respectively:

- *Zero-sum-game*: the amount gained by one game player is the same as the amount lost by the other game player. In this case, cumulate revenue is not possible for their cooperation.
- *Non-zero-sum game*: the amount gained by one game player is not equal to the amount lost by the other game player/s. This means that the gains of one player cannot be deduced from the gains of the other players.

Depending on the knowledge about the strategy of the other players, solution strategies such as Nash equilibrium or Stackelberg game can be devised.

3.7.Software.

There are some commercial tools for general optimization purposes, including GAMS (General Algebraic Modeling System, *(Rosenthal et al., 2012)*, AMPL (A Mathematical Programming Language, *(Fourer et al., 2002)*, AIMMS (Advanced Interactive Multidimensional Modeling System, *(Roelofs, 2010)*, Matlab and the recently developed PYOMO. All of them share similar characteristics (general mathematical language, use different solvers to solve the modeled problems, etc.). In this Thesis, GAMS has been selected since is the most widely used modeling and optimization software in the PSE field, and thus, promotes future comparisons.

3.7.1. GAMS – General Algebraic Modeling System

In addition to its popularity, GAMS has some important characteristics that promote its selection:

- The pool of solvers available can be updated, thus, once the model is developed; several solvers are available to optimize the problem.
- The user interface is very friendly and simple which promotes its readability for both humans and machines. Thus, links between different software's are feasible such as import and export data from/to Microsoft Excel and MATLAB.
- Allows unambiguous statements of algebraic relationships.
- The ability to extend formulations aimed to solve small size problems to address large-scale ones at low coding effort.

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

3.7.2. Solvers

Many solvers can be used to solve NLP problems such as MINOS, CONOPT, IPOT, KNITRO, etc. Similarly, some other solvers are used to address convex and non-convex problems, including DICOPT (convex/non-convex), GloMIQO (convex/non-convex quadratic), BARON (convex/non-convex), and SCIP (convex/non-convex), among others. The main solvers used in this Thesis and included in the GAMS library are displayed in Table 3.2.

Table. 3.2. Typical AHP numerical equivalences/preferences.

	LP	MIP	NLP	MINLP
BARON	x	x	x	x
CONOPT	x		x	
CPLEX	x	x		
DICOPT				x
SCIP		x	x	x

3.8. Final remarks.

In this chapter, different optimization techniques have been outlined. The main ideas behind each technique have been briefly introduced in order to provide the reader with a general understanding of the theory involved in the solution techniques applied in this Thesis. In order to implement mathematical formulation in optimization software (i.e., GAMS), one requires having a good understanding of their principles, to interpret results as well as to debug skills. For that reason, special emphasis has been made to these topics. Particularly in this Thesis, the combination of MO and uncertainty approaches frameworks has been developed. Additionally solution identification strategies have been proposed.

Part II:

Efficient Multi-Objective Strategies

Chapter 4

Fuzzy programming as advanced MOO approach

Despite the efficiency of the current multi-objective approaches to assess more than two objectives simultaneously, their application has been limited to optimize (increase or reduce) the objective value. However, these approaches are useful to address complex sustainability problems, since they have the potential to improve the process management by considering both, the quantified impact and its effects over further process conditions. The above becomes more relevant, especially when one of the objectives affects directly a limited and/or non-renewable resource (such as water and energy).

In this chapter, a multi-objective optimization strategy based on a fuzzy formulation is proposed for the sustainable design and planning of water supply chains in urban areas. As opposed to other models that attempt to minimize water consumption, this study seeks to minimize the water stress index, which quantifies the impact of freshwater consumption over the water reservoirs considering the geographical conditions of the location where the withdrawals take place. The capabilities of this approach are illustrated through its application to a real case study based on the city of Morelia in Mexico, in which the use of alternative water sources along with an appropriate water distribution plan allows reducing the pressure over natural reservoirs.

4.1. The Role of Multi-Objective approaches in the design and management of water SC's

The massive water requirements are driving to the fast depletion of worldwide available freshwater, which compromises the water availability for the near future. Thus, one of the key global sustainability challenges is the efficient management and conservation of water, since it is the essential resource for all anthropogenic activities worldwide. Water scarcity affects differently each geographic region across the world due to the uneven spatial distribution of groundwater availability as well as the region-specific climatic conditions. Therefore, strategies that take into account the spatial features of water consumption are needed to promote a sustainable water use. For the particular case of industrial processes, the following three main challenges must be addressed:

(i) The integration of water reuse/recycle strategies in industrial processes;
(ii) The development and application of efficient redesign/retrofit techniques to wastewater treatment processes; and
(iii) The integration of water efficiency indexes in decision-support strategies.

PSE community is able to tackle these challenges by adopting a holistic systems-based analysis. Such an approach should seek for an integrated solution by minimizing the global impact while considering feasibility constraints imposed by universal physical laws and current regulations. In particular, MOO has been applied for the design and planning of a wide variety of industrial systems (including water networks) *(Grossmann and Guillén-Gosálbez, 2010)*. For example *Zhang et al. (2014)* identify the potential benefits of reusing wastewater in regional sectors by performing a trade-off between the recovered wastewater, regeneration costs and pollutants reduction. Later on, the process challenges associated to the use of alternative water source (such as collected rainwater) have been assessed considering three conflicting objectives (economic, freshwater consumption and land use) *(Rojas-Torres et al., 2015)*. More recently, the scope of the study was enlarged to optimize the energy-water of hydrologic power plants considering economic, environmental and social objectives *(González-Bravo et al., 2016)*. Furthermore, multi-objective models were applied to optimize the use of water in agriculture concerning wheat production *(Galán-Martín et al., 2017)*.

The overwhelming majority of formulations dealing with water issues (either preservation or conservation ones) considers directly the freshwater consumption as the environmental impact associated with the water withdrawals. Nevertheless, the impact of freshwater withdrawals over water availability depends on multiple factors and not only in the quantity. Thus, sophisticated environmental indices that better express the cause-effect relationships between water use and environmental impact have been promoted. In this line, the water stress index (WSI) was proposed to model the impact of water consumption over the availability in its sources *(Pfister et al., 2009)*. Similar metrics have been proposed to use the water consumption level as a way to quantify the real impact of water consumption considering the regional aspects of the withdrawals. Until now, water efficiency indexes were never included as an environmental objective in a multi-objective (MO) water management problem. Hence, there is significant room for improvement in the way water management is optimized, particularly regarding the selection of appropriate environmental metrics.

Besides the definition of a customized environmental objective function, MOO methods need additional improvements for the detailed analysis of the solution within the Pareto frontier, and the further identification of the best option among them. Alternatively, the number of Pareto solutions can be systematically narrowed down following other approaches, including, Pareto filters *(Pozo et al., 2012; Antipova et al., 2015)*, ELECTRE methods *(Rogers et al., 2010)* and data envelopment analysis *(Limleamthong et al., 2016)*. Traditional MOO and narrow down methods have been described in detail in Chapter 3.

Seeking to overcome the typical limitations of MOO and solution reduction methods, fuzzy programming appears as a promising alternative to reduce the complexity of MOO models while promoting the generation of well-balanced solutions. In the recent past, these approaches have been applied to solve manufacturing *(Karsak and Kuzgunkaya, 2002)* and energy systems problems *(Mazur, 2007)*. Similarly, MO-fuzzy formulations have been used for the planning of heat/cooling networks considering linear and non-linear operating costs and energy requirements *(Sakawa and Matsui, 2013; Ehsani et al., 2016)*. Despite all the studies on fuzzy approaches to address MOO problems, two main challenges remain unsolved. First, the proper definition of membership functions to capture the objectives' behavior and their associated impact (cause-effect). Second, how to properly incorporate the decision-makers' preferences in the fuzzy model.

This chapter proposes a novel approach for the optimal retrofit and planning of water distribution networks in urban areas based on a MO-fuzzy formulation that makes use of nonlinear membership functions. Three conflicting objectives are considered: fob_1, economic profit (*Profit*), fob_2, water consumption (*WC*) and fob_3, land usage (*LU*). The first criterion is commonly optimized in industrial processes reflecting the economic dimension of sustainability. The other two quantify environmental aspects, with the third one measuring as well the level of complexity of the network and the ease of operation. fob_1 and fob_3 are formulated assuming linear membership functions following traditional fuzzy methods. For fob_2, a nonlinear membership function is defined that links the *WC* to the water availability. Hence, one of the main contributions of this chapter is the adoption of a mathematical approach to capture the cause-effect relationship between water consumption and the associated impact (rather than using WC as a proxy of environmental impact).

4.2. Problem statement

This chapter addresses the re-design and operation of a water network system considering both, its economic performance and the environmental impact (see Fig. 4.1). To derive the mathematical formulation, a standard high-level network is considered encompassing natural water sources k that play the role of suppliers (including dams, springs and deep wells). The SC also includes industrial u, agricultural h and domestic j sites acting as water consumers along with potential sites for storage tanks and artificial ponds (indexed with the subscripts l and n, for agricultural and domestic sites, and b and w, for industrial sites, respectively).

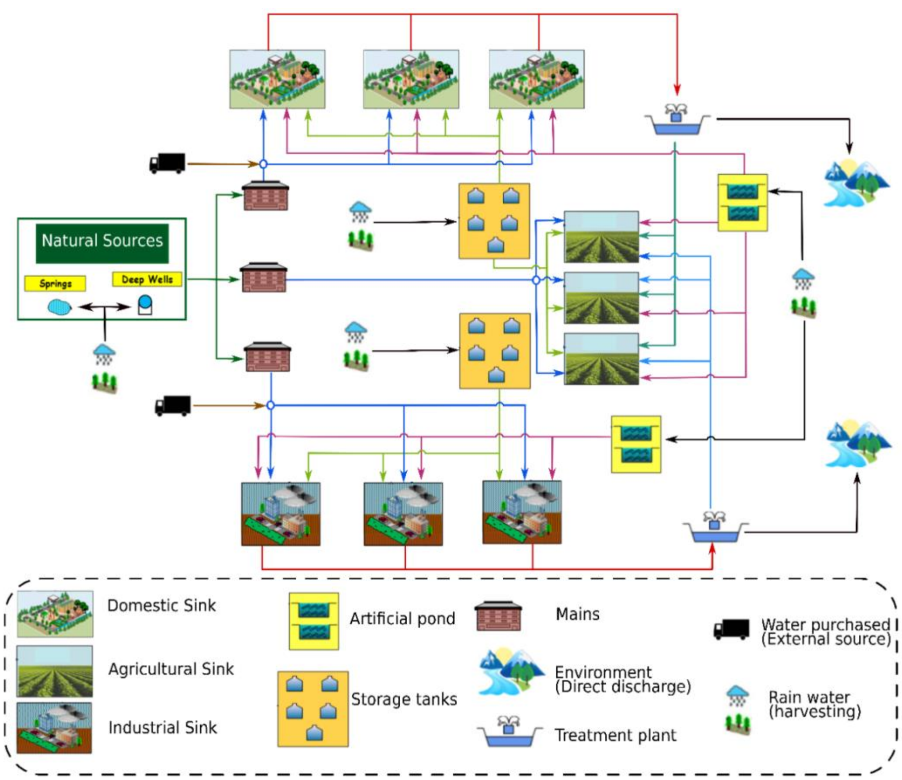

Fig. 4.1. Superstructure for water distribution at the macroscopic level.

Natural freshwater sources, k, can be recharged by direct precipitation, runoff water and by natural tributaries m. Water from natural sources is treated in central facilities (henceforth know as mains) and distributed to industrial u, agricultural h and/or domestic j sites. Reclaimed water can be either, used to meet the agricultural demands (without previous treatment) or be directly discharged to the environment. Water can be acquired from external places, which distribute it directly to the final users whenever natural sources cannot satisfy the water demand. Harvested rainwater is stored in different facilities (storage tanks and artificial ponds).

The goal of the analysis is to identify the best design and planning decisions in terms of its economic performance and water perseveration while reducing the land usage given the average capacity of natural and alternative sources, water demands, purchasing prices and process constraints.

4.3.Mathematical formulation

The following equations model the water network shown in Fig. 4.1. In particular, mass and energy balances for each part of the network are next described.

4.3.1. Mass balances

Natural water sources

Eq. (4.1) accounts for the water in natural repositories ($G_{k,t}$) using an inlet-outlet analysis. In particular, $r_{m,k,t}$ represents the water inlets from all the affluent m that contribute to flows k, while $p^{g}_{k,t}$ quantifies the water collected from both, the rainfall and runoff water. Similarly, the output water is quantified through the sum of the water sent to domestic, agricultural and industrial sites ($g^{d}_{k,t}$, $g^{a}_{k,t}$ and $g^{i}_{k,t}$, respectively), the water losses ($v^{g}_{k,t}$) and over-flooding ($Drop^{g}_{k,t}$). For simplicity, water losses (due to evaporation, filtration, and losses in the distribution process), are fixed at 20% of the total collected water, while the over-flooding is defined as the amount of water exceeding the maximum capacity of source k.

$$G_{k,t} - G_{k,t-1} = \sum_{m \in M} r_{m,k,t} + p^{g}_{k,t} - g^{d}_{k,t} - g^{a}_{k,t} - g^{i}_{k,t} - v^{g}_{k,t} - Drop^{g}_{k,t} \qquad (4.1)$$

The rainfall ($ROWV_{k,t}$) and runoff water ($DPWV_{k,t}$) can be calculated as follows.

$$p^{g}_{k,t} = ROWV_{k,t} + DPWV_{k,t} \qquad k \in K, t \in T \qquad (4.2)$$

Notice that both, the runoff water and rainfall are calculated from the total annual precipitation (P_t), and the collection area (A_k), considering a certain coefficient $C_e$as described in Eq. (4.3) and Eq. (4.4).

$$ROWV_{k,t} = P_t \cdot A^{ROW}_{k} \cdot C_e \qquad k \in K, t \in T \qquad (4.3)$$

$$DPWV_{k,t} = P_t \cdot A^{DPW}_{k} \cdot C_e \qquad k \in K, t \in T \qquad (4.4)$$

Particularly in this case study $C_e = 0.1435$, which can be obtained (with indirect methods) from the annual precipitation and the parameter K, which takes into account the type and use of land.

Storage tanks

The mass balance for storage tanks follows the same logic than the balance for natural sources. Thus, Eq. (4.5) models the water stored for domestic/agricultural use ($S_{l,t}$).

$$S_{l,t} - S_{l,t-1} = s_{l,t}^{in} - \sum_{j \in J} s_{l,j,t}^{out,d} - \sum_{h \in H} s_{l,h,t}^{out,a} \qquad \forall l \in L, \forall\, t \in T \tag{4.5}$$

$s_{l,t}^{in}$ accounts for the harvested rainwater, while $s_{l,j,t}^{out,d}$ and $s_{l,h,t}^{out,a}$ represent the water sent for domestic and agricultural use, respectively. In the same way, the balance for storage tanks in industrial facilities is as follows.

$$SI_{b,t} - SI_{b,t-1} = si_{b,t}^{in} - \sum_{u \in U} si_{b,u,t}^{out,i} \qquad \forall b \in B, \forall\, t \in T \tag{4.6}$$

Artificial ponds

The mass balances for artificial ponds are equivalent to those applied to storage tanks. For domestic and agricultural use, the balance is the following:

$$A_{n,t} - A_{n,t-1} = a_{n,t}^{in} - \sum_{j \in J} a_{n,j,t}^{out,d} - \sum_{h \in H} a_{n,h,t}^{out,a} \quad \forall n \in N, \forall\, t \in T \tag{4.7}$$

Where $A_{n,t}$ represents the amount of stored water in pond n at period t. $a_{n,t}^{in}$ corresponds to harvested rainwater, while $a_{n,j,t}^{out,d}$ and $a_{n,h,t}^{out,a}$ represent the water sent to domestic and agricultural users. For industrial users, the balance is stated as follows:

$$AI_{w,t} - AI_{w,t-1} = ai_{w,t}^{in} - \sum_{u \in U} ai_{w,u,t}^{out,i} \quad \forall w \in W, \forall\, t \in T \tag{4.8}$$

Mass balance in mains

The mains can be considered as a pretreatment site in which all the natural water flows are treated to attain the quality required by their final users, as shown by Eqs. (4.9) to (4.11).

$$\sum_{k} g_{k,t}^{d} = \sum_{j \in J} f_{j,t} \qquad t \in T \tag{4.9}$$

$$\sum_{k} g_{k,t}^{a} = \sum_{h \in H} r_{h,t} \qquad t \in T \tag{4.10}$$

$$\sum_{k} g_{k,t}^{i} = \sum_{u \in U} q_{u,t} \qquad t \in T \tag{4.11}$$

Where $f_{j,t}$, $r_{h,t}$ and $q_{u,t}$ represent the inlet water for domestic (j), agricultural (h) and industrial (u) sinks, respectively, at time t.

Domestic/agricultural sinks and domestic treatment plant

The demand for domestic use ($D_{j,t}^{ds}$) can be satisfied using natural sources (domestic main) as well as reused/harvested water (storage tanks and/or artificial ponds) as described in Eq. (4.12).

$$D_{j,t}^{ds} = f_{j,t} + \sum_{l \in L} s_{l,j,t}^{out,d} + \sum_{n \in N} a_{n,j,t}^{out,d} + fpch_{j,t} \quad j \in J, t \in T \tag{4.12}$$

Notice that water can also be purchased from external sites (if required), as denoted by $fpch_{j,t}$. In particular, Eq. (4.13) describes the mass balance in the domestic sinks, which contains two terms.

The first one ($cw_{j,t}^{d}$) accounts for the water consumed/lost during process/transportation, while the second one ($int_{j,t}^{in}$) represents the wastewater generated in domestics sinks.

$$D_{j,t}^{ds} = cw_{j,t}^{d} + int_{j,t}^{in} \qquad j \in J, t \in T \tag{4.13}$$

Notice that wastewater can be regenerated in a wastewater treatment plant for its further use in agricultural sinks (int_{t}^{out}) or prior to being disposed (cw_{t}^{tp}).

$$\sum_{j} int_{j,t}^{in} = int_{t}^{out} + cw_{t}^{tp} \qquad t \in T \tag{4.14}$$

The regenerated water (int_{t}^{out}) can be sent to any agricultural sink as described in Eq. (4.15).

$$int_{t}^{out} = \sum_{h} int_{h,t}^{out,ag} \qquad t \in T \tag{4.15}$$

Similarly than for domestic use, agricultural demands can be satisfied by different sources as shown in Eq. (4.16).

$$D_{h,t}^{as} = r_{h,t} + \sum_{l \in L} s_{l,h,t}^{out,a} + \sum_{n \in N} a_{n,j,t}^{out,a} + rpch_{j,t} + int_{h,t}^{out,ag} + inti_{h,t}^{out,i} \quad h \in H, t \in T \tag{4.16}$$

Where $int_{h,t}^{out,ag}$ and $inti_{h,t}^{out,i}$ represent the regenerated water from domestic and industrial treatment plants. Notice that a “non-output” situation is assumed which means that all the inputs flows for the agricultural sinks are consumed.

Industrial sinks and treatment plants

Industrial sinks balances follow the same logic as domestic and agricultural ones (See Eq. (4.17)).

$$D_{u,t}^{di} = q_{u,t} + \sum_{b \in B} si_{b,u,t}^{out,i} + \sum_{w \in W} ai_{w,u,t}^{out,i} + qpch_{u,t} \quad u \in U, t \in T \tag{4.17}$$

Here, $qpch_{u,t}$ quantifies the water purchased from external sites. The water consumed/lost in the production process ($cw_{u,t}^{di}$) as well as wastewater produced ($inti_{u,t}^{in}$) are also considered.

$$D_{u,t}^{di} = cw_{u,t}^{di} + inti_{u,t}^{in} \qquad \forall u \in U, \forall\, t \in T \tag{4.18}$$

The treatment plant balances are described in Eqs. (4.19) and (4.20).

$$\sum_{u} inti_{u,t}^{in} = inti_{t}^{out} + cwi_{t}^{tp} \qquad t \in T \tag{4.19}$$

$$inti_{t}^{out,i} = \sum_{h} inti_{h,t}^{out,i} \qquad t \in T \tag{4.20}$$

Storage tanks and artificial ponds

Maximum capacity levels are defined by S_{l}^{max} and A_{n}^{max} for storage tanks and artificial ponds, respectively (only for domestic and agricultural use). Similarly, SI_{b}^{max} and AI_{w}^{max} represent the maximum capacity for storage tanks and artificial ponds for industrial purposes. Eqs. (4.21) to (4.28) guarantee a storage accumulation below the maximum capacity.

$$S_l^{max} \geq S_{l,t}, \qquad l \in L, \qquad t \in T \tag{4.21}$$

$$A_n^{max} \geq A_{n,t}, \qquad n \in N, \qquad t \in T \tag{4.22}$$

$$S_l^{max} \geq s_{l,t}^{in}, \qquad l \in L, \qquad t \in T \tag{4.23}$$

$$A_n^{max} \geq a_{n,t}^{in}, \qquad n \in N, \qquad t \in T \tag{4.24}$$

$$SI_b^{max} \geq SI_{b,t}, \qquad b \in B, \qquad t \in T \tag{4.25}$$

$$AI_w^{max} \geq A_{w,t}, \qquad w \in W, \qquad t \in T \tag{4.26}$$

$$SI_b^{max} \geq si_{b,t}^{in}, \qquad b \in B, \qquad t \in T \tag{4.27}$$

$$AI_w^{max} \geq ai_{w,t}^{in}, \qquad w \in W, \qquad t \in T \tag{4.28}$$

The installation (or not) of storage tanks is controlled using a binary variable ($z_{l,t}^{s}$, for domestic and agricultural usage, and $z_{b,t}^{si}$ for industrial one) as displayed in Eq. (4.29) and Eq. (4.31). A similar approach was used for artificial ponds using $z_{n,t}^{a}$ for domestic/agricultural use and $z_{w,t}^{ai}$for industrial purposes, as seen in Eqs. (4.30) and (4.32).

$$\sum_t z_{l,t}^{s} \leq 1, \qquad \forall l \in L \tag{4.29}$$

$$\sum_t z_{n,t}^{a} \leq 1, \qquad \forall n \in N \tag{4.30}$$

$$\sum_t z_{b,t}^{si} \leq 1, \qquad \forall b \in B \tag{4.31}$$

$$\sum_t z_{w,t}^{ai} \leq 1, \qquad \forall w \in W \tag{4.32}$$

Installing storage tanks and/or artificial ponds has an important impact on the cost function as shown in Eqs. (4.33) and (4.34).

$$Cost_l^{s} = \left(\sum_t K_{F_{l,t}} \cdot VP_{l,t} \cdot z_{l,t}^{s}\right) \cdot A + \left(\sum_t K_{F_{l,t}} \cdot VP_{l,t} \cdot Zag_{l,t}^{s}\right)^{\alpha} \cdot B, \qquad \forall l \in L \tag{4.33}$$

$$Cost_n^{a} = \left(\sum_t K_{F_{n,t}} \cdot VP_{n,t} \cdot z_{n,t}^{a}\right) \cdot C + \left(\sum_t K_{F_{n,t}} \cdot VP_{n,t} \cdot Zag_{n,t}^{a}\right)^{\alpha} \cdot D, \qquad \forall n \in N \tag{4.34}$$

In Eqs. (4.33) to (4.34), both, A and B are parameters used to calculate the fixed and variable costs of storage tanks ($Cost_l^s$), while C and D have the same purpose for artificial ponds costs ($Cost_n^a$). α accounts for economies of scale, while, K_F is used to annualize the investment in each facility (described as $K_{F_{n,t}} = 1/(1+i)^t$). The total investment for storage installation is represented through the variable VP, while $Zag_{l,t}^s$ is an additional variable used to linearize the cost functions through the Big-M reformulation (see Eqs. (4.35) to (4.40)). Eqs (4.33) to (4.34) describe the costs of domestic/agricultural use. Until now, domestic, agricultural and industrial related equations have been included. However, for simplicity, from now on just domestic/agricultural equations will be described since the equations describing the industrial use follow the same logic as the domestic/agricultural ones.

$$Zag_{l,t}^{s} \leq S_{l}^{max} + ML_{l,t} \cdot \left(1 - z_{l,t}^{s}\right), \qquad \forall l \in L, \forall t \in T \tag{4.35}$$

$$Zag_{l,t}^{s} \geq S_{l}^{max} - ML_{l,t} \cdot \left(1 - z_{l,t}^{s}\right), \qquad \forall l \in L, \forall t \in T \tag{4.36}$$

$$Zag_{l,t}^{s} \leq ML_{l,t} \cdot \left(z_{l,t}^{s}\right), \qquad \forall l \in L, \forall t \in T \tag{4.37}$$

$$Zag_{n,t}^{a} \leq A_{n}^{max} + MN_{n,t} \cdot \left(1 - z_{n,t}^{a}\right), \qquad \forall n \in N, \forall t \in T \tag{4.38}$$

$$Zag_{n,t}^{a} \geq A_{n}^{max} - MN_{n,t} \cdot \left(1 - z_{n,t}^{a}\right), \qquad \forall n \in N, \forall t \in T \tag{4.39}$$

$$Zag_{n,t}^{a} \leq MN_{n,t} \cdot \left(z_{n,t}^{a}\right), \qquad \forall n \in N, \forall t \in T \tag{4.40}$$

From Eqs. (4.35) to (4.40), ML and MN represent a very large number that acts as an upper bound on the volume of the installed tanks and artificial ponds, respectively. Thus, when binary variable $z_{l,t}^{s}$ is 1, variables $Zag_{l,t}^{s}$ take the value of the maximum volume of storage S_{l}^{max} and the model calculates the installation cost of the storage tank; otherwise, the installation cost is zero. In addition to the economic impact, the installation of storage devices and artificial ponds has an impact on the land use that is given by the surface occupied by these repositories, as described in Eq. (4.41).

$$S_{l}^{max} = ARS_{l} \cdot ATS_{l}, \qquad \forall l \in L \tag{4.41}$$

Variable ARS_l denotes the land use required for the storage tanks installed, while ATS_l denotes the tanks height of these tanks. Since the effect of such a factor over land use is significant, a set of constraints for the tanks height were included. In addition to the occupied surface, the harvesting equipment's area has been explicitly calculated using the nominal area (A_n^a) (as displayed in Eqs. (4.42) to (4.43)). Note that the total collected rainwater is hence a function of these areas. Similarly, to storage tanks ATN_n denote the height of the artificial pond.

$$A_{n}^{max} = ARL_{n} \cdot ATN_{n}, \qquad \forall n \in N \tag{4.42}$$

$$APA_{n} = \sum_{t} z_{n,t}^{a} \cdot A_{n}^{a}\,, \qquad \forall n \in N \tag{4.43}$$

As commented before, the same logic is applied to the installation of storage tanks and artificial ponds for industrial use.

4.3.2. Objective functions

The model includes three objective functions, being the water sales revenue, the water consumption and the land use (associated with the storage devices). A detailed description of the objective functions calculation is presented below.

Economic Objective

The economic objective is calculated from the revenues and expenditures associated with the water management (Eq. (4.44)). The profit is obtained by summing the water sales for domestic, agricultural, and industrial purposes ($WaterSales$) while expenses account for the treatment ($TreatmentCost$), distribution ($PipingCost$) and the installation/operation costs associated with artificial tanks ($StorageCost$).

$$Profit = WaterSales - TreatmentCost - StorageCost - PipingCost \tag{4.44}$$

Particularly, $WaterSales$ is calculated as follows.

$$
\begin{aligned}
WaterSales = &\left(\sum_k \sum_t g_{k,t}^{d} + \sum_l \sum_j \sum_t s_{l,j,t}^{out,d} + \sum_n \sum_j \sum_t a_{n,j,t}^{out,d}\right) \cdot DSC \\
&+ \left(\sum_k \sum_t g_{k,t}^{a} + \sum_l \sum_h \sum_t s_{l,h,t}^{out,a} + \sum_n \sum_h \sum_t a_{n,h,t}^{out,a} + \sum_h \sum_t int_{h,t}^{out,ag}\right) \cdot ASC \\
&+ \left(\sum_k \sum_t g_{k,t}^{i} + \sum_b \sum_u \sum_t si_{b,u,t}^{out,i} + \sum_w \sum_u \sum_t ai_{w,u,t}^{out,i} + \sum_h \sum_t inti_{h,t}^{out,i}\right) \cdot ISC \\
&+ \left(\sum_j \sum_t fpch_{j,t} + \sum_h \sum_t rpch_{h,t} + \sum_u \sum_t qpch_{u,t}\right) \cdot PSC
\end{aligned}
\tag{4.45}
$$

Where DSC and ASC are the prices of water for domestic and agricultural purposes, respectively. ISC is the price of water for industrial users, and PSC is the price for the water purchased from external suppliers. The treatment operations are applied to guarantee a satisfactory water quality level, thus, treatment cost can be estimated using Eq. (4.46).

$$
\begin{aligned}
TreatmentCost = &\left(\sum_k \sum_t g_{k,t}^{d}\, CTND + \sum_k \sum_t g_{k,t}^{a}\, CTNA + \sum_k \sum_t g_{k,t}^{i} CTNI\right) \\
&+ \left(\sum_l \sum_j \sum_t s_{l,j,t}^{out,d} + \sum_n \sum_j \sum_t a_{n,j,t}^{out,d}\right) \cdot CTAD \\
&+ \left(\sum_l \sum_h \sum_t s_{l,h,t}^{out,a} + \sum_n \sum_h \sum_t a_{n,h,t}^{out,a}\right) \cdot CTAA \\
&+ \left(\sum_b \sum_u \sum_t si_{b,u,t}^{out,i} + \sum_w \sum_u \sum_t ai_{w,u,t}^{out,i}\right) \cdot CTAI \\
&+ \left(\sum_h \sum_t int_{h,t}^{out,ag} + \sum_h \sum_t inti_{h,t}^{out,i}\right) \cdot CTPA \\
&+ \left(\sum_j \sum_t fpch_{j,t}\, CTFP + \sum_h \sum_t rpch_{h,t}\, CTRP + \sum_u \sum_t qpch_{h,t} CTQP\right) \\
&+ \left(\sum_t Cw_t^{tp} + \sum_t Cw_t^{tpi}\right) \cdot CTPE
\end{aligned}
\tag{4.46}
$$

Where CTND, CTNA and CTNI are the fixed treatment costs for natural streams to be used for domestic, agricultural and industrial purposes, respectively. Similarly, CTAD and CTAA are the rainwater treatment costs for domestic and agricultural purposes, respectively, while CTAI is for industrial use. CTP is the wastewater regeneration cost for agricultural use and CTPE is the cost of wastewater treatment. Finally, CTFP, CTRP, and CTQP are the costs for domestic, agricultural, and industrial use respectively.

Storage tanks are allowed as a way to ensure the water demand satisfaction. Their associated cost is calculated considering the installation/operation cost of artificial reservoirs for both domestic and agricultural ($Cost_l^s$ and $Cost_n^a$ for tanks and ponds, respectively) as well as for industrial use ($Cost_b^{si}$ and $Cost_w^{ai}$ for tanks and artificial ponds, respectively).

$$StorageCost = \sum_l Cost_l^s + \sum_n Cost_n^a + \sum_b Cost_b^{si} + \sum_w Cost_w^{ai} \tag{4.47}$$

The water transportation between locations is described in Eq. (4.48).

$$\begin{aligned} PipingCost = & \sum_l \sum_j \sum_t s_{l,j,t}^{out,d}\, PCSTD + \sum_n \sum_j \sum_t a_{n,j,t}^{out,d}\, PCASD \\ & + \sum_l \sum_h \sum_t s_{l,h,t}^{out,a}\, PCSTA + \sum_n \sum_h \sum_t a_{n,h,t}^{out,a}\, PCASA \\ & + \sum_b \sum_u \sum_t si_{b,u,t}^{out,i}\, PCSTI + \sum_n \sum_h \sum_t ai_{w,u,t}^{out,i}\, PCASI \\ & + \sum_k \sum_t g_{k,t}^d\, PCND + \sum_k \sum_t g_{k,t}^a\, PCNA + \sum_k \sum_t g_{k,t}^i\, PCNI \\ & + \sum_h \sum_t int_{h,t}^{out,ag}\, PCTW + \sum_j \sum_t fpch_{j,t}\, PFP \\ & + \sum_h \sum_t rpch_{h,t}\, PRP + \sum_u \sum_t qpch_{u,t}\, PQP \\ & + \sum_h \sum_t inti_{h,t}^{out,i}\, PCTI \end{aligned} \tag{4.48}$$

Where PCSTD is the unit transportation cost between the storage tank and domestic sink. PCASD represents the unitary pumping cost from the artificial pond to the domestic sink. PCSTA is the unit cost of the pipeline and pumping from the storage tank to agricultural sink. PCASA denotes the unit cost of piping and pumping from an artificial pond to agricultural sink. PCSTI is the unit cost of piping and pumping from industrial storage tank to industrial sink; PCASI is the unit cost of piping and pumping from industrial artificial pond to industrial sink; and PCND, PCNA, and PCNI are the unit costs of piping and pumping from natural sources to domestic, agricultural, and industrial mains, respectively. The cost of piping and pumping purchased water for different users is represented by PFP (domestic), PRP (agricultural), and PQP (industrial). Finally, PCTW (domestic) and PCTI (industrial) are the unit costs of piping and pumping from treatment plants to agricultural sinks.

<u>Environmental Objective</u>

The environmental objective is represented in Eq. (4.49).

$$\begin{aligned} WC = & \sum_k \left(NaturalFlowrate_k^d + NaturalFlowrate_k^a + NaturalFlowrate_k^i \right) \\ & + \sum_j WaterPurchased_j + \sum_h WaterPurchased_h + \sum_u WaterPurchased_u \end{aligned} \tag{4.49}$$

Where the natural and purchased water flows entering to each main are calculated in Eqs. (4.50-4.55).

$$NaturalFlowrate_k^d = \sum_t g_{k,t}^d \tag{4.50}$$

$$NaturalFlowrate_k^a = \sum_t g_{k,t}^a \tag{4.51}$$

$$NaturalFlowrate_k^i = \sum_t g_{k,t}^i \tag{4.52}$$

$$WaterPurchased_j = \sum_t fpch_{j,t} \tag{4.53}$$

$$WaterPurchased_h = \sum_t rpch_{h,t} \tag{4.54}$$

$$WaterPurchased_u = \sum_t qpch_{u,t} \tag{4.55}$$

Land Use Objective

The land use objective is presented in Eq. (4.56).

$$\begin{aligned} LU = \sum_l ARS_l + \sum_b ARSI_b + \sum_n ARL_n + \sum_w ARI_w \\ + \sum_n APA_n + \sum_w API_w \end{aligned} \tag{4.56}$$

4.4.Methodology

The proposed fuzzy-based approach comprises three main steps as shown in Fig. 4.2. First, a MOO model is developed in step 1, which is reformulated into a single-objective optimization (SOO) one by using membership functions (step 2). Finally, the SOO model is solved in step 3 using any optimization strategy. A detailed description of each step is provided in the ensuing subsections.

4.4.1. Definition of the MOO model

The mathematical model presented herein capitalizes on the mixed-integer linear programming (MILP) formulation introduced by Rojas-Torres et al. (2015). The model seeks to optimize simultaneously the *Profit*, *WC* and *LU* objectives described in the multi-dimensional objective function as presented in model *M*.

$$(M) \qquad Max[Profit, -WC, -LU]$$

$$s.t.\ constraints\ 4.1 - 4.56$$

$$x \in R; y \in (0,1)$$

From model *(M)*, variables *x* denote operating and design decisions, while binary variables *y* model the existence (or not) of artificial storage devices. Model *(M)* can be solved by standard MOO methods. As will be later discussed in the next subsection, environmental objective *(WC)* does not account for the spatial specificity of the impact, and therefore it is replaced by the water stress index *WSI*, which provides a better estimate of the "true" impact of water consumption.

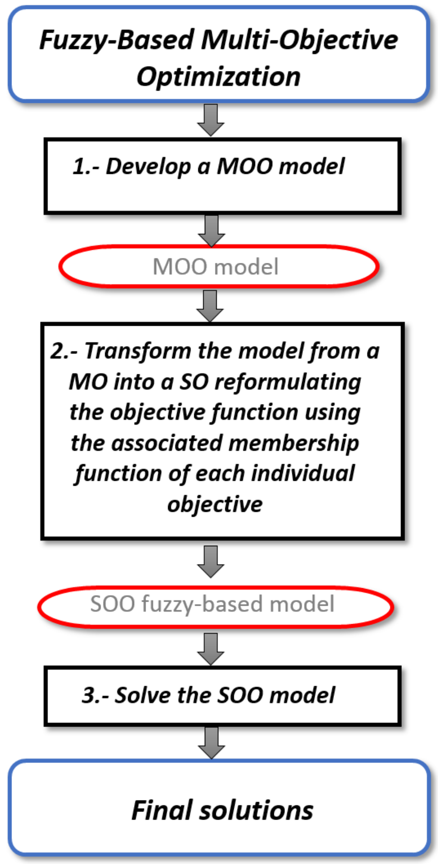

Fig. 4.2. Algorithm for the proposed strategy.

4.4.2. Fuzzy-based model

A fuzzy-based strategy has been used as an alternative to solve the model *(M)* by reformulating the objective function. Particularly, a membership function is defined for each objective using the general expression *(Zimmermann, 1978)* displayed in Eq. (4.57). A detailed description of the idea behind Fuzzy based approaches is presented in Section 3.3.2. For clarity of this section let's highlight that fuzzy formulation has as a main advantages its capability to relax the non-linear objectives behaviour while properly representing the cause-effect relationships. Nevertheless, the fuzzy approach is efficient to identify a well-balanced solution

$$\lambda_{ob}(x_{ob}) = \begin{cases} 1 & if\ x_{ob} \geq \overline{b}_{ob} \\ 1 - (\overline{b}_{ob} - x_{ob})/(\overline{b}_{ob} - \underline{b}_{ob}) & if\ \underline{b}_{ob} < x_{ob} < \overline{b}_{ob} \\ 0 & if\ x_{ob} \leq \underline{b}_{ob} \end{cases} \tag{4.57}$$

Where x_{ob} represents the performance for objective ob, while $\lambda_{ob}(x_{ob})$ can be interpreted as the normalized degree of x_{ob} within the limits for the specific objective ($ob \in \{Profit, WC, LU\}$). The value of $\lambda_{ob}(x_{ob})$ is expressed in the range zero to one, where zero corresponds to the minimum value and one to the maximum one. Moreover, $\overline{b}_{ob}$ and $\underline{b}_{ob}$ represent the objective boundaries (maximum and minimum value, respectively). Eq. (4.57) is applied to the objectives to be maximized; otherwise, the membership function follows the form in Eq. (4.58).

$$\lambda_{ob}(x_{ob}) = \begin{cases} 1 & if\ x_{ob} \leq \underline{b}_{ob} \\ (\bar{b}_{ob} - x_{ob})/(\bar{b}_{ob} - \underline{b}_{ob}) & if\ \underline{b}_{ob} < x_{ob} < \bar{b}_{ob} \\ 0 & if\ x_{ob} \geq \bar{b}_{ob} \end{cases} \tag{4.58}$$

These membership forms facilitate the introduction of the objective fuzziness into the formulation. Notice that Eqs. (4.57) and (4.58) obeys a Γ-shaped fuzzy formulation, which is appropriate in cases where the impact increases linearly with the objective value (as in this particular application).

When assessing environmental burdens, a linear relationship is seldom found between burdens (e.g. emissions, materials consumption and land and water use) and their associated environmental impact. This is because damage assessment models are often nonlinear, yet they are simplified via linear equations to facilitate their use. Therefore, rather than using WC as a proxy of environmental impact, as was done in former studies *(Rojas-Torres et al., 2015)*, herein the environmental performance is modeled via the *WSI*. In order to calculate the *WSI*, the ratio *WC* to total water availability (WA) is first determined as described in Eq. (4.59).

$$WTA = \frac{WC}{WA} \tag{4.59}$$

By definition, *WSI* describes a nonlinear relation with respect to WTA in which for small values of WTA (i.e. small water consumptions) the water reservoirs ensure water supply for future processes. On the contrary, for larger values of WTA (for example, > 0.2), any increment in the water consumption will significantly compromise the water availability for future applications; finally, for large values in WTA (>0.9) the impact becomes irreversible and even when there is still water available in the reservoirs, it is likely that other processes will operate under water limitations. The most appropriate expression to represent this *WSI* behavior is a sigmoidal function as the shown in Eq. (4.60), which provides a continuous range between 0.01 and 1 as discussed in the literature *(Pfister et al., 2009)*. Therefore, Eq. (4.60) can then be used as membership function for quantifying the impact of water consumption:

$$WSI = \frac{1}{1 + e^{-6.4*WTA}\left(\frac{1}{0.01} - 1\right)} \tag{4.60}$$

The environmental objective related to water consumption is then calculated via Eq. (4.61):

$$\lambda_{WC}(x_{WC}) = 1 - WSI \tag{4.61}$$

Finally, the model *(M)* is reformulated into the model *(M2)* as follows:

$$(M2) \qquad Max\left[OB = \sum_{ob} \lambda_{ob}(x_{ob})\right]$$

The overall algorithm is then summarized as:

4. Solve model *(M)* individually for each objective $ob \in OB$. Let $\bar{b}_{ob}$and $\underline{b}_{ob}$ be the maximum and minimum values of each objective, respectively.
5. Reformulate the objective functions using the membership functions in Eqs. (4.57-4.58) and Eq. (4.61).
6. Merge the membership functions to define a SO problem (model (*M2*)).
7. Solve the resulting nonlinear problem using any available solver.

Due to the nonlinear mathematical representation of the *WSI*, the model takes the form of a mixed-integer nonlinear programming formulation (MINLP). Since, there are only two nonlinear terms

(Eqs. (4.59-4.60)), the MINLP can be easily approximate into a MILP by using well-known piecewise techniques. This method, which reformulates univariate nonlinear terms into piecewise linear functions defined using binary variables, was already applied to other problems addressed by the authors *(Pozo et al., 2010)*. Note that it is also possible to apply global optimization solvers to the original MINLP problem, yet the aforementioned reformulation greatly facilitates the solution procedure. A qualitative analysis of the piecewise linearization used in this study is presented in Appendix B.1.

4.5. Case study: Design of water SC's

The proposed formulation is illustrated through its application to a design and planning problem of a water management system in a real urban area. The city of Morelia (Michoacán, Mexico) was selected as a case study due to the high freshwater cost and the severe overexploitation suffered in the last decades. Particularly, 12 natural water sources were considered, out of which ten are deep wells, one a spring and the last one a dam. In order to prevent water depletion, water usage was forced to lie below 80% of the current capacity. The water price is US\$1.4/m^3 *(Zhang et al., 2014)*, while wastewater generated in domestic and industrial sinks is treated to satisfy partially the agricultural demand and the rest is disposed to the environment.

The problem addressed seeks the optimal distribution of water sources that satisfy the domestic, agricultural, and industrial demands for a five-year time horizon (with monthly discretization). A constant increase in water demand of 0.27% (over the average current demand) was considered. Similarly, a linear decrease in precipitation was assumed, with a 3% reduction over the average historical values. We follow the same geographical assumptions as in a former study with the same case study *(Rojas-Torres et al., 2015)*. The city was divided into five areas and the population and location of both industrial and agricultural users were uniformly distributed. Due to the current water usages for each sector, up to 20 storage tanks were considered for domestic and agricultural activity, whereas 20 tanks are allowed for industrial purposes. Similarly, six artificial ponds can be installed for domestic and agricultural users, and six artificial ponds for industrial users.

Additional parameters values are provided in Appendix B.2. The model optimizes simultaneously the design of the SC network and the planning decisions. For comparison purposes, the problem is first solved following a standard MOO approach and then the proposed fuzzy-based method is applied to illustrate its advantages.

4.5.1. Fist approach: Traditional multi-objective method.

For this first case, the well-known ε-constraint method was used to produce a set of Pareto solutions in the space of the three original objectives, *Profit*, *WC*, and *LU* *(Ehrgott, 2005)*. The SO-MILP form of the model *(M)*, contains 34,911 equations, 44,571 continuous variables and 3,120 binary variables and was implemented in GAMS 23.9 and solved with CPLEX 12.4 on a Windows XP computer with Intel®Core™i7 CPU(920)3.4GHz processor with 16.00GB of RAM. It takes approximately 500 seconds to identify the global optimum in every instance. 45 Pareto points were generated, as shown in Fig. 4.3a, in which nadir and utopia points have been also included. To provide additional visual support, a 3-D surface is generated from the set of Pareto frontiers (Fig. 4.3b). Notice that the generation of such a surface is not an accurate prediction of the global Pareto surface, however provides a useful overview.

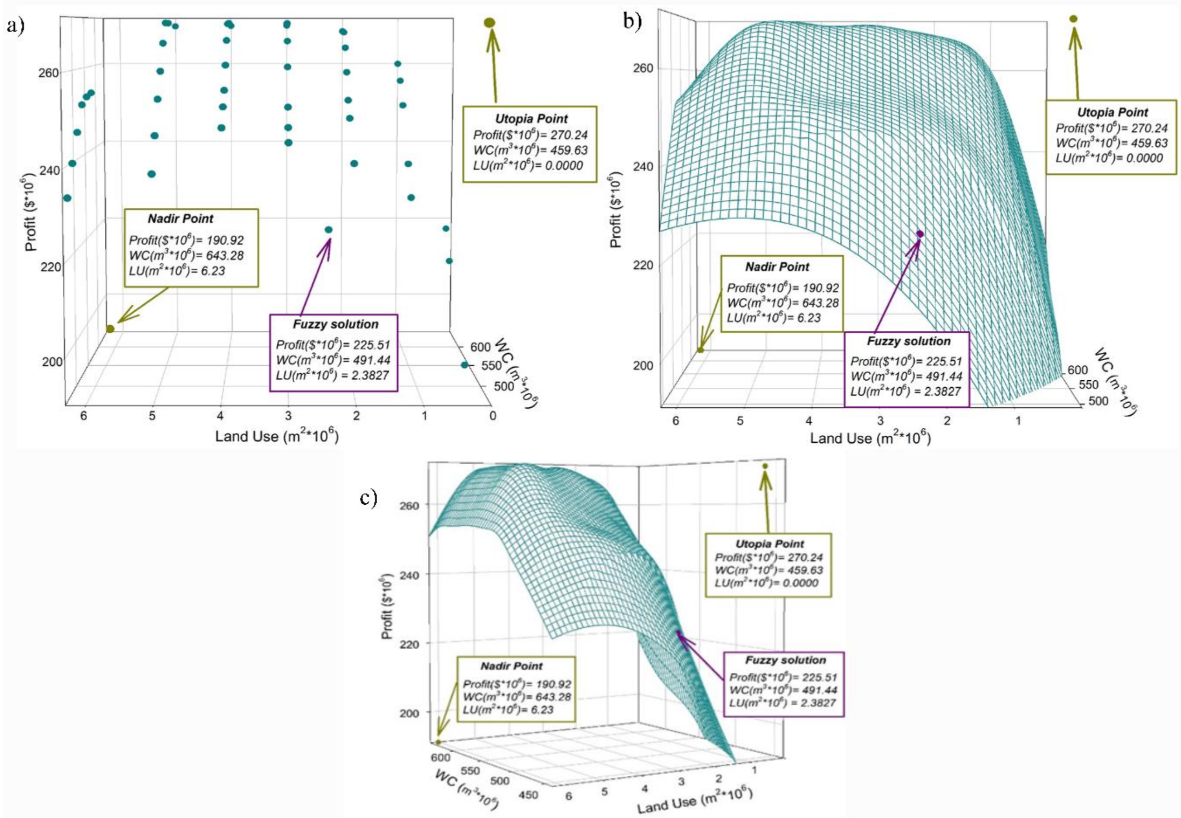

Fig. 4.3. Left. Pareto frontiers for the three objectives under analysis. Right) Projected Pareto surface.

In general, Fig. 4.3 shows that the *LU* and *WC* decrease at the expense of compromising the *Profit* performance. Within the *LU* range, the *Profit* varies about \$70x10^6 (from \$219.15 x10^6 to \$270.26x10^6), while the *WC* oscillates in a range of 183x10^6m^3 (from 459.63x10^6m^3 to 643.28x10^6m^3). The extreme solutions and some intermediate ones are discussed in detail in a previous work *(Rojas-Torres et al., 2015)*. In essence, in order to reduce the environmental impact, it is needed to install 20 storage tanks (upper bound according to the problem formulation) and use some amount of reclaimed water to partially satisfy the freshwater demands (up to 10% of the total consumption). In addition, most of the water needed is covered purchasing water from external suppliers (around 70%) in order to maintain a high level of water in the local water repositories. Thus, the high transportation costs and the large number of storage tanks/land use required deteriorate the performance in both, the *Profit* and *LU* objectives. From this set of solutions and many potential more that could be generated within the aforementioned ranges, decision-makers should select the most appealing one according to their preferences. This would introduce subjectivity into the process and emphasize the need to manage their preferences. In order to simplify this process, the fuzzy-based approach is applied as describes in the next subsection.

4.5.2. Second approach: Fuzzy-Based method

Here, the three objectives were modelled using their respective membership functions. The SO-MINLP model (model *M2*) contains 35,050 equations, 44,708 continuous variables and 3,125 binary variables and it was implemented in the same computer as before. It took approximately 1,500 seconds to find the optimal solution. The obtained solution (henceforth known as fuzzy solution) attains a performance 43%, 82% and 62% of the best possible values for *Profit*, *WC* and *LU*, respectively (\$225.517x10^6, 491.437x10^6m^3 and 2.382x10^6m^2). The above solution obtained through the proposed fuzzy-based approach represents a single point within the Pareto frontier and its graphical representation/allocation is displayed in Fig. 4.3. From such a graphic it can be noticed how the final fuzzy solution lies within the global Pareto frontier/surface, even if it is not within the individual Pareto frontiers for the bi-objective combinations. Additionally, by changing the perspective of the Pareto surface (Fig. 4.3c), it can be noticed how the fuzzy solution is one of the feasible dominant solutions that approximate to the utopia point. Notice that the fuzzy formulation tries to provide a balanced solution, however its performance is conditioned by the decision maker assumptions (as proved in the following section). In addition, Fig. 4.4 represents the corresponding normalized radar plot in order to illustrate the performance of the fuzzy solution.

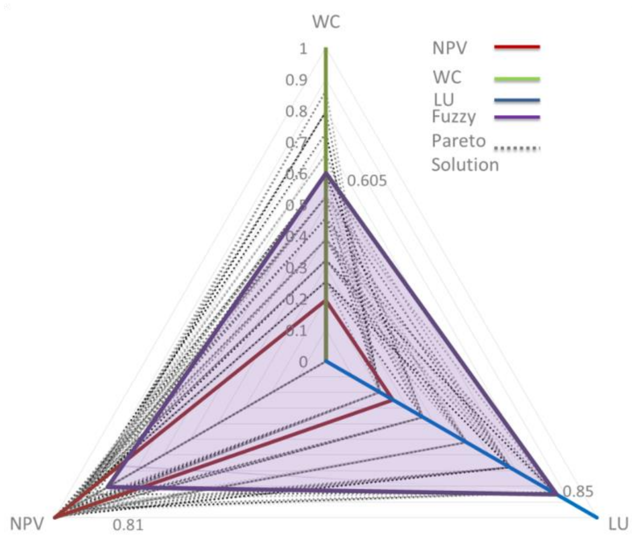

Fig. 4.4. Radar plot comparing the performance for the individual optimization of each objective and the fuzzy approach.

In order to analyze and compare the resulting designs, the solution with the highest *Profit* in the first case is used as a reference point (henceforth known as *Reference* solution). Such a design attains \$270.24x10^6, 661.437x10^6m^3 and 4.766x10^6m^2 for *Profit*, *WC* and *LU*, respectively. Compared to this solution, the fuzzy solution leads to savings of 170.862x10^6m^3 and 2.38x10^6m^2 in freshwater and land use, respectively, but at the expense of reducing in \$44.723x10^6 the economic performance.

4.5.3. Reference and fuzzy-based design comparison

The solution with the highest *Profit* in the first case is the best feasible solution, thus, it will be used as a reference for comparison purposes (henceforth known as *Reference* solution). Such a design attains \$270.24x10^6, 661.437x10^6m^3 and 4.766x10^6m^2 for *Profit*, *WC* and *LU*, respectively. Compared to this solution, the fuzzy solution leads to savings of 170.862x10^6m^3 and 2.38x10^6m^2 in freshwater and land use, respectively, but at the expense of reducing in \$44.723x10^6 the economic performance.

The resulting designs are displayed in Figs. 4.5 and 4.6, respectively. By comparing them, three main differences can be highlighted. First, for domestic and agricultural purposes, the fuzzy design requires two artificial ponds, while for the reference design six are installed. Moreover, water from artificial ponds in the reference and fuzzy designs amount to 5.99x10^6 m^3 and 6.86x10^6 m^3, respectively. On the other hand, the reference design allocates 15 and 20 storage tanks for domestic/agricultural and industrial use, respectively, while the fuzzy one includes 20 for both of them. The storage and artificial ponds capacities had a significant impact on the economic performance due to their installation and transportation costs ($867,260 higher for the fuzzy solution). However, the fuzzy design collects and distributes 9.83x10^{6}m^3 of harvested rainwater, 30% higher than the reference case. The use of these alternative water sources reduces the environmental impact at the expense of increasing the installation cost. A similar behavior was found in the artificial ponds and storage tanks for industrial usages.

The final and most important difference concerns the amount of freshwater consumed in agricultural activities. In the fuzzy solution, the water consumed in agriculture is fully satisfied using regenerated water from treatment plants, ultimately attaining freshwater savings of 21.03x10^6 m^3 compared to the reference solution. This reduces the environmental and land use impacts at the expense of sacrificing economic benefits, as there is also an increment in water treatment/distribution/storage costs (which amount to $27.347x10^6). Although the purchase of water was an option available, it was not selected in any of the optimal solutions. This was expected, considering the high external prices and limited availability of resources.

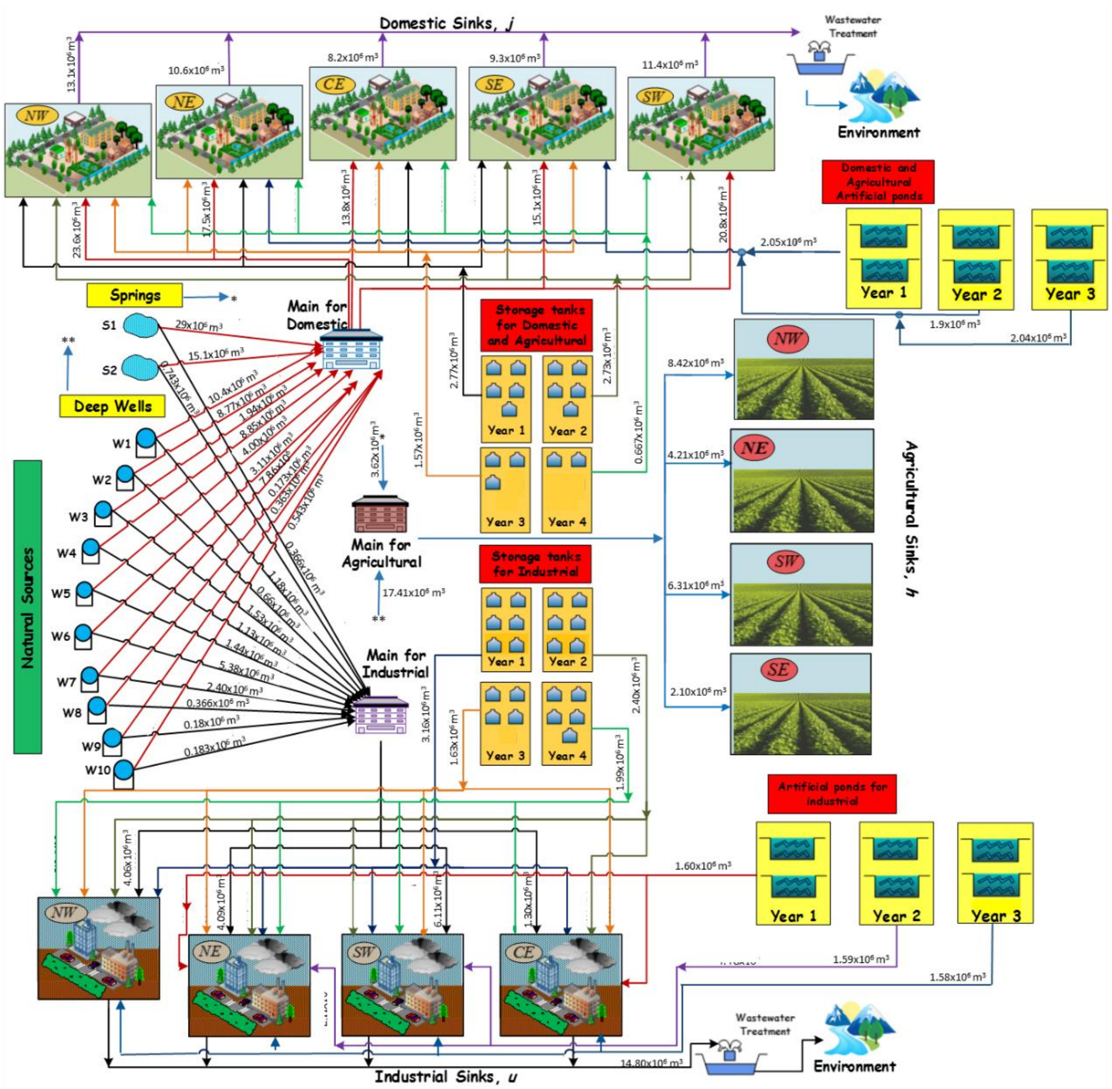

Fig. 4.5. Configuration of solution with highest Profit value for case 1.

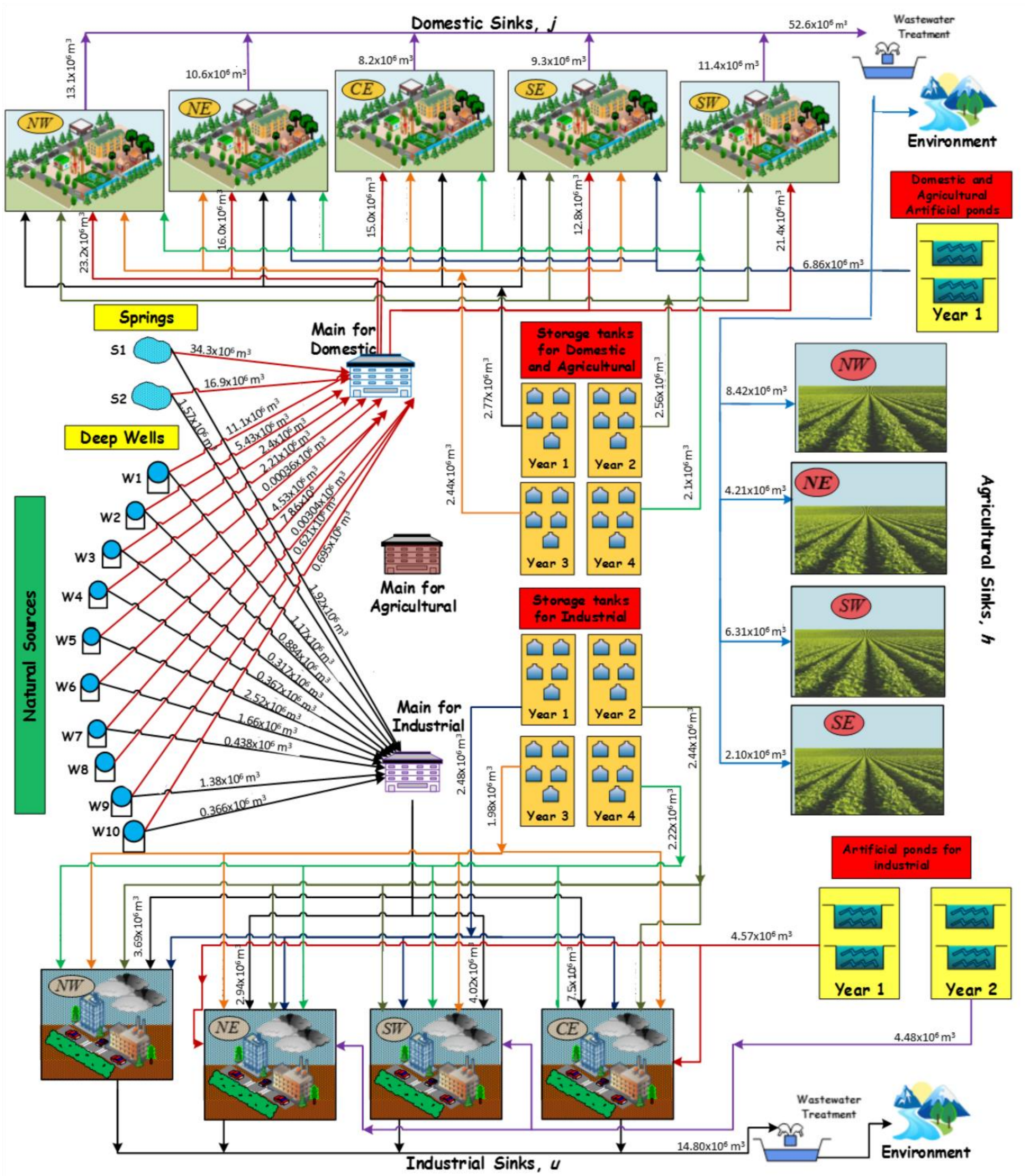

Fig. 4.6. Optimal overall configuration obtained through the fuzzy-based formulation.

In order to stress even more the capabilities of the proposed formulation, its flexibility and robustness are evaluated in the following subsections.

4.5.4. Comparison among different non-linear membership functions

Here, in addition to the already commented sigmoidal function, an exponential impact associated with the LU objective ($\lambda_{LU} = Log_{10}(LU)$) has been considered and represented in Fig. 4.8. Alike in the sigmoidal case, here, the same piecewise approximation (i.e. using five fixed intervals) was used to relax the nonlinearities.

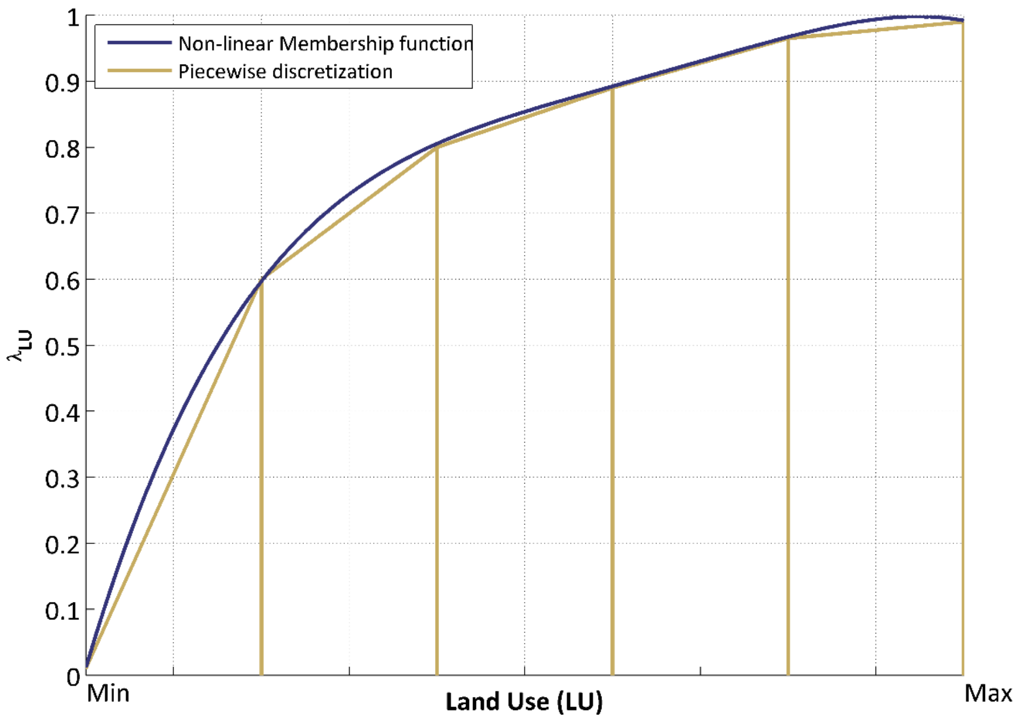

Fig. 4.8. LU representation using our cause-effect approach (Blue line) and the fixed piecewise discretization used (gold line).

Thus, using the LU exponential function, two particular situations can be defined and compared afterward. First, the single non-linear membership function situation (SNLMF), when a sigmoidal behavior for *WC* was assumed (the one explained in previous subsections). For the second case, the exponential membership function for *LU* was considered in addition to the sigmoidal one (defined as double non-linear membership function situation (DNLMF)). After solving model *M2* for the DNLMF case, the resulting objective values are displayed in Table 4.1, together with the ones from the SNLMF solution.

Table 4.1. Results for single and double non-linear membership function cases.

	Fuzzy-Based Optimization			
	SNLMF	Performance	DNLMF	Performance
Profit	0.862	$225.51\text{x}10^{6\,a}$	0.846	$221.51\text{x}10^{6\,a}$
WC	0.873	$491.44\text{x}10^{6\,b}$	0.702	$525.34\text{x}10^{6\,b}$
LU	0.618	$2.00\ \text{x}10^{6\,c}$	0.736	$1.00\ \text{x}10^{6\,c}$

[a] Values expressed in \$; [b] Values expressed in m^3; [c] Values expressed in m^2

From Table 4.1, it is evident that the definition of the membership function has a significant effect on the final solution. The position of solutions for SNLMF and DNLMF within the Pareto set is represented in Fig. 4.9. By comparing these points, it can be concluded that the optimal solution moves mainly along the *LU* axis. In fact, the *LU* performance improves significantly when compared with the SNLMF case (improvement of 11.8%) at the expense of reducing the *Profit* and *WC* performances (about 0.2 and 17%, respectively). The above proves that the fuzzy-based strategy is sensitive enough to account for different nonlinear cause-effect membership functions, which represents a feasible option to aid decision-support tasks.

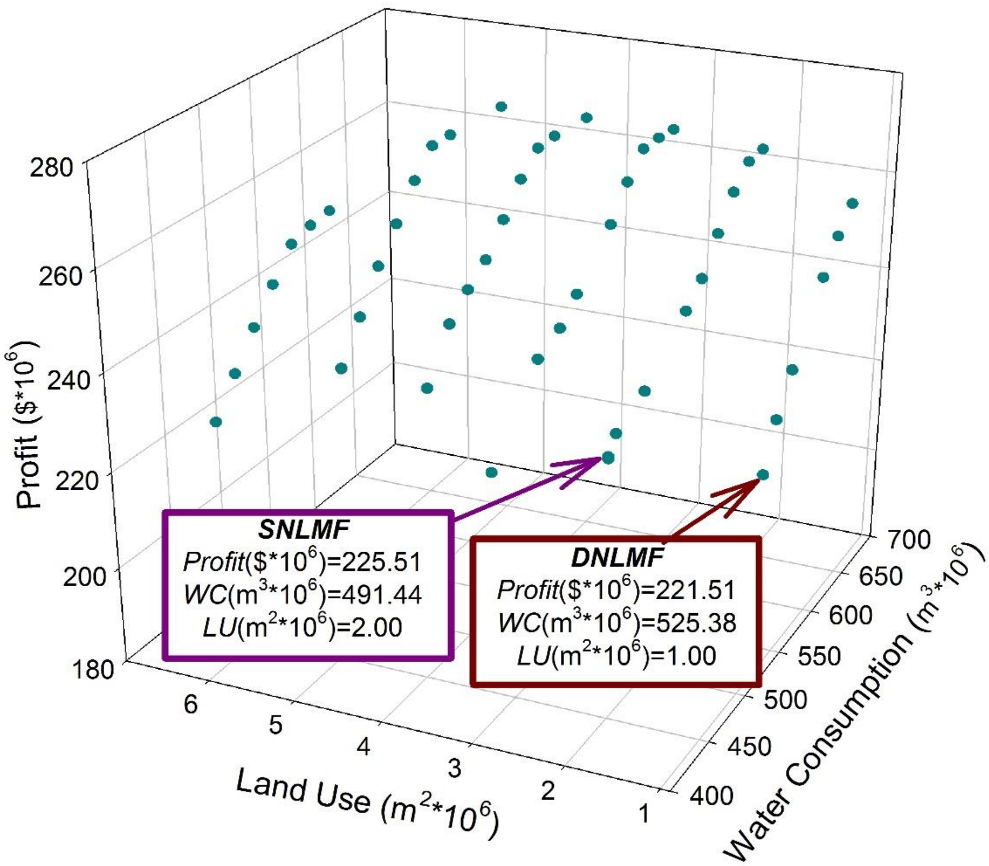

Fig. 4.9. LU representation using our cause-effect approach (Blue line) and the fixed piecewise discretization used (gold line).

Similarly to the use different non-linear membership functions, other factors may also affect the final result while using fuzzy-based approach, such as the decision maker preferences as evaluated next.

4.5.5. Effect of different objective preferences.

Alike in the previous subsection, here, two different cases were defined in which different weighting values were assumed for the economic objective, in order to promote the evaluation and discussion of the approach sensitivity. The preferences are considered by introducing a coefficient for each objective (WF_{ob}) into the model *M2* leading to the following model (*M3)*.

$$(M3) \qquad Max\ OB = \sum_{ob} \Big(\big(WF_1 * \lambda_1(x_1)\big), \big(WF_2 * \lambda_2(x_2)\big), \dots, WF_{ob} * \lambda_{ob}(x_{ob}) \Big)$$

Table 4.2 displays these values. For the first case, the economic performance was assumed twice important than the rest of them, while for the other case *Profit* is half as important as the other objectives. The performance for each objective is obtained by solving model *(M3)* and is presented in Table 4.2.

Table 4.2. Decision maker preferences for each objective.

	First case		Second case		Reference	Fuzzy (Original)
	Weight	*Performance*	*Weight*	*Performance*	*Performance*	*Performance*
Profit	2	$220.39x10^{6a}$	0.5	$222.35x10^{6a}$	$270.24x10^{6a}$	$225.52x10^{6a}$
WC	1	$529.06x10^{6b}$	1	$522.76x10^{6b}$	$661.48x10^{6b}$	$491.48x10^{6b}$
LU	1	$0.906\ x10^{6c}$	1	$0.997\ x10^{6c}$	$4.766\ x10^{6c}$	$2.382\ x10^{6c}$

[a]Values expressed in \$; [b]Values expressed in m^3; [c]Values expressed in m^2

Numerical results in Table 4.2 confirm that the preference for each value significantly conditions the final solution obtained.

4.6. Concluding remarks

A fuzzy-based formulation addressing the water management in urban areas was presented, whose main novelty is the incorporation of the water stress index as cause-effect oriented objective and the use of the fuzzy theory to simplify the post-optimal analysis of the Pareto set of solutions.

The capabilities of the proposed approach were illustrated through the design and planning of a real water management system in an urban area (city of Morelia in Mexico). The case study accounts for rainwater harvesting and regenerated wastewater as alternative water sources for satisfying water demands (at industrial, domestic, and agriculture sectors).

Numerical results show that the final design reduces natural freshwater consumption by installing storage devices and using alternative water sources. Altogether, the proposed tool identifies solutions entailing savings of up to 13% and 38% in water consumption and land use, reinforcing the idea that water reclamation and harvested rainwater are promising and feasible options to reduce the use of freshwater in agricultural activities, even during drought seasons.

The successful application of this tool to urban water management can open up applications to other industrial problems where sustainability criteria need to be accounted during the analysis. Nevertheless, these results also prove that this method completely skips the consideration of decision-maker preferences. Consequently, additional contributions are needed addressing/proposing an efficient integrated approach capable of identifying a unique and representative solution explicitly considering the decision maker interests.

4.7. Nomenclature

Abbreviations

MOO	Multi-objective optimization
SC	Supply chain
MO	Multi-Objective
MINLP	Mixed integer non-linear programming
PSE	Process system engineering
SO	Single-Objective
SOO	Single-Objective Optimization
WSI	Water Stress Index
AHP	Analytical hierarchical processes
ELECTRE	ELimination Et Choix Traduisant la REalité (ELimination and Choice Expressing Reality)

SNLMF	Single non-linear membership function
DNLMF	Double non-linear membership function

Index

b	Set for location of industrial storage tanks $(b\|b=1,\dots,B)$
h	Set for agricultural sinks $(h\|h=1,\dots,H)$
j	Set for domestic sinks $(j\|j=1,\dots,J)$
k	Set for natural sources $(k\|k=1,\dots,K)$
l	Set for location of storage tanks $(l\|l=1,\dots,L)$
m	Set for tributaries $(m\|m=1,\dots,M)$
n	Set for location of artificial ponds $(n\|n=1,\dots,N)$
t	Set for time periods $(t\|t=1,\dots,T)$
u	Set for industrial sinks $(u\|u=1,\dots,U)$
w	Set for location of industrial artificial ponds $(w\|w=1,\dots,W)$
ob	Set for objectives $(ob\|ob=1,\dots,OB)$

Parameters

A_n^a	Collection area in location *n* for artificial ponds a
A_n^{max}	Maximum capacity of artificial ponds *a* in location *n*
A_l^s	Collection area in location *l* for storage tanks *s*
A_k^{ROW}	Area of collection for runoff water for natural source *k*
A_k^{DPW}	Area of collection for direct precipitation for natural source *k*
AI_w^{max}	Maximum capacity of industrial artificial ponds AI in location *w*
ASC	Cost of water for agricultural use
ATN_n	Depth of artificial ponds in location *n*
ATS_l	Height of storage in location *l*
$CTAA$	Treatment cost for rainwater for agricultural use
$CTAI$	Treatment cost for rainwater for industrial use
$CTFP$	Treatment cost for water purchased with domestic use
$CTND$	Treatment cost for natural sources with domestic use
$CTNA$	Treatment cost for natural sources with agricultural use
$CTNI$	Treatment cost for natural sources with industrial use
$CTAD$	Treatment cost for rainwater for domestic use
$CTPA$	Treatment cost for regeneration of wastewater for agricultural use
$CTPE$	Treatment cost for regeneration of wastewater for final disposal
$CTRP$	Treatment cost for water purchased with agricultural use
$CTQP$	Treatment cost for eater purchased with industrial use
$D_{h,t}^{as}$	Agricultural users *h* demands in time *t*
$D_{u,t}^{di}$	Industrial users *u* demands in time *t*
$D_{j,t}^{ds}$	Domestic users *j* demands in time *t*
$DPWV_{k,t}$	Water collected from direct precipitation in natural sources *k* in time *t*
DSC	Water sale cost for domestic use
ISC	Cost of water for industrial use
$K_{F\,l,t}$	Factor to take into account the annualized investment for storage tanks in location *l* in time *t*
$K_{F\,n,t}$	Factor to take into account the annualized investment for artificial ponds in location *n* in time *t*
$ML_{l,t}$	Large number with allow to constraint the volume for storage tanks in location *l* in time *t*
$MN_{n,t}$	Large number to constraint the volume of artificial ponds in location *n* and time *t*
P_t	Precipitation over time period *t*
P^{total}	Annual precipitation

$PCSTD$	Unit cost of transport from storage tank *l* to domestic sink *j*
$PCASD$	Unit cost of pumping from artificial pond *n* to domestic sink *j*
$PCSTA$	Unit cost of pipeline and pumping from storage tank in location *l* to agricultural sink *h*
$PCASA$	Unit cost of transport water from artificial pond in location *n* to agricultural sink *h*
$PCSTI$	Unit cost of transport water from industrial storage tank in location *b* to industrial sink *h*
$PCASI$	Unit cost of transport water from industrial artificial ponds in location *w* to industrial sink *u*
$PCND$	Unit costs for transport from natural sources *k* to domestic main
$PCNA$	Unit costs for transportation of water from natural sources *k* to agricultural main
$PCNI$	Unit cost of water transportation from natural sources *k* to industrial main
$PCTW$	Unit water transportation cost from treatment plant to agricultural sink *h*
$PCTI$	Unit water transportation cost from industrial treatment plant to agricultural sink *h*
PFP	Unit water transportation cost from external water vendor to domestic users *j*
PQP	Unit water transportation cost from external water vendor to industrial users *u*
PRP	Unit water transportation cost from external water vendor to agricultural users *h*
PSC	Water sale cost for water purchased sent to users
$p_{k,t}^{g}$	Water collected from direct precipitation and runoff water in sources *k* at time *t*
$r_{m,k,t}$	Segregated flow rate from the tributaries *m* to natural sources *k* over time period *t*
$ROWV_{k,t}$	Runoff water collection in natural sources *k* over time period *t*
S_{l}^{max}	Maximum capacity of storage tanks *s* in location *l*
SI_{b}^{max}	Maximum capacity of industrial storage tanks *si* in location *b*
$VP_{l,t}$	Factor to consider the value of investment for storage tank in location *l* and time *t*
$VP_{n,t}$	Factor to consider the value of investment for artificial ponds in location *n* and time *t*
$\bar{b}_{ob}$	Upper bound for objective *ob*
$\underline{b}_{ob}$	Lower bound for objective *ob*
A	Fixed cost for storage tank
B	Variable cost for storage tank
C	Fixed cost for artificial ponds
D	Variable cost for artificial ponds
WF_{ob}	Weighting criteria for each objective.

Variables

$A_{n,t}$	Existing water in artificial ponds *a* in location *n* at time *t*
$A_{n,t-1}$	Existing water in artificial ponds *a* in location *n* in previous time period *t-1*
$a_{n,t}^{in}$	Water obtained from rainfall sent to artificial ponds *a* in location *n* and time *t*
$a_{n,j,t}^{out,d}$	Segregated flow rate from artificial ponds *a* in location *n* sent to domestic users *j* in time *t*
$a_{n,h,t}^{out,a}$	Segregated flow rate from artificial ponds *a* in location *n* to agricultural users *h* in time *t*
$AI_{w,t}$	Existing water in industrial artificial ponds *ai* in location *w* and time *t*
$AI_{w,t-1}$	Existing water in artificial ponds *ai* in location *w* in previous time *t-1*

$ai_{w,t}^{in}$	Water obtained from rainfall sent to artificial industrial ponds *ai* in location *w* and time *t*
$ai_{w,u,t}^{out,i}$	Segregated flow rate from industrial artificial ponds *ai* in location *w* sent to industrial users *u* at time *t*
APA_n	Total area occupied by artificial ponds in industrial location *n*
API_w	Total area occupied by artificial industrial ponds in location *w*
ARI_n	Area occupied by the artificial ponds in location *n*
ARI_w	Area occupied by the artificial industrial ponds in location *w*
ARS_l	Area occupied by the storage tank in location *l*
$ARSI_b$	Area occupied by the industrial storage tanks in location *b*
C_e	Runoff coefficient
$Cost_n^a$	Cost of artificial ponds *a* in location *n*
$Cost_w^{ai}$	Cost of industrial artificial ponds *ai* in location *w*
$Cost_l^s$	Cost of storage tank *s* in location *l*
$Cost_b^{si}$	Cost of industrial storage tank *si* in location *b*
$cw_{j,t}^d$	Water consumed and losses in domestic sinks *j* in time *t*
$cw_{u,t}^{di}$	Water consumed and losses in industrial sink *u* in time *t*
cw_t^{tp}	Water reclaimed in domestic treatment plant and sent to final disposal in time *t*
cwi_t^{tp}	Water reclaimed in industrial plant and sent to final disposal in time *t*
$Drop_{k,t}^g$	Water that exceeds the maximum capacity of natural sources *k* in time *t*
$f_{j,t}$	Segregated flow rate sent from the domestic main to the domestic users *j* in time *t*
fob_{ob}	Objective function.
$fpch_{j,t}$	Segregated flow rate of water purchased sent to domestic users *j* in time *t*
$G_{k,t}$	Existing water in natural sources *k* in time *t*
$G_{k,t-1}$	Existing water in natural sources *k* in time *t*-1
$g_{k,t}^a$	Segregated flow rate from the natural sources *k* to main agricultural *a* in time *t*
$g_{k,t}^d$	Segregated flow rate from the natural source *k* to main domestic *d* in time *t*
$g_{k,t}^i$	Segregated flow rate from the natural source *k* to main industrial *i* in time *t*
$int_{j,t}^{in}$	Wastewater sent from site *j* to treatment plant in time *t*
$inti_{u,t}^{in}$	Wastewater sent from site *u* to treatment plant in time *t*
int_t^{out}	Wastewater sent to treatment plant in time *t*
$int_{h,t}^{out,ag}$	Water reclaimed in industrial treatment plant and sent to agricultural sinks *h* in time t
$inti_{h,t}^{out,i}$	Water reclaimed in industrial treatment plant and sent to agricultural sink *h* in time *t*
$q_{u,t}$	Segregated flow rate sent from the industrial main to the industrial users *u* in time *t*
$qpch_{u,t}$	Segregated flow rate of water purchased sent to industrial users *u* in time *t*
$r_{h,t}$	Segregated flow rate sent from the agricultural main to the agricultural users *h* in time t
$rpch_{h,t}$	Segregated flow rate of water purchased sent to agricultural users *h* in time *t*
$S_{l,t}$	Existing water in storage tanks *s* in location *l* in time *t*
$S_{l,t-1}$	Existing water in storage tanks *s* in location *l* in time *t*-1
$s_{l,t}^{in}$	Water obtained from rainfall sent to storage tanks *s* in location *l* in time *t*
$si_{b,t}^{in}$	Water obtained from rainfall sent to industrial storage tanks *si* in location *b* and time *t*
$s_{l,h,t}^{out,a}$	Segregated flow rate from storage tanks *s* in location *l* sent to agricultural users *h* in time *t*
$s_{l,j,t}^{out,d}$	Segregated flow rate from storage tanks *s* in location *l* sent to domestic users *j* in time *t*

$SI_{b,t}$	Existing water in industrial storage tanks SI in location b in time *t-1*
$SI_{b,t-1}$	Existing water in industrial storage tanks SI in location *b* in time *t-1*
$si_{b,u,t}^{out,i}$	Segregated flow rate from industrial storage tanks *si* in location *b* sent to industrial users *u* in time *t*
$v_{n,t}^{a}$	Water losses in artificial ponds *a* in time *t*
$v_{w,t}^{ai}$	Water losses in artificial industrial ponds *ai* in time *t*
$v_{k,t}^{g}$	Water losses in natural sources *k* in time *t*
$v_{l,t}^{s}$	Water losses in storage tanks *s* in time t
$v_{b,t}^{si}$	Water losses in industrial storage tanks *si* in time *t*
WTA_{k}	Ratio of water usage at reservoir *k*
WA_{k}	Water available at reservoir *k*
$WC_{u,k}$	Water consumption at repository *k* for industrial sites *u*
$WC_{h,k}$	Water consumption at repository *k* for agricultural sites *h*
$WC_{j,k}$	Water consumption at repository *k* for domestic sites *j*
$WA_{k,t}$	Water available at reservoir *k* for time *t*
$WC_{u,k,t}$	Water consumption at repository *k* for industrial sites *u* and time *t*
$WC_{h,k,t}$	Water consumption at repository *k* for agricultural site *h* and time *t*
$WC_{j,k,t}$	Water consumption at repository *k* for domestic site *j* and time *t*
x_{ob}	Best possible value for each objective *ob*
λ_{ob}	Performance degree of optimal value for objective *ob*
$Zag_{l,t}^{s}$	Variable for installing storage tanks in location *l* in time *t*
$Zag_{n,t}^{a}$	Variable for installing artificial ponds in location *n* at time *t*
$WaterSales$	Total profit from water sales
$TreatmentCosts$	Total cost associated to treatment processes
$PipingCost$	Total cost associated to piping of water
$StorageCost$	Total cost for water storage tasks
$NaturalFlowrate_{k}^{d}$	Inlet flow rate of freshwater to domestic site
$NaturalFlowrate_{k}^{a}$	Inlet flow rate of freshwater to agricultural site
$NaturalFlowrate_{k}^{i}$	Inlet flow of freshwater to industrial site
$WaterPurchased_{j}$	Purchased amount of freshwater for domestic site
$WaterPurchased_{h}$	Purchased amount of freshwater for agricultural site
$WaterPurchased_{u}$	Purchased amount of freshwater for industrial site.

Binary Variables

$z_{n,t}^{a}$	Variable to select the installation of artificial ponds *a* in location *n* at time *t*
$z_{w,t}^{ai}$	Variable to select the installation of artificial industrial ponds *ai* in location *w* in time *t*
$z_{l,t}^{s}$	Variable for installing storage tanks *s* in location *l* at time *t*
$z_{b,t}^{si}$	Variable for installing industrial storage tanks *si* in location *b* in time *t*

Chapter 5

Comparing and Extending Multi-Criteria decision-making strategies

The increasing pressure on design and planning green processes promoting the best possible economic performance force companies to make an efficient and detailed analysis prior to taking any decision. As proved in the previous Chapter, traditional decision-support approaches, such as Fuzzy ones have been proved effective for this purpose; however, they consider one objective as the most important one while neglecting the effect of the additional criteria's. Such a limitation, hinders the application of traditional approaches for systems in which multiple actors are involved in the decision making process. Thus, besides the management of the technical difficulties associated with a SC design/planning optimization, this Chapter addresses the advantages and disadvantages of two decision-support strategies under cooperative and competitive market schemes (i.e. centralized and decentralized respectively).

5.1.Challenges in Decision-support frameworks

Along with the management of water resources discussed in the previous chapter, the integrated management of water networks merged into energy production process is also a key challenge for the process sustainability *(Matson, 2001)*. As commented before, MOO approaches are necessary for any solution framework addressing sustainability problems due to its capacity to evaluate simultaneously multiple objectives of different nature *(You et al., 2012)*. These frameworks commonly use the ε-constraint method as a first step to build the Pareto frontier while further steps perform a selection/identification of the best option within these points. Even if MOO approaches have been extensively studied, both, the definition of an adequate number of objectives and the absence of a systematic identification procedure remains as open issues. In order to address them while assisting the decision-making task, the fractional formulation and ELECTRE-IV method have been used as advanced MO optimization alternatives. Details regarding these techniques can be found in Chapter 3.

Notwithstanding the huge number of MOO studies, most of them have been applied to the management of problems under cooperative stakeholder's environment (i.e. centralized scheme). For example, the Fuzzy approach presented in the previous Chapter fails to produce a well-balanced solution when each participant has the freelance take its own decisions based on their individual interests, due to the lack of information available to represent such a behavior. Thus, in order to strictly consider a freelance attitude of each participant (i.e. non-cooperative problem); a leader-follower relationship was modeled through a bi-level formulation leading to the so-called Stackelberg game *(Bard, 1998; Dempe, 2002)*. In such a mathematical representation, the data used to represent the lower-level part of the problem conditions the upper-level performance, ultimately, compromising the global optimality of the resulting solution *(Sinha et al., 2018)*. Thus, integrated optimization frameworks combining MO and MCDM appear as a promising alternative to approach the solution of this kind of problems *(Kumar et al., 2017)*. These frameworks should be able to produce a set of feasible solutions and identify the best one considering simultaneously the individual objectives of each entity/participant in a time-effective way.

Therefore, in this Chapter a detailed comparison regarding the advantages and limitations of different decision-making frameworks was performed. In particular, both, a mathematical programming strategy based on the fractional formulation and the ELECTRE-IV method (as a post-optimization approach) were compared. To stress the methods differences and discuss them, two different real-life process and business environments were assumed (cooperation and competition). Finally, to promote a useful comparison, a case study based on a shale gas SC design and planning problem was used for both strategies. A brief background de on this kind of problems is next provided.

5.2. Motivating example: Water management for shale gas exploitation.

The search for natural gas alternatives has been promoted by the increasing energy demand. In this line, the shale gas production processes have caught the attention of both industry and academia. Shale gas is typically embedded in shale rocks, which must be fractured to extract enough gas for commercial purposes. Hydraulic fracturing is the most commonly used technique in which a fluid (a solution of almost 95% water) at high pressure is pumped into the wellbore *(Yang et al., 2014)*. Based on historical data, it is estimated that, each year, the shale gas extraction requires between 12 and 20 million gallons of freshwater per wellbore *(Jiang et al., 2014)*, from which, 0.5 to 5 million returns to the surface as highly contaminated wastewater *(Rahm and Riha, 2012)*. Even if at a first sight, the above may seems as a small amount (Less than 1% of any small reservoir which is around 1.5 billion gallons); each shale gas plant has at least 10 wellbores leading to major water preservation issue. Currently only the U.S. and Canada exploit the shale gas production; however, it is expected that in the coming years such an industry increase exponentially, particularly in these countries with highest repositories (Countries such as China, Argentina, Algeria, and México) *(Gao and You, 2017)*. Apart from the geographic issues (i.e. availability and recoverability challenges) there are three additional factors explaining the low use of shale gas production processes:

- (i) Low economic efficiency (due to the low prices of natural gas and fossil fuels) *(Cafaro and Grossmann, 2014; Drouven and Grossmann, 2016)*,
- (ii) High environmental impact (due to the high water consumption) and
- (iii) The presence of multiple uncertainty sources (i.e. wastewater quality) *(Gao and You, 2017)*.

A recent study on shale gas processes *(Gao et al., 2017)* stress the multiple strategies used to optimize its design and operations in a sustainable way. These environmentally friendly designs take into account the quality of both, wastewater and recovered wastewater streams, and use this information to promote reuse/recycle activities. Fig 5.1 illustrates a global water network associated to a Shale gas plant. Nevertheless, the combination of environmental and economic objectives has been inefficiently applied for this kind of problems, compromising the solution reliability. In order to achieve an accurate representation, the explicit satisfaction of multiple decision criteria, as well as non-linear behaviors (i.e. wastewater treatment efficiencies and operational costs), in a single solution is required. Therefore, robust MOO tools applicable to flexible water systems integrated with other industrial processes (e.g. energy-production) are needed and, in fact, PSE community is particularly well positioned to deal with such challenges.

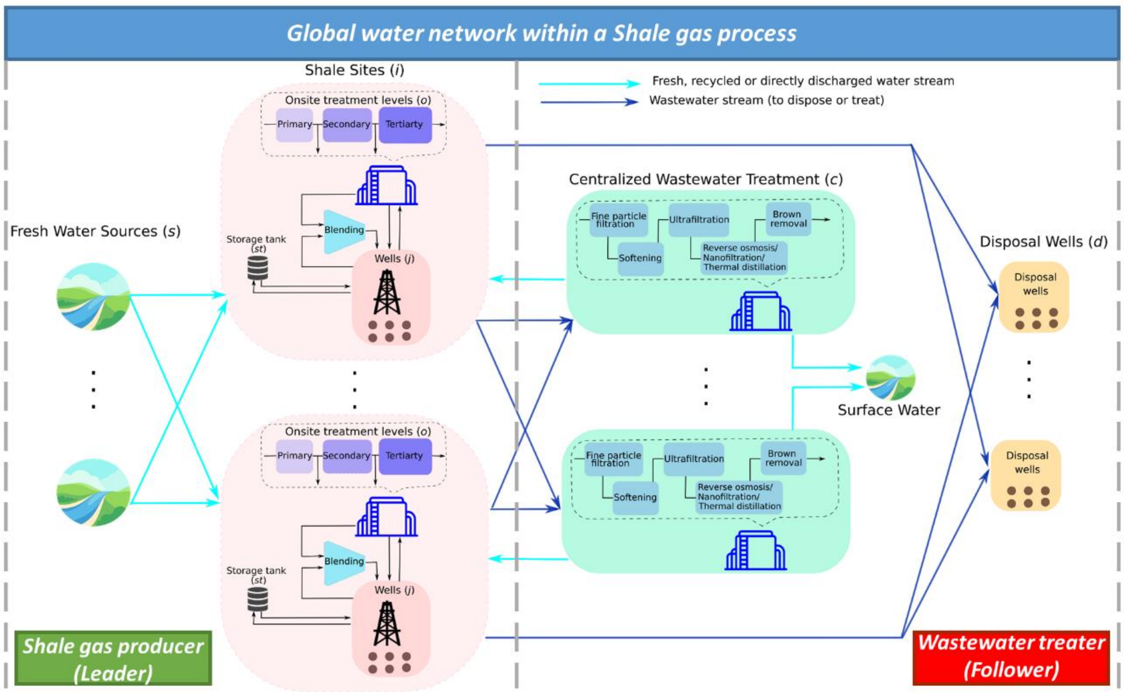

Fig. 5.1. Water network associated to a Shale gas process.

5.3. Problem statement

The network associated to a water supplier-consumer SC is considered, based on the generalization of the system illustrated in Fig. 5.1. It includes a set of freshwater sources $s \in S$ from which supplier s can satisfy the freshwater requirements of consumer sites $i \in I$ in which a set of specific consumption points can be chosen $j \in J$. The wastewater produced can be treated either in centralized wastewater treatment facilities (CWT; $c \in C$), disposal wells ($d \in D$) or onsite treatment plants. Notice that each onsite treatment plant consist on a set of treatment levels ($o \in O$) in order to satisfy the output water quality. The water flows are managed through different transportation modes ($m \in M$). The use and allocation of wastewater storage tanks ($st \in ST$) is assumed as feasible before any treatment process for reuse and/or mixing purposes. A defined set of capacities for the onsite treatment plant and transportation modes ($q \in Q$ and $r \in R$, respectively) are used. It is considered that recovered wastewater partially satisfy the site demands (Dem_{ij}). Notice that Fig. 5.1 actually represents a two “players” decentralized scheme in which the water consumer is defined as a leader while the wastewater treatment plant belongs to the follower. However, in essence, the same SC configuration can be used for centralized and decentralized approaches.

Disregarding the specific approach to be used, the following assumptions have been considered for this problem:

- Profit from water consumer production is considered as a known parameter in accordance with the work of *(Yang et al., 2014)*.
- All the investment decisions are made at the beginning of the project.
- The freshwater has the same composition disregarding the water sources.
- There are no time delays due to operational tasks.

Similarly, the information regarding freshwater availability and cost at each source, water requirements and wastewater production profile, unit operating cost, capacity, reused water recovery factor at each treating facility, capital investment and unit operating cost for each transportation mode is assumed to be known beforehand.

The main purpose is to optimize the design and planning of the water network within the water consumer (e.g.: shale gas) production network, considering three main objectives functions: net present profit, freshwater consumption, and their economic ratio. Such an optimization promotes a balanced solution between cost-effectiveness and freshwater conservancy; however, a further and deeper analysis will be performed evaluating these objectives together with a set of additional performance indicators (such as installing, handling and operating costs). Finally, the results comparison is given in Section 5.

5.4.Mathematical formulation

The mathematical model representing the water production, consumption, treatment, and disposal networks was inspired in the one reported by *Gao and You, (2015)*. The main difference in this model is the specific consideration of the non-linear effect of the pollution level of the wastewater flows over the final treatment cost and process efficiencies. Nevertheless for continuity purposes, the mass and energy balances are presented.

5.4.1. Mass and energy balances

The total water requirements are satisfied using either freshwater and/or reused water from treatment sites (onsite and CWT) as displayed in Eq. (5.1)

$$\sum_{s\epsilon S}\sum_{m\epsilon M} fw_{s,i,m,t} + \sum_{c\epsilon C}\sum_{m\epsilon M} wtcr_{i,c,m,t} + \sum_{o\epsilon O} LO_o \cdot wto_{i,l,o,t} = \sum_{j\epsilon J} RW_{i,j,t} \qquad \forall i,t \qquad (5.1)$$

The total freshwater acquired from sources s and distributed to consumption site i at time period t is calculated in the first term ($fw_{s,i,m,t}$). Particularly, the recycled water sent from CWT facilities to consumption site i at period t is represented by $wtcr_{i,c,m,t}$, while the one treated onsite correspond to $wto_{i,l,o,t}$ which is the third factor in the left-hand side of Eq. (5.1). Remarkably, regenerated water coming from CWT already accounts for an efficiency value, while onsite treatment plants employ a recovery factor for each level o (LO_o). Finally, the right-hand side of the equation describes the water demand for consumption at site i at period t ($RW_{i,j,t}$).

Eq. (5.2) calculates the total wastewater generated by summing the one coming from the consumption points at time t and the one stored in previous periods. In order to maintain the conservation law, this value should be equal to the total water sent to the different water treatment/disposal options (CWT, disposal, onsite treatment, and storage).

$$\sum_{j\epsilon J} WP_{i,j,t} + ws_{i,t-1} = \sum_{c\epsilon C}\sum_{m\epsilon M} wtc_{i,c,m,t} + \sum_{d\epsilon D}\sum_{m\epsilon M} wtd_{i,d,m,t} + \sum_{o\epsilon O} wto_{i,o,t} + ws_{i,t} \qquad \forall i,t \qquad (5.2)$$

Particularly, $WP_{i,j,t}$ denotes the amount of wastewater generated at site i and period t with a TDS concentration ranging between defined values according to the case study. $wtc_{i,c,m,t}$, $wtd_{i,d,m,t}$ and $wto_{i,o,t}$ represents the amount of wastewater transported by mean m to water management facility c, d or o (CWT, disposal and onsite treatment respectively) at time period t. Finally, $ws_{i,t}$ denotes the amount water stored at site i at period t.

Here, it is assumed that CWT facilities the management of treated water either disposing it directly to surface water bodies or recycling it to consumer sites for reuse as described in Eq. (5.3).

$$\sum_{i\epsilon I}\sum_{m\epsilon M} LC_{i,t} \cdot wtc_{i,c,m,t} = wtcd_{c,t}\sum_{i\epsilon I}\sum_{m\epsilon M} wtcr_{i,c,m,t} \qquad \forall c,t \qquad (5.3)$$

Here, the recovery efficiency for the CWT facility was described as ($LC_{i,t}$) while $wtcd_{c,t}$ calculates the amount of treated water at CWT facility c disposed directly to the surface. The total freshwater supply should be lower or equal to the water availability on freshwater sources as described in Eq. (5.4), where, $FR_{s,t}$, accounts for the freshwater availability.

$$\sum_{i\epsilon I}\sum_{m\epsilon M} fw_{s,i,m,t} \leq FR_{s,t} \qquad \forall s,t \qquad (5.4)$$

The freshwater distribution should be lower or equal than the total capacity of transportation mode m ($tsc_{s,i,m,r}$) as described in Eq. (5.5).

$$fw_{s,i,m,t} \leq \sum_{r\epsilon R} tsc_{s,i,m,r} \qquad \forall s,i,m,t \qquad (5.5)$$

Similarly, Eq. (5.6) and (5.7) quantifies the amount of wastewater transported from site i to the different wastewater management facilities c and d (CWT and disposal respectively) constrained by the total capacity of transportation mode m. Such a capacity is represented by $tcc_{i,c,m,r}$ and $tdc_{i,d,m,r}$ for CWT and disposal respectively.

$$wtc_{i,c,m,t} \leq \sum_{r\epsilon R} tcc_{i,c,m,r} \qquad \forall i,c,m,t \qquad (5.6)$$

$$wtd_{i,d,m,t} \leq \sum_{r\epsilon R} tdc_{i,d,m,r} \qquad \forall i,d,m,t \qquad (5.7)$$

Additionally to the transportation capacities, the total amount of wastewater treated or disposed at each CWT or disposal facility cannot exceed its capacity ($WC_{c,t}$ and $WD_{d,t}$, respectively) as shows in Eqs. (5.8) and (5.9).

$$\sum_{i\epsilon I}\sum_{m\epsilon M} wtc_{i,c,m,t} \leq WC_{c,t} \qquad \forall c,t \qquad (5.8)$$

$$\sum_{i\epsilon I}\sum_{m\epsilon M} wtd_{i,d,m,t} \leq WD_{d,t} \qquad \forall c,t \qquad (5.9)$$

Similarly, the amount of water treated onsite is bounded by the capacities of onsite treatment facilities where $oc_{i,o,q}$ denotes the capacity of level o with capacity range q for treating wastewater at site i.

$$wto_{i,o,t} \leq \sum_{q \epsilon Q} oc_{i,o,q} \qquad \forall i, l, t \quad o \epsilon O \qquad (5.10)$$

Notice that, $o \epsilon O$ is a subset of onsite treatments that are capable of treating wastewater at defined TDS concentration ranges. The identification of the most promising distribution links are formulated using binary variables and considering the associated bounding constraints. For example, if transportation mode m is installed between freshwater source s to site i, its freshwater transportation amount cannot exceed the availability of corresponding freshwater source ($FR_{s,t}$); otherwise, the transportation amount should be zero (Eq. (5.11)). Notice that the capacity of each transportation mode is predefined using a set of nominal capacity ranges r.

$$fw_{s,i,m,t} \leq \sum_{r \epsilon R} xs_{s,i,m,r} \cdot FR_{s,t} \qquad \forall s, i, m, t \qquad (5.11)$$

The binary variable $xs_{s,i,m,r}$ determines the installation (or not) of transportation mode m between water source s and site i. If $xs_{s,i,m,r} = 1$, transportation mode m with capacity range r is installed between water source s and site i; otherwise not installed.

The same logic is applied to connect site i and CWT and disposal facilities as shown in Eqs. (5.12) and (5.13) respectively.

$$wtc_{i,c,m,t} \leq \sum_{r \epsilon R} xc_{i,c,m,r} \cdot WC_{c,t} \qquad \forall i, c, m, t \qquad (5.12)$$

$$wtd_{i,d,m,t} \leq \sum_{r \epsilon R} xd_{i,d,m,r} \cdot WD_{d,t} \qquad \forall i, d, m, t \qquad (5.13)$$

The nominal capacities are used to limit the operation of the transportation modes as described in the following equation.

$$MS_{s,i,m,r-1} \cdot xs_{s,i,m,r} \leq tsc_{s,i,m,r} \leq MS_{s,i,m,r} \cdot xs_{s,i,m,r} \qquad \forall s, i, m, r \qquad (5.14)$$

From there, $MS_{s,i,m,r}$ represents the maximum capacity of transportation mode m with capacity range r from source s to site i. We have similar constraints for the capacity of transportation mode m from site i to CWT and Disposal wastewater management facilities, given by

$$MC_{i,c,m,r-1} \cdot xc_{i,c,m,r} \leq tcc_{i,c,m,r} \leq MC_{i,c,m,r} \cdot xc_{i,c,m,r} \qquad \forall i, c, m, r \qquad (5.15)$$

$$MD_{i,d,m,r-1} \cdot xd_{i,d,m,r} \leq tdc_{i,d,m,r} \leq MD_{i,d,m,r} \cdot xd_{i,d,m,r} \qquad \forall i, d, m, r \qquad (5.16)$$

The installation (or not) of onsite treatment plants are also bounded by the corresponding capacity range as described by the following inequality.

$$WO_{i,o,q-1} \cdot y_{i,o,q} \leq oc_{i,o,q} \leq WO_{i,o,q} \cdot y_{i,o,q} \qquad \forall i, o, q \qquad (5.17)$$

Here, $y_{i,o,q}$ is the binary variable that determines the installation of onsite treatment facilities. Notice that, only one capacity range is allowed for transportation mode m at each transportation link.

$$\sum_{r\epsilon R} xs_{s,i,m,r} \leq 1 \qquad \forall s,i,m \tag{5.18}$$

$$\sum_{r\epsilon R} xc_{i,c,m,r} \leq 1 \qquad \forall i,c,m \tag{5.19}$$

$$\sum_{r\epsilon R} xd_{i,d,m,r} \leq 1 \qquad \forall i,d,m \tag{5.20}$$

$$\sum_{q\epsilon Q} y_{i,o,q} \leq 1 \qquad \forall i,o \tag{5.21}$$

5.4.2. Economic constraints

The economic benefit associated with the production SC is described in Eq. (5.22).

$$NP = \sum_{i\epsilon I}\sum_{j\epsilon J}\sum_{t\epsilon T} \frac{SP_{i,t} \cdot WP_{i,j,t} \cdot CC_{i,j,t}}{(1+DR)^t} \tag{5.22}$$

NP stands for the total net present profit gained by production excluding the water management cost. $SP_{i,t}$ denotes the average revenue per unit of final product production at site i at period t while $WP_{i,j,t}$ represents the wastewater generation profile for consumer j at consumption site i and time period t. Finally, $CC_{i,j,t}$ is a coefficient that correlates the water and final product production profiles for consumer j at site i and *DR* is a commonly used discount rate per period.

The total cost in the water SC is described in Eq. (5.23). In particular, it is considered the total net present cost for freshwater acquisition (c_{water}), water/wastewater transportation ($c_{transport}$), and wastewater handling ($c_{handling}$).

$$cw = c_{water} + c_{transport} + c_{handling} \tag{5.23}$$

The detailed formulations of the individual terms are following described. Eq. (5.24) represents the total net present cost for freshwater acquisition in which WA_s denotes the unit freshwater acquisition cost from freshwater source s.

$$c_{water} = \sum_{s\epsilon S}\sum_{i\epsilon I}\sum_{m\epsilon M}\sum_{t\epsilon T} \frac{WA_s \cdot fw_{s,i,m,t}}{(1+DR)^t} \tag{5.24}$$

The total net present cost for water transportation is described by equations (5.25)–(5.31), representing the transportation cost between freshwater sources to production sites and from these sites to either CWT facilities or disposal wells. The general form for the total net present cost for water transportation is presented in Eq. (5.25).

$$\begin{aligned} c_{transport} = c_{trans-var}^{source} + c_{trans-cap}^{source} + c_{trans-var}^{cwt} \\ + c_{trans-cap}^{cwt} + c_{trans-var}^{disposal} + c_{trans-cap}^{disposal} \end{aligned} \tag{5.25}$$

From Eq. (5.25), $c_{trans-var}^{source}$ calculates the total variable freshwater transportation cost as described in Eq. (5.26), in which $TS_{s,i,m}$ represents the unit transportation cost of freshwater.

$$c_{trans-var}^{source} = \sum_{s\epsilon S}\sum_{i\epsilon I}\sum_{m\epsilon M}\sum_{t\epsilon T}\frac{TS_{s,i,m} \cdot fw_{s,i,m,t}}{(1+DR)^t} \tag{5.26}$$

The total investment required for freshwater transportation ($c_{trans-cap}^{source}$) follows a nonlinear behavior, thus, a piecewise formulation has been included in the cost function to provide an accurate approximation of the original nonlinear cost curve (Eq. (5.27)).

$$\begin{aligned} c_{trans-cap}^{source} = &\sum_{s\epsilon S}\sum_{i\epsilon I}\sum_{m\epsilon M}\sum_{r\epsilon R} FS_{s,i,m,r-1} \cdot xs_{s,i,m,r} \\ &+\sum_{s\epsilon S}\sum_{i\epsilon I}\sum_{m\epsilon M}\sum_{r\epsilon R}\left(tsc_{s,i,m,r} - MS_{s,i,m,r-1} \cdot xs_{s,i,m,r}\right) \\ &\cdot\left(\frac{FS_{s,i,m,r} - FS_{s,i,m,r-1}}{MS_{s,i,m,r} - MS_{s,i,m,r-1}}\right) \end{aligned} \tag{5.27}$$

Where, $FS_{s,i,m,r}$ is the reference capital investment for transportation mode m between the freshwater source and production site with capacity range r.

A similar structure than in Eq. (5.25) has been used for the case of wastewater transportation costs. In particular, Eq. (5.28) and (5.29) represents the transportation cost to CWT and disposal facilities respectively where $TC_{i,c,m}$ and $TD_{i,d,m}$ denotes the unitary cost of water transported using mode.

$$c_{trans-var}^{cwt} = \sum_{i\epsilon I}\sum_{c\epsilon C}\sum_{m\epsilon M}\sum_{t\epsilon T}\frac{TC_{i,c,m} \cdot \left(wtc_{i,c,m,t} + wtcr_{i,c,m,t}\right)}{(1+DR)^t} \tag{5.28}$$

$$c_{trans-var}^{disposal} = \sum_{i\epsilon I}\sum_{d\epsilon D}\sum_{m\epsilon M}\sum_{t\epsilon T}\frac{TD_{i,d,m} \cdot wtd_{i,d,m,t}}{(1+DR)^t} \tag{5.29}$$

The computation of the total capital cost required to distribute wastewater from and to water management facilities follows the same structure than Eq. (5.28). CWT facilities ($c_{trans-cap}^{cwt}$) are given by Eq. (5.30), while disposal wells total capital investment costs ($c_{trans-cap}^{disposal}$) are described through Eq. (5.31) where $FC_{i,c,m,r}$ and $FC_{i,d,m,r}$ denotes the reference capital investment respectively.

$$\begin{aligned} c_{trans-cap}^{cwt} = &\sum_{i\epsilon I}\sum_{c\epsilon C}\sum_{m\epsilon M}\sum_{r\epsilon R} FC_{i,c,m,r-1} \cdot xc_{i,c,m,r} \\ &+\sum_{i\epsilon I}\sum_{c\epsilon C}\sum_{m\epsilon M}\sum_{r\epsilon R}\left(tcc_{i,c,m,r} - MC_{i,c,m,r-1} \cdot xc_{i,c,m,r}\right) \\ &\cdot\left(\frac{FC_{i,c,m,r} - FC_{i,c,m,r-1}}{MC_{i,c,m,r} - MC_{i,c,m,r-1}}\right) \end{aligned} \tag{5.30}$$

$$\begin{aligned} c_{trans-cap}^{disposal} = &\sum_{i\epsilon I}\sum_{d\epsilon D}\sum_{m\epsilon M}\sum_{r\epsilon R} FD_{i,d,m,r-1} \cdot xd_{i,d,m,r} \\ &+\sum_{i\epsilon I}\sum_{d\epsilon D}\sum_{m\epsilon M}\sum_{r\epsilon R}\left(tdc_{i,d,m,r} - MD_{i,d,m,r-1} \cdot xd_{i,d,m,r}\right) \\ &\cdot\left(\frac{FD_{i,d,m,r} - FD_{i,d,m,r-1}}{MD_{i,d,m,r} - MD_{i,d,m,r-1}}\right) \end{aligned} \tag{5.31}$$

The total cost associated to wastewater management is modeled as the summation of both, capital and operating costs for onsite treatment, as well as operating costs for CWT, disposal wells, and onsite storage facilities (Eq. (5.32)).

$$c_{handling} = c_{onsitetreat}^{capital} + c_{onsitetreat}^{operating} + c_{cwt} + c_{disposal} \tag{5.32}$$

The onsite treatment total investment ($c_{onsitetreat}^{capital}$) is calculated using a piecewise linear interpolation formulation as shown in Eq. (5.33).

$$\begin{aligned} c_{onsitetreat}^{capital} = & \sum_{i \epsilon I} \sum_{o \epsilon O} \sum_{q \epsilon Q} FO_{i,o,q-1} \cdot y_{i,o,q} \\ & + \sum_{i \epsilon I} \sum_{o \epsilon O} \sum_{q \epsilon Q} \left(oc_{i,o,q} - WO_{i,o,q-1} \cdot y_{i,o,q} \right) \\ & \cdot \left(\frac{FO_{i,o,q} - FO_{i,o,q-1}}{WO_{i,o,q} - WO_{i,o,q-1}} \right) \end{aligned} \tag{5.33}$$

$FO_{i,o,q}$ denotes the reference capital investment for level o onsite treatment with capacity range q at production site i; $WO_{i,o,q}$ denotes maximum capacity for a level o in the onsite treatment facility with capacity range q at site i.

Operational cost for onsite treatment ($c_{onsitetreat}^{operating}$) is described in Eq.(5.34) where $VO_{i,o,t}$ is the unitary cost of treating wastewater treated by level o onsite treatment.

$$c_{onsitetreat}^{operating} = \sum_{i \epsilon I} \sum_{o \epsilon O} \sum_{t \epsilon T} \frac{VO_{i,o,t} \cdot wto_{i,o,t}}{(1 + DR)^t} \tag{5.34}$$

The total operational cost for CWT facilities (c_{cwt}) is described in Eq. (5.35) where $VC_{i,c,t}$ is the unitary cost of treating wastewater by CWT.

$$c_{cwt} = \sum_{i \epsilon I} \sum_{c \epsilon C} \sum_{m \epsilon M} \sum_{t \epsilon T} \frac{VC_{i,c,t} \cdot wtc_{i,c,m,t}}{(1 + DR)^t} \tag{35}$$

Similarly, the total cost of disposal wells ($c_{disposal}$) is calculated by Eq. (5.36) using the unitary cost for dispose of wastewater at a disposal well.

$$c_{disposal} = \sum_{i \epsilon I} \sum_{d \epsilon D} \sum_{m \epsilon M} \sum_{t \epsilon T} \frac{VD_{i,d,t} \cdot wtd_{i,d,m,t}}{(1 + DR)^t} \tag{5.36}$$

Finally, the freshwater mass balance is calculated in Eq. (5.37) in which the term nfw denotes the net freshwater consumption.

$$nfw = \sum_{s \epsilon S} \sum_{i \epsilon I} \sum_{m \epsilon M} \sum_{t \epsilon T} fw_{s,i,m,t} - \sum_{c \epsilon C} \sum_{t \epsilon T} wtcd_{c,t} \tag{5.37}$$

Note that the water treated by CWT facilities and discharge directly to surface is actually returning to the natural water cycle, and, therefore, does not contribute to freshwater consumption.

5.4.3. Objective functions

Multi-objective function.

The MO problem considered consists in the maximization of total profit while reducing the freshwater consumption for the water supply chain network (henceforth known as model *(MOP)*) as represented in the following objective function:

$$(MOP) \qquad \max \quad \{Profit; -nfw\}$$

$$s.t. \qquad Eqs.(5.1) - (5.37)$$

Where, $Profit$, represents the economic revenue of the process, while nfw accounts for the net freshwater consumption. It is important to comment that $Profit$ was calculated as $Profit = NP - cw$. NP denotes the profit of final product production excluding water management cost and cw denotes the total cost of the water network.

Fractional objective function.

In the case of the fractional approach, a single objective function that maximizes the profit per unit of freshwater consumption was formulated leading to a single objective mixed integer linear fractional programming (SO-MILFP) which will be known as model *(F)* for the entire chapter. The form of the model *(F)* is given by:

$$(F) \qquad \max \quad Frac = \frac{Profit}{nfw}$$

$$s.t. \qquad Eqs.(5.1) - (5.37)$$

Here, the $Profit$ and the *nfw* takes the same meaning that in the model *(MOP)*.

Non-cooperative objective function.

A non-cooperative objective assuming a decentralized scheme (see Fig. 5.1) was also considered seeking for the simultaneous maximization of the individual profit of at least two entities (one leader and one follower). Even if additional entities and/or objectives could be considered, this study limits its scope to an economic performance for each entity. To efficiently calculate these individual performances, the mathematical model should be extended to include a new subset that represents the SC members ($sc \in L$; $sc \in F$) as well as their respective constraints (Eqs. (5.38.)-(5.42)).

$$Profit_L = NP_{sc} - cw_{sc} \qquad \forall sc \in L \qquad (5.38)$$

$$Profit_F = Sales_{sc'} - cw_{sc'} \qquad \forall sc' \in F \qquad (5.39)$$

$$Sales_{sc'} = \sum_{t \in T} price_{sc',t} \cdot Q_{sc',t} \qquad \forall sc' \in F \qquad (5.40)$$

$$cw_{sc} = (Cwater_{sc} + Ctran_{sc} + Chan_{sc} + Sales_{sc'}) \qquad \forall sc \in L \qquad (5.41)$$

$$cw_{sc'} = Chan_{sc'} \qquad \forall sc' \in F \qquad (5.42)$$

Particularly, Eqs. (5.38) and (5.39) calculate the economic benefit for the leader and follower respectively while Eq. (5.40) represents the total revenue for the follower. Eqs. (5.41) and (5.42) describe the water management and acquisition costs for each SC member. It is important to mention that the leader costs include water purchase, transport, production, and the "disposal/treatment", while the follower ones are only associated with the operational tasks. Notice that the "disposal/treatment" term ($Sales_{sc'}$) affects both objectives ($Profit_L$ and $Profit_F$) representing the non-cooperative behavior and the conflict of interests between entities. Thus, the resulting MO-MILP problem has the following form and it is henceforth known as Non-Cooperative model *(NC)*:

$$(NC) \qquad \max \quad \{Profit_L; Profit_F\}$$

$$s.t. \qquad Eqs. (5.1) - (5.42)$$

5.4.4. Wastewater recovery representation

The level of pollution in wastewater flows typically has a non-linear impact over the final treatment cost and process efficiencies. Therefore, without loss of generality, it is assumed a sigmoidal and exponential behavior for the process efficiency and recovered wastewater price respectively *(Alleman, 2010; Veil, 2010; Acharya et al., 2011)*. Eqs. (5.43) and (5.44) present the non-linear functions modeling these behaviors for the CWT facilities while Fig. 5.2 shows their graphical representation.

$$LC = 0.75 - \left(\frac{0.25}{1 + e^{-0.0009(x-50000)}}\right) \tag{5.43}$$

$$VC = 1 - (4.5)^{-(x/3500)} \tag{5.44}$$

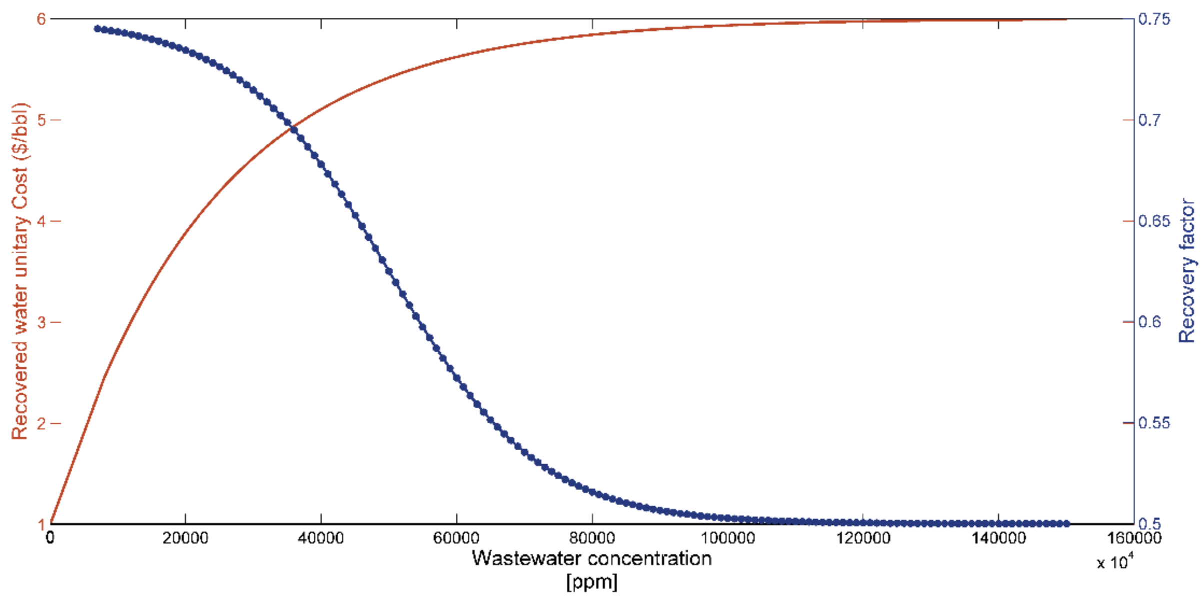

Fig. 5.2. The recovered wastewater cost and plant efficiency non-linear behaviors.

Even if Eqs. (5.43) and (5.44) leads to a MINLP, these non-linearity's can be relaxed using the well-known piecewise approximation, which is based on dividing the non-linear space into a sufficiently large amount of partitions and considering each one as an individual linear function. The efficient number of divisions is obtained by systematically increasing them until a minimum accuracy level is reached. However, since the accuracy of the piecewise formulation is out of the scope of this work a set of five equidistant points was used in this problem.

5.5. Solution strategy

To make a useful decision support tool evaluation, a set of optimal solutions has been first obtained by solving the model *(MOP)* using the ε-constraint method (resulting in the well-known Pareto frontier). Afterward, the ELECTRE-IV method has been used to systematically compare all the Pareto solutions to each other and identify the one that best reflects the decision-maker preferences. In the case of fractional approach, the solution is obtained directly after optimizing the model *(F)* that seeks for the maximum profit per unit of fresh water consumed. It is important to notice that both decision-making strategies identify a dominant solution (i.e. belonging to the Pareto frontier), thus, the final solutions (and decision-strategies) can be effectively compared.

This chapter also addresses the capabilities of the ELECTRE-IV method as a decision-support strategy for decentralized problems, thus, the optimal solution of the model *(NC)* was compared with the one identified using the ELECTRE-IV method. Such a comparison evaluates the effect of considering the leader and follower economic benefits independently as decision criteria. The general comparison methodology is illustrated in Fig. 5.3.

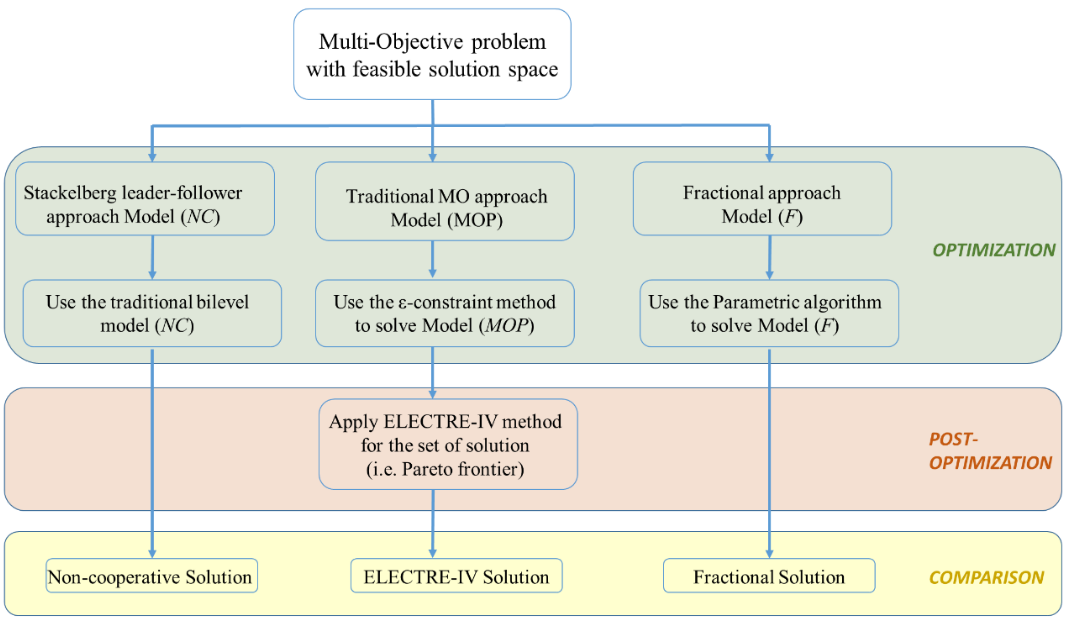

Fig. 5.3. General methodology diagram.

The results obtained after each step are discussed in the following subsections as well as their comparison. The detailed information of the particular solution approaches was presented in Chapter 3.

5.5.1. The fractional objective solution approach

The solution of models *(MOP)* and *(NC)* employs common methods described in Chapter 3; however, the solution of the model *(F)* requires a tailor-made approach as described in this section. First, notice that model *(F)* is clearly a sort of MINLP problem, in which its global optimization can be computationally tractable by applying Dinkelbach's algorithm *(You et al., 2009)*. However, the recent study of *Gao and You, (2015)* has proven the time-effective performance of parametric algorithms to solve MILFP problems, thus, one of these parametric algorithms was used, which is briefly described as follows.

Parametric algorithm

The parametric algorithm used consists of four main steps. In the first one, the original MILFP problem is transformed into an equivalent parametric MILP problem, denoted as function $F(\Omega)$. Such a function can be defined as the difference between the numerator and the denominator multiplied by a parameter (Ω). It is important to highlight that, when $F(\Omega) = 0$, the MILP problem has a unique optimal solution, which is the same as the global optimal solution of the original MILFP problem. Therefore, in the second step both a counter and a parameter are initialized ($n = 0$ and $\Omega = |n|$, respectively). Additionally, in the second step, an optimality gap is defined ($\delta = 0$). The third step seeks for the solution of the MIFLP problem finding the root of the equation (i.e. $F(\Omega) = 0$). In this particular case, the Newton's method is used to solve this problem; however, any other numerical root-finding methods can be applied. For the exact Newton's method applied, each parametric MILP sub-problem was solved to the global optimum (0% optimality gap). Afterwards, an iterative procedure was performed until $F(\Omega)$ equals zero. Finally, the fourth step corresponds to the definition of the optimal solution of this problem. The full procedure of this parametric algorithm is described as follows.

1. Modify the original MIFLP to an equivalent parametric MILP problem. For this particular case, the MILP formulation will be $F(\Omega) = \max\{(NP - cw) - \Omega \cdot (nfw)\}$
2. Let n be a counter for the Newton method and δ the optimality gap equal to 0%. Initialize $\Omega = |n|$.
3. Solve $F(\Omega)$.
   3.1. If $|F(\Omega)| \leq \delta$, stop, global optimality was found. Else:
   3.2. Let $\Omega = \frac{NP-cw}{nfw}$, and return to step 3.
4. Let solution x_n^* be the optimal solution of this problem (design and planning variables). It is important to notice that from the above algorithm, the objective value is represented by Ω.

For more details about the parametric algorithm used in this study, readers are referred to *(Gao and You, 2015)*.

5.6. Case Study

The capabilities of the proposed solution approaches were illustrated using a case study based on Marcellus shale play. The use of this case study does not only contribute to illustrating the similarities and limitations of both, the fractional and ELECTRE-IV base decision-support systems but also highlighting their effect on the optimal water management strategy. The optimal results provide the basis for a useful discussion and comparison of the corresponding optimization strategies.

This medium-scale case study consists of a network of two freshwater sources, three shale sites, and 10 water consumption wells in each site. Freshwater availability was estimated based on historical data taking into account the seasonal fluctuation. As wastewater treatment facilities, three CWT and 10 disposal wells were considered. Wastewater TDS concentration is assumed to vary within 8,000 and 150,000 mg/L based on the range of TDS concentration at fracturing stages. Due to geographic distribution, Marcellus shale play has disposal wells located far away from the shale sites, therefore these wells became an unlikely (but not impossible) option due to the high transportation cost. The onsite treatment contains three levels (primary, secondary, and tertiary one). For the primary and secondary levels, water is partially treated, and a certain amount of freshwater water is required to reduce the TDS concentration and satisfy the reuse specification. For tertiary level, around 20% make-up water is required to reach a low enough value for the inlet TDS concentration to be treatable (around 120,000 mg/L). The connections between each one of the treatment levels have been oversimplified by assuming that the TDS concentration in the wastewater conditions the treatment level to be applied in the first instance. More precisely, primary treatment receives water with TDS concentration lower than 20,000 mg/L; secondary treatment treats water with TDS concentration lower than 40,000 mg/L, and tertiary treatment is able to treat wastewater of any TDS concentration ranges (<120,000 mg/L). Pipelines and trucks are assumed as transportation modes for freshwater management, but only trucks are allowed for transporting wastewater from shale sites to CWT facilities and disposal wells. Three nominal capacities were considered for pipelines as well as for each level of onsite treatment facilities. The planning horizon is 10 years weekly discretized (520 periods). The main parameters used are included in the Appendix B.3.

The mathematical model has been written in GAMS and the problem was solved using CPLEX 11.0 on a PC Intel CoreI i7-2600M CPU 2.70 GHz and 16.00 GB of RAM. The absolute optimality tolerance for all solvers is set to zero. The optimality tolerance for the outer loop in the parametric algorithm is set to 10^{-4}.

5.6.1. MOO results

Here, *Profit* and *nfw* were considered as objectives. According to the ε-constraint algorithm (described in Chapter 3), first, the model *MOP* has to be optimized for each objective individually (SO optimization) and their results represent the bounds for the feasible solution space (see Table 5.1).

Table 5.1. Economical and freshwater consumption performance for the individual optimizations.

	Max $Profit$	Min nfw
$Profit(\$ \cdot 10^6)$	83.164	75.903
$nfw(bbl \cdot 10^6)$	6.239	4.975

To apply the ε-constraint method, the $Profit$ was considered as main objective while the level of nfw was constrained at each iteration. According to Table 5.1, nfw ranges between 4.97 and 6.25 millions of barrels of freshwater representing the feasible space within which the objective could be constrained. Particularly, 12 constrained points were used producing the same number of solutions as displayed in Fig. 5.4. Notice that each point represents different design and management decisions.

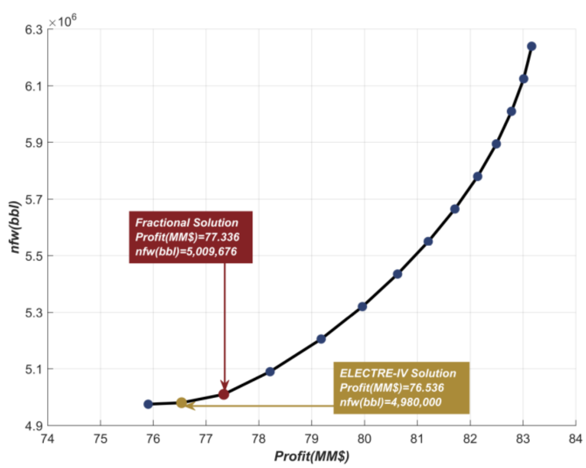

Fig. 5.4. Pareto set of solutions for the $Profit$ vs nfw problem. Red dot represents the solution obtained after using the Fractional approach. Golden dot represents the best overall solution identified with the ELECTRE-IV method.

From Fig. 5.4 it is observed that as the freshwater consumption increases, the profit increases as well, proving their conflicting behavior. At this point, the decision maker has to compare all the solutions and select the one that better represents his preferences. The above justifies the evaluation and comparison of two different decision-making strategies.

First method: Fractional objective

The objective ($Frac$) represents the relation between *Profit* and *nfw*. Their individual performances were obtained and displayed in Table 5.2, which henceforth will be known as *Fractional* solution. In this section, a description of the objective performances will be discussed, however, the optimal design decisions and their impact over the water management strategy will be analyzed in the next subsections.

Table 5.2. Economical and freshwater consumption performances for the fractional optimization.

	Max $Frac$
$Frac(\$/bbl)$	15.473
$nfw(bbl \cdot 10^6)$	5.009
$Profit(\$ \cdot 10^6)$	77.336

The value of $Frac$ is $15,437 per thousand barrels of freshwater consumed which represents a profit of more than $15.4 per barrel. About 5MM Bbl of freshwater along the complete time horizon were required to achieve economic benefits of $77,336,340. In Fig. 5.4 the position of the *Fractional* solution within the Pareto curve was displayed proving that, the fractional formulation totally bypasses the decision-making effort and identifies a feasible optimal solution for bi-objective optimization problems. However, the fractional formulation assumes a significant preference for the objective in the numerator disregarding the potential undesirable/poor performance for the denominator objective. Since such a preference is completely uncontrollable, the quality of the resulting solution in terms of decision maker interests is compromised. By analyzing the idea behind the fractional formulation such a limitation can be clarified, in which the solution identified corresponds to the point with the minimum slope for a defined curve (in this case Pareto curve). Thus, the position of the Pareto curve within the solution space determines the solution obtained, being the fixed process conditions the ones that modify such a position (like fixed cost). Consequently, the fractional approach may promote the identification of undesirable solutions from the decision maker perspective. In order to stress even more such an issue a definition of seven increasing fixed costs were included in the model *(F)*. The results are displayed in Table 5.3.

Table 5.3. Economical and freshwater consumption performances for the fractional optimization (expressed in x10^6).

	Model (MOP)		*Model (F)*	Fixed cost added to the total cost in *Model (F)*						
				0.02	2.00	10.0	20.0	40.0	60.0	80.0
	Case 0	Case 0’	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case7	Case 8
Total Water cost ($)	0.13	1.55	0.25	0.25	0.25	0.30	0.40	0.35	0.16	0.13
Management Cost ($)	0.295	7.63	6.02	6.02	6.00	5.92	5.74	4.22	1.61	0.295
Fractional Objective	13.33	15.28	15.57	15.57	15.17	13.56	11.55	7.60	3.87	0.51
Profit ($)	83.20	75.80	77.40	77.40	75.50	67.50	57.70	39.20	21.80	3.16
Withdrawal (bbl)	6.24	4.96	4.97	4.97	4.97	4.98	4.99	5.16	5.64	6.24
NP ($)	83.46	83.46	83.46	83.44	81.46	73.46	63.46	43.46	23.46	3.46

In Table 5.3, the first two columns represent the anchor points of the original Pareto curve obtained by optimizing the *Profit* and *nfw* individually in the model (*MOP*). Column 3 (i.e. Case 1) shows the results of solving the original fractional model *(F)* while for the rest of the columns an increment in the fixed costs for the wastewater management process was assumed. Logically lower basic benefits (*Profit*) were obtained after each cost increment; however, it was surprising that the freshwater consumed (*nfw*) increases as well. The above can be explained since the economic margin is shortened at each iteration thus transportation and/or treatment costs are reduced to the minimum (or not used) and, consequently, large amounts of freshwater are used instead. Additionally, if the fixed cost is as high as the original basic benefit (*Profit* equal or near to zero), the design/operating decisions from the optimum fractional solution matches with the decisions of the extreme solution that maximizes the *Profit* (first column). As pointed out, these results suggest that modifying the fixed cost "moves the scales" the Pareto space and, consequently, the fractional approach is affected. More importantly, it is proved that fractional approach presents an uncontrollable preference for the economic objective. A graphical representation of such an issue is displayed in Fig. 5.5.

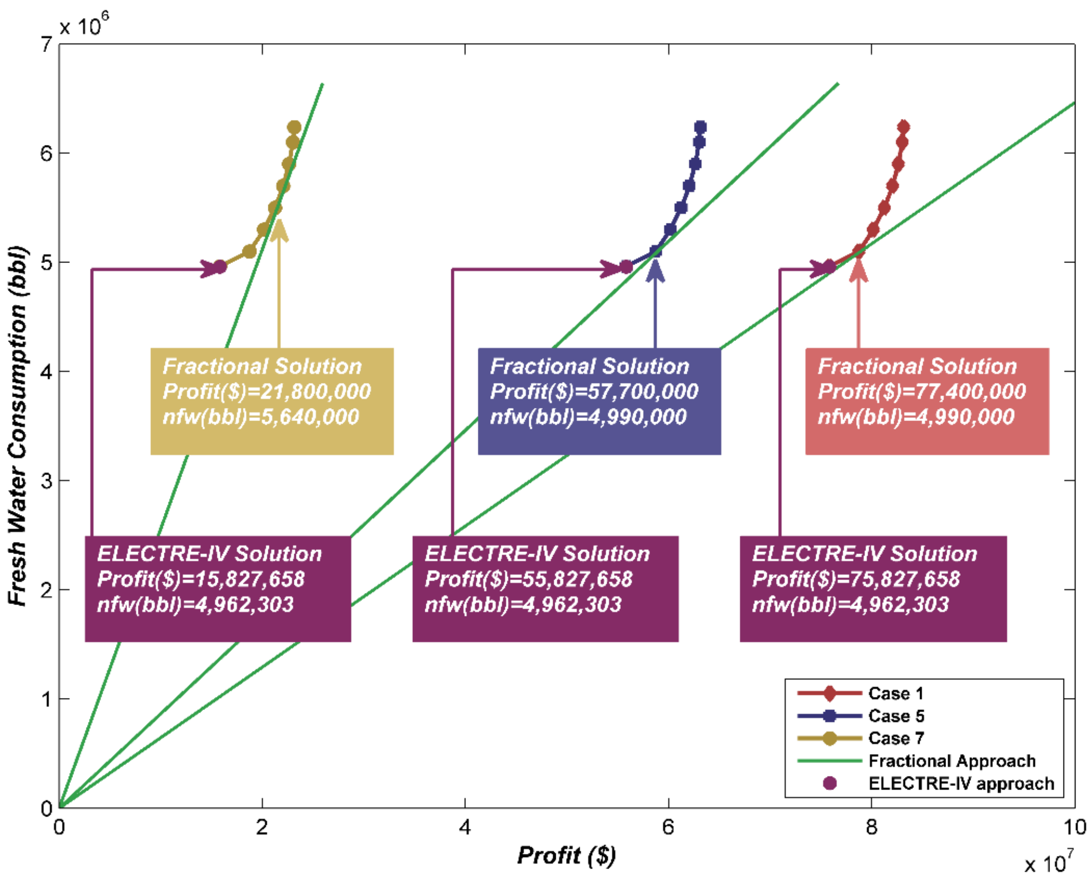

Fig. 5.5. Effect of fixed cost over fractional approach behavior.

The results prove that the solution obtained using the fractional approach remains efficient only if a strict control of the fixed costs is performed and/or when the fixed cost is sufficiently small to be neglected. However, when the fixed cost is unknown or significantly variable across the time, the fractional approach is not suitable (for example in non-cooperative problems where some of the decisions may change to react to other players decisions). In summary two main drawbacks can be pointed out; first, its application is limited to bi-objectives problems; and second, the specific formulation of the fractional problem gives an indirect preference to one objective conditioning the final solution. Consequently, it is evident that there is a need for a robust methodology that expands the application of the fractional methodology to evaluate multiple objectives while reflecting the decision maker interests/criteria. In this line, the ELECTRE-IV method is a promising alternative as supported by the numerical results presented in the following sections.

Second method: ELECTRE-IV

In order to identify a solution that satisfies the decision maker expectations within the Pareto frontier the ELECTRE-IV method has been used. In accordance with the procedure described in Chapter 3, the preference, indifference and infeasible thresholds for each one of the objectives used in this section are presented in Table 5.4.

Table 5.4. Thresholds values for the three objectives considered in this case study.

Thresholds	Objective's value	
	$Profit$ ($\$\cdot 10^6$)	nf ($bbl \cdot 10^6$)
Indifference (*qt*)	79.0	4.90
Preference (*pt*)	83.0	5.30
Veto (*vt*)	100.0	5.40

These thresholds must reflect realistic decision-maker preferences for each criterion. In this particular case, the indifference threshold for the $Profit$ has been defined by adding close to 50% of the difference between the economic bounds (i.e. maximum and minimum economic performance) to the lowest feasible value ($\$75.9\text{x}10^6$). The above is assumed since in most of the real-life problems, the decision maker trend to avoid solutions with the lowest economic performances. Following the same logic, the preference threshold is set close to the maximum feasible value. Finally, since $Profit$ is a maximization objective it is undesirable to remove solutions with high performances, thus, the veto threshold was set as a big number (larger than the maximum value). On the other hand, for the minimization of the freshwater consumption the thresholds definition is different. Particularly, the indifference and preference thresholds were assumed as $4.9\text{x}10^6$bbl and $5.3\text{x}10^6$bbl respectively. In order to drive the search to a solution with the lower consumption as possible, a veto threshold of $5.40\text{x}10^6$ bbl was defined even if there are feasible solutions with higher values. Such a veto threshold promotes that, unless there is no other better option, a solutions with freshwater consumption, higher than $5.40\text{x}10^6$ bbl will hardly be selected. Thus, using these thresholds, the 14 optimal solutions were evaluated by applying the ELECTRE-IV method. It is important to highlight, that the selection of different thresholds will influence in the final solution selected and they can be tailor-made to represent the decision maker preferences.

After applying the ELECTRE-IV method, a solution within the set of Pareto options that satisfies the decision maker preferences as much as possible was found (henceforth known as *ELECTRE-IV* solution). In such a solution the $Profit$ value was \$ 76,536,340, the nfw about 4,980,000 bbl, and their relation ($Frac$) reach a value of 15.36 \$/bbl. Notice that the identified solution produce a $Profit$ value below the preference thresholds and, in particular, it lies within the indifference range (between $\$77\text{x}10^6$ and $\$79\text{x}10^6$). The above means that the economic objective cannot be completely satisfied but still represents a good outcome according to the defined decision maker expectations. Such a solution was identified as the best one by systematically defining the degree of preference satisfaction of each objective as a function of the outranking relationships. In other words, the strategy identifies the solution that has a "lower negative impact" on the decision maker preferences by accepting a reduction in the $Profit$ to significantly reduce the freshwater consumption. Notice that even if the relation $Profit/nfw$ is lower than in the *Fractional* solution, ultimately the ELECTRE-IV method produces a balanced solution. In Fig. 5.4, *Fractional* and

ELECTRE-IV solutions are displayed. The above proves that, with the ELECTRE-IV method, both objectives are equally important, avoiding any subjective preference.

Alike the fractional approach, ELECTRE-IV method was applied for the seven different Pareto curves obtained as a result of considering several fixed costs in the water management. Notice that the thresholds for the economic objective must be proportionally modified to lie within the feasible "solution space". The above allows evaluating the effect of the Pareto space in the performance of the ELECTRE-IV method. In Fig. 5.5 the position of the solutions obtained using the ELECTRE-IV method are displayed. Notice that even if the objective performance were different (i.e. the Pareto solution space is different) the associated design/management decisions are maintained. Therefore it is proved that ELECTRE-IV method not only provides a reliable and robust solution for bi-criteria problems but also bypass the uncontrollable preference assumption made in the fractional approach without compromising the quality of the final solution.

In order to stress the sensibility of the ELECTRE-IV method, in the following subsection, a solution selection procedure is illustrated by considering additional decision criteria (not only the objectives themselves). Additionally, an analysis of the capabilities of the ELECTRE-IV method to identify a solution that works for a non-cooperative environment is exploited.

5.6.2. Capabilities of ELECTRE-IV method.

In this section, the capabilities of the solution identification method are emphasized assuming different interesting real-life conditions. Nevertheless, first, the definition of the feasible set of solutions has to be generated, as explained next.

Analysis of multiple objectives

Here, additionally to *Profit* and *nfw*, the effect of their relation to the optimization is exploited (*Frac*). As well as in previous sections, a table containing the results for the individual optimization problem *MOP* for each objective is presented and used as feasible area boundaries (Table 5.5).

Table 5.5. Performance of the three objectives under analysis for their individual optimizations.

	Max $Profit$	min nfw	max $Frac$
$Profit$ ($\$ \cdot 10^6$)	83.16	74.97	77.34
nfw ($bbl \cdot 10^6$)	6.239	4.998	5.009
$Frac$ ($\$/bbl$)	13.33	14.99	15.43

Similarly, the $Profit$ was considered as main objective while nfw and $Frac$ performance were constrained within the feasible space. Both objectives were constrained at 12 defined points within their feasible ranges (between 4.998×10^6 and 6.239×10^6 bbl, and 13.33 and 15.43 for nfw and $Frac$ respectively). In this case, the Pareto frontiers obtained may be projected to build a sort of 3D-surface (see Fig. 5.6). Notice that the projection in the $Frac$ axis has a clear a linear trend since this objective depends directly form the remaining objectives. It is worth to comment that these projections are not an accurate representation of the Pareto surface, but provide a good approach.

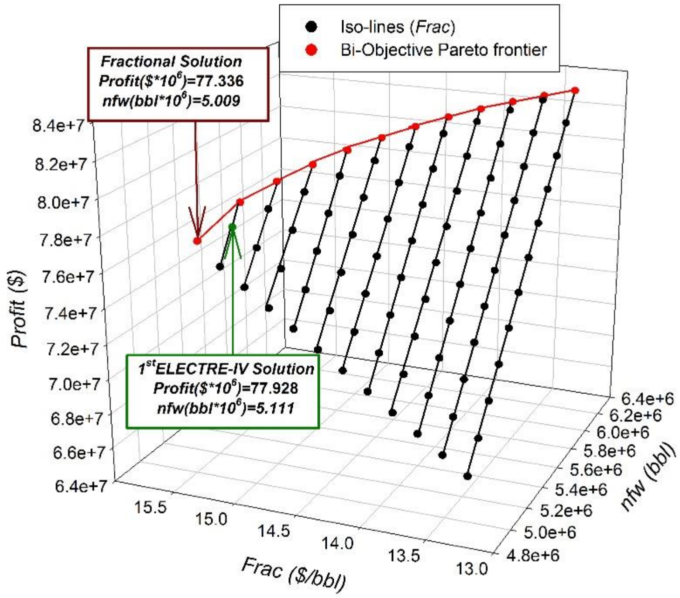

Fig. 5.6. Pareto surface for the three-objective problem highlighting the *Fractional* and *1st ELECTRE-IV* solutions.

From Fig. 5.6 it can be observed that the *Fractional* solution corresponds to one anchor point (best value for *Frac*). However, it is clear that the decision maker challenge has significantly increased in complexity (compared with Fig. 5.4). Thus, the ELECTRE-IV method has been applied to identify the best solution for the three conflicting objectives simultaneously.

Solution identification

In this section, similar assumptions were made for the definition of the preference thresholds for both $Profit$ and nfw. For the case of $Frac$ an increment of 15% to the minimum bound was defined for the indifference threshold since it is an objective to be maximized. The preference and veto thresholds were defined following the same assumptions that in the previous section for $Profit$ (see Table 5.6).

Table 5.6. Thresholds values for the three objectives considered in this case study.

Thresholds	Objective's value		
	$Profit$ (\$$\cdot 10^6$)	nf $(bbl \cdot 10^6)$	$Frac$ (\$$/bbl$)
Indifference (*qt*)	79.0	4.90	13.73
Preference (*pt*)	83.0	5.30	15.30
Veto (*vt*)	100	5.40	18.45

Using the data in Table 5.6, the ELECTRE-IV method was applied to evaluate the 144 resulting optimal solutions. Thus, a unique solution was found (henceforth known as *1st-ELECTRE-IV* solution) in which the $Profit$ value was \$77,928,589, the nfw about 5,111,595 bbl, and their relation is of 15.245 \$/bbl. By comparing the *Fractional* and *1st ELECTRE-IV* solutions it can be noticed that the second one leads to a *Profit* increment while reducing the other two objectives performance (See Fig. 5.6). Remarkably, $Profit$ and nfw lie in the range of indifference and preference values, while $Frac$ reach a value in the preference range, proving again that ELECTRE-IV method identified a balanced solution. Despite the differences in the objectives performance, both strategies identify solutions close each other in the solution space. The above proves that under the same conditions the fractional approach and ELECTRE-IV method show a good performance. However, the second method is particularly useful to consider more than three decision criteria without compromising the quality of the final solution. The above is significantly important for real industrial applications in which, for example, all the operations may have additional constraints that restrict the solution (for example, budget limitations). In order to stress even more the sensitivity of the solution selection method a set of additional decision criteria were considered and not only the objectives themselves.

Additional criteria during solution identification

In this section, a set of budget limitations were considered. In particular, key factors such as water acquisition, transportation, and wastewater treating costs were considered as selection criteria. Thus, additionally to the pursuit for the highest profit, it is assumed that water acquisition, transportation, and wastewater treating costs should not exceed 0.155, 5 and 3 million of dollars respectively, as presented in Table 5.7. The rest of thresholds (preference and indifference) are defined following similar assumptions than in the previous subsection.

Table 5.7. Thresholds values for the three objectives and the additional criteria considered.

Thresholds	Objective's value			Additional Criteria's value		
	$Profit$ (\$)[a]	nf (bbl)[a]	$Frac$ $(\$/bbl)$	*Acquisition(\$)*[a]	*Transport(\$)*[a]	*Operating(\$)*[a]
Indifference (qt)	79.0	4.90	13.73	0.135	0.100	0.001
Preference (pt)	83.0	5.30	15.30	0.140	0.900	1.00
Veto (vt)	100	5.40	18.45	0.155	5.00	3.00

[a]Values at expressed in x10^6

After applying the ELECTRE-IV method, a solution was identified (henceforth known as *2nd-ELECTRE-IV* Solution) and its associated performance is presented in Table 5.8. From such a solution, notice that all the criteria lie within the defined thresholds except for the operating cost. The above suggest that this is the only solution that better balances all the criteria, even if the operating cost is significantly undesirable.

Table 5.8. Optimal criteria values for the selected solution.

Criteria/Objective	Value
$Profit$(\$)[a]	79.870
nf (bbl)[a]	5.305
$Frac$ $(\$/bbl)$	15.054
Acquisition(\$)[a]	0.145
Transport(\$)[a]	0.414
Operating(\$)[a]	3.029

[a]Values at expressed in x10^6

Comparing the two ELECTRE solutions (*1stELECTRE-IV* and *2nd-ELECTRE-IV)* it is evident that a significant increase in the economic performance at an expense of increasing the total freshwater consumption was obtained. Such a behavior was expected considering that the additional constraints associated with transportation and wastewater regeneration costs force the solution to use freshwater. However, the identified solution still represents an attractive compromise according to the decision maker preferences. For example, from the six decision criteria, three of them ($Profit, Frac$ and $Transport$) lie in the indifference-preference range, while the rest presents values in the preference region. Fig. 5.7 provides a visual aid to identify the effect of the additional criteria and allows a comparison with *Fractional* and *1stELECTRE-IV* solutions.

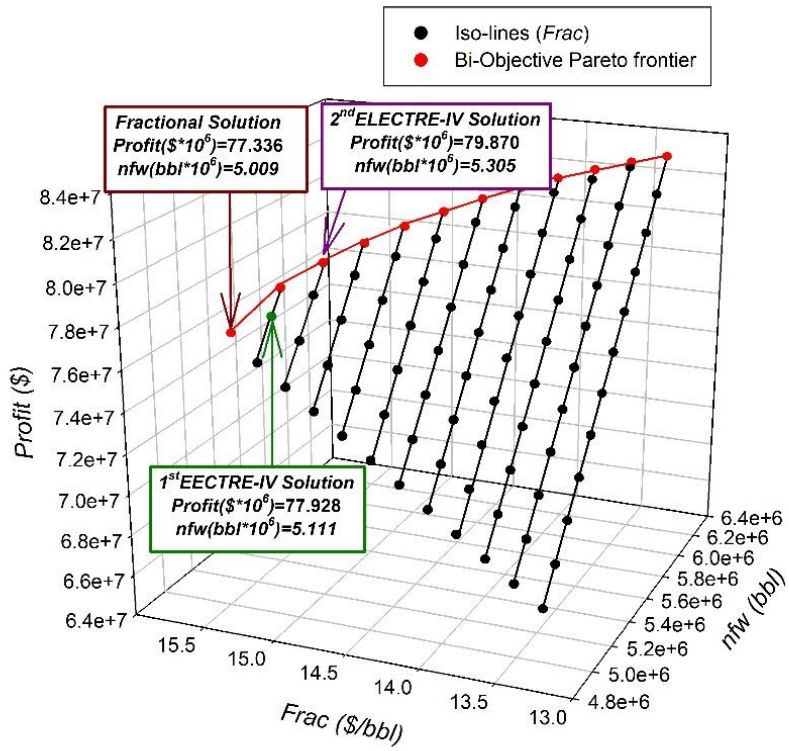

Fig. 5.7. Pareto surface for the three-objective problem. *Fractional*, *1stELECTRE-IV* and *2ndELECTRE-IV* solution are highlighted.

These results prove that the ELECTRE-IV method is sensitive enough to account systematically for additional constraints satisfying the decision maker preferences. Therefore, it is possible to identify a single solution in a time-effective way. Nevertheless, two main drawbacks can be highlighted: (i) The ELECTRE-IV method do not guarantee a single solution but it ensures a reduced set of feasible ones. Therefore and even if ELECTRE-IV method represents an important advantage for the decision maker, a more determinant tool is still needed. (ii) Even if the application of the ELECTRE-IV method is very fast and reliable, the computational effort associated to the production of the "pool of solutions" hinder its acceptance in the dynamic industrial problems, due to its nature of post-optimization tool. Consequently, a combination of the ELECTRE-IV method with other fast/accurate MOO strategies is an open and hot topic for the PSE community.

Analysis of non-cooperative environment

In this section, the model *(NC)* was solved considering as objectives only the economic benefit of both entities, the leader, and follower (i.e. $Profit_L$ and $Profit_F$) disregarding the performance of the environmental objective. The resulting solution will henceforth know as *NC-solution*, and its associated objective performances are displayed In Table 5.9 together with the global economic value ($Profit$).

NC-solution leads to $83,164,560 and $444.04 for $Profit_L$ and $Profit_F$ respectively. Additionally, even if the nature of both objectives was economic, the global water consumption and the relation between global profit and water consumption were also collected (nfw=6,238,823 and $Frac$=13.33). Since the economic benefit was considered as objective, it is not surprising that the final solution for the model *(NC)* is very similar to the solution obtained through the economic optimization of model (MOP) (i.e. the best *Profit*). From the results in Table 5.7 and the position of the *NC-solution* within the solution space (See Fig. 5.8) two main aspects should be emphasized:

Table 5.9. Economic performance of the individual entities and the global system.

	$Global$	$Leader$	$Follower$
$Profit$ (\$)	83,165,014	83.16456	444
nfw $(bbl \cdot 10^6)$	6.239	-	-
$Frac$ $(\$/bbl)$	13.33	-	-

(i) The obtained solution from the bi-level model matches with the extreme solution of the bi-objective Pareto frontier. However, this is not typical, since the solution of a bi-level problem does not guarantee a Pareto solution of the collaborative case. In this particular situation, the solution belongs to such a frontier due to the lack of additional constraints associated with the formulation of follower part in the model (*NC*).

(ii) The undesirable follower's performance (very low economic benefit) still represents an optimal solution for the considered model conditions/constraints, but obviously the follower's performance may be improved. Thus, even if it is clear that a very basic and crude example was used, the obtained results can be used to demonstrate the capabilities of the proposed methodology as described in the following section.

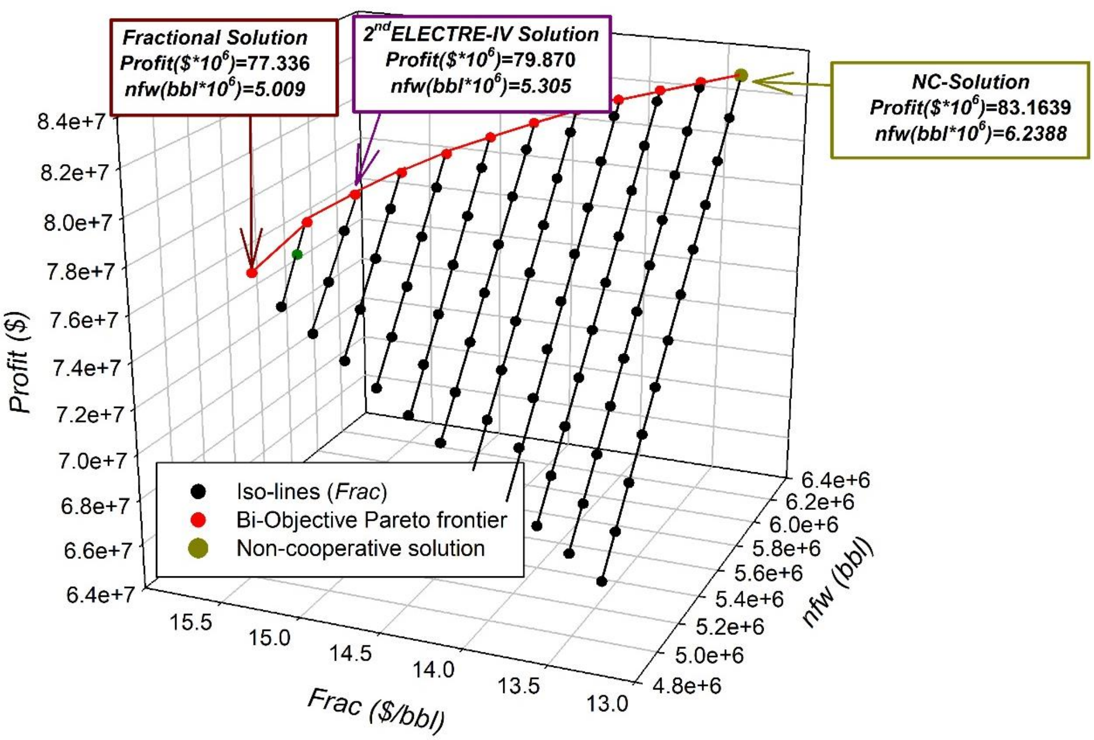

Fig. 5.8. *NC-Solution* within the Pareto surface for the three objective problem.

As commented before, from Fig. 5.8 it can be observed that the *NC-solution* is near to the economic optimization of the collaborative model *(MOP)* (best value for *Profit*). However, in order to prove once again the capabilities of the ELECTRE-IV method, the entire set of Pareto points will be evaluated to identify the solution that shows better performance for both entities simultaneously.

Solution identification

In this section, the solution with the highest profit level for both entities is identified. In order to avoid undesirable solutions, it was assumed that leader and follower profits should not be lower than 79.0 and 0.2 million dollars respectively, as presented in Table 5.10. The rest of thresholds (preference and indifference) are defined following similar assumptions than in previous sections.

Table 5.10. Thresholds values for the global and individual objectives for the non-cooperative situation.

Thresholds	Global objective	Individual objectives	
	$Profit$ (\$$\cdot 10^6$)	$Profit_L$ (\$$\cdot 10^6$)	$Profit_F$ (\$$\cdot 10^6$)
Indifference (*qt*)	79.0	79.0	0.2
Preference (*pt*)	83.0	83.0	1.00
Veto (*vt*)	100	100	10

After applying the ELECTRE-IV method, the solution henceforth known as *NC-ELECTRE-Solution* was identified and the associated performances are displayed in Table 5.11. Notice that the economic performance of the leader is slightly lower than the global one for this selected solution (around 0.2%). The above is logical considering that in the global perspective all the network cost were extracted to the shale gas revenues, while in the non-cooperative scheme, only some of the costs are applied (those belonging to the leader). Thus, the leader reaches a higher individual profit. Additionally, notice that the *NC-ELECTRE-Solution* promotes a high follower profit (higher than the *NC-Solution*). Since the follower part of the problem is associated with the wastewater plant, a significant amount of regenerated water was used and consequently reducing the freshwater use. These performances are deeper discussed in the next section in which a detailed comparison of the resulting designs is presented.

Table 5.11. Optimal values for the identified solution of a non-cooperative environment.

Criteria/Objective	Value
$Profit(MM\$)$	81.487
$Profit_L(MM\$)$	81.283
$Profit_F(MM\$)$	0.204
$nfw\ (MMbbl)$	5.528
$Frac\ (\$/bbl)$	14.67

Comparing the *NC-ELECTRE-Solution* against the *NC- Solution* makes evident that a more balanced solution was obtained at the expense of reducing the economic performance of the system. Particularly, *NC-ELECTRE-Solution* obtains a value of 14.67 \$/bbl while *NC- Solution* is only 13.33\$/bbl proving that the identified solution using ELECTRE-IV method takes a better economic profit per unit of freshwater consumed. Both objectives ($Profit$ and nfw) were significantly affected, and in particular, a reduction of 2 millions of dollars in global benefits and 0.7 millions of barrels of freshwater were obtained. Thus, despite the significant reduction in the global economic performance of the system, a more balanced solution was obtained promoting a win-win situation. Therefore, even if the Pareto points were obtained under a global perspective, the ELECTRE-IV method is flexible enough to identify the solution that produce “better” performances for a non-cooperative environment. In Fig. 5.9 the position of the *NC-ELECTRE-Solution* within the solution space is presented and compared with the *NC-Solution.*

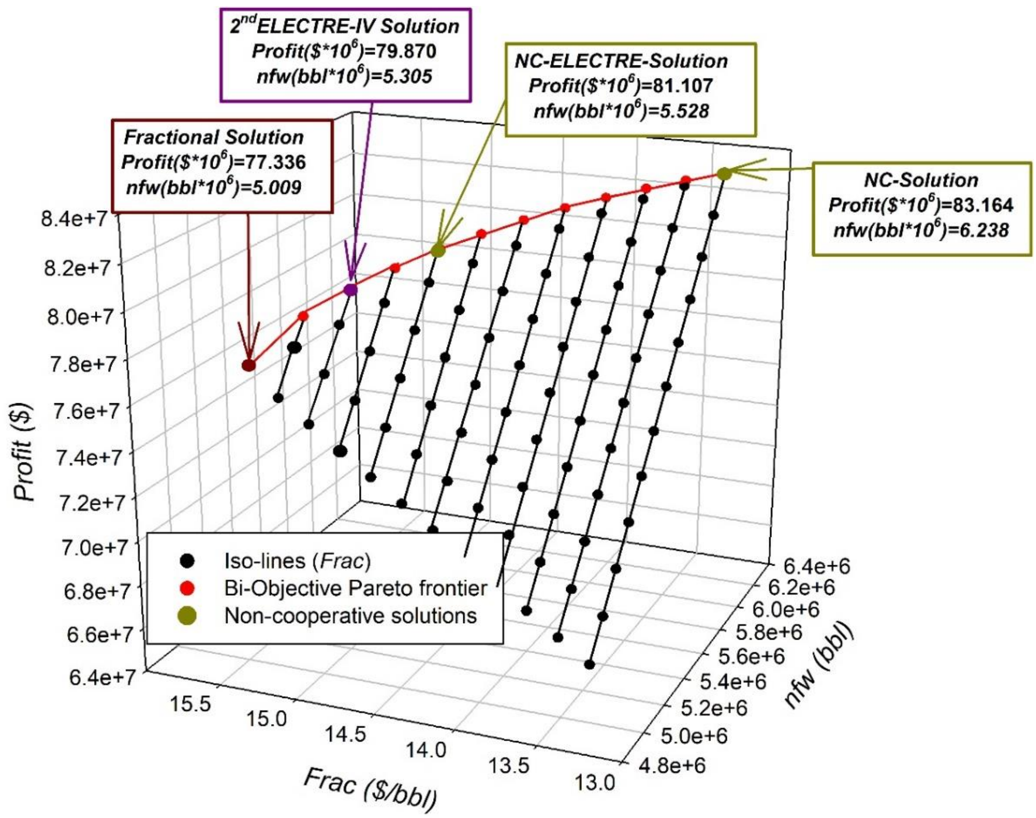

Fig. 5.9. Pareto surface for the three objectives problem highlighting the *Fractional*, *2ndELECTRE-IV*, *NC-Solution,* and *NC-ELECTRE-Solution*s.

The identification of a well-balanced solution for non-cooperative environments demonstrates ones again the utility of ELECTRE-IV method to account for additional constraints to be satisfied following the decision maker preferences.

5.7.Networks comparison

In order to provide a further analysis of the solutions obtained using the proposed solution approaches, a comparison of the resulting designs associated with the water management decisions for the cooperative and non-cooperative scenarios are presented. In particular, this section focuses on the comparison of the design associated with the *Fractional and 2nd-ELECTRE-IV* solutions for the cooperative scenario. Similarly, the designs for the *NC-Solution* and *NC-ELECTRE-Solution* are compared for the non-cooperative scenario.

5.7.1. Cooperative environment

Fractional solution design

The optimal water supply chain network in obtained as solution of the MILFP problem (*Fractional* solution) is shown in Fig. 5.10. All the shale sites acquire freshwater from source one, which is the cheapest one. The obtained water management strategy combines the CWT and onsite treatment for water regeneration purposes. As commented before, in this case no disposal well is available within a short distance and, therefore, it is not surprising that the underground injection option was not selected due to the high transportation cost.

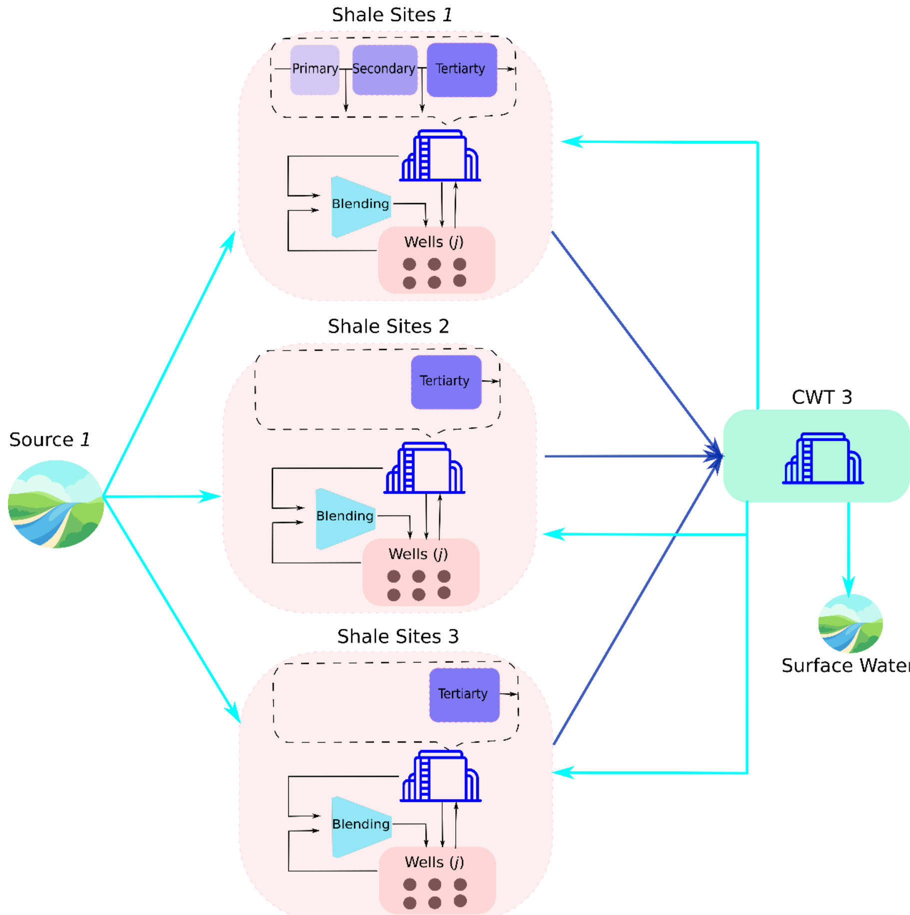

Fig. 5.10. Water supply chain network for model (*F*).

The profit obtained per barrel of freshwater is of $15.437. The associated cost for freshwater supply tasks, including acquisition and transportation, is $250,653. This value represents only a 5% of the overall distribution and management (treatment and disposal) cost. The reuse of water from onsite treatments is the main reason of the significantly freshwater savings; however, a high treatment cost of $5,007,958 is required (around 80% of the total water network cost).

By analyzing the network in detail, it can be noticed that the optimal water network transports all the freshwater through pipelines. Despite the high capital investment required for construction, this option is acceptable since a long time period is considered and such a high investment is compensated with its lower transportation cost during the 10 years period. Additionally, the smallest and cheapest capacity was employed for the pipeline capacity (30,000 bbl).

On the other hand, planning decisions (water handling) includes the choice of different water management options for a specific amount of wastewater. In this particular case, onsite treatments were preferred over the CWT option for reuse purposes. Onsite treatments simultaneously reduced the transportation cost and freshwater consumption by treating wastewater onsite and blending it with smaller amounts of freshwater for reuse. CWT option was used in the final design, however, it is used almost exclusively for disposal purposes and the small amount of recovered water (<586 bbl/year) is used when onsite treatment cannot satisfy the demands. The above can be explained since the "double" transportation cost for a "round trip" to/from CWT makes its selection unlikely even considering their low wastewater treatment cost. As to the detailed breakdown of total water management cost, the CWT facilities contribute to 6% of the overall cost for water management while onsite treatment accounts for 81% of the total cost, including capital investment and operating cost. Finally, the extensive application of onsite treatment and reuse highly relieved the stress on freshwater withdrawal while satisfying the required operational conditions.

2nd-ELECTRE-IV Design

The optimal water supply chain network associated with the solution of the model (*MOP)* (i.e. *2nd-ELECTRE-IV*) is shown in Fig. 5.11. Alike the Fractional design, all the shale sites acquire freshwater from "Sources 1". Also, the associated water management strategy uses a combination of onsite and CWT units for regeneration/reuse purposes for all the shale sites. Due to the lack of close disposal wells, in addition to the additional constraint to the transportation cost, it is not surprising that the underground injection option was not selected.

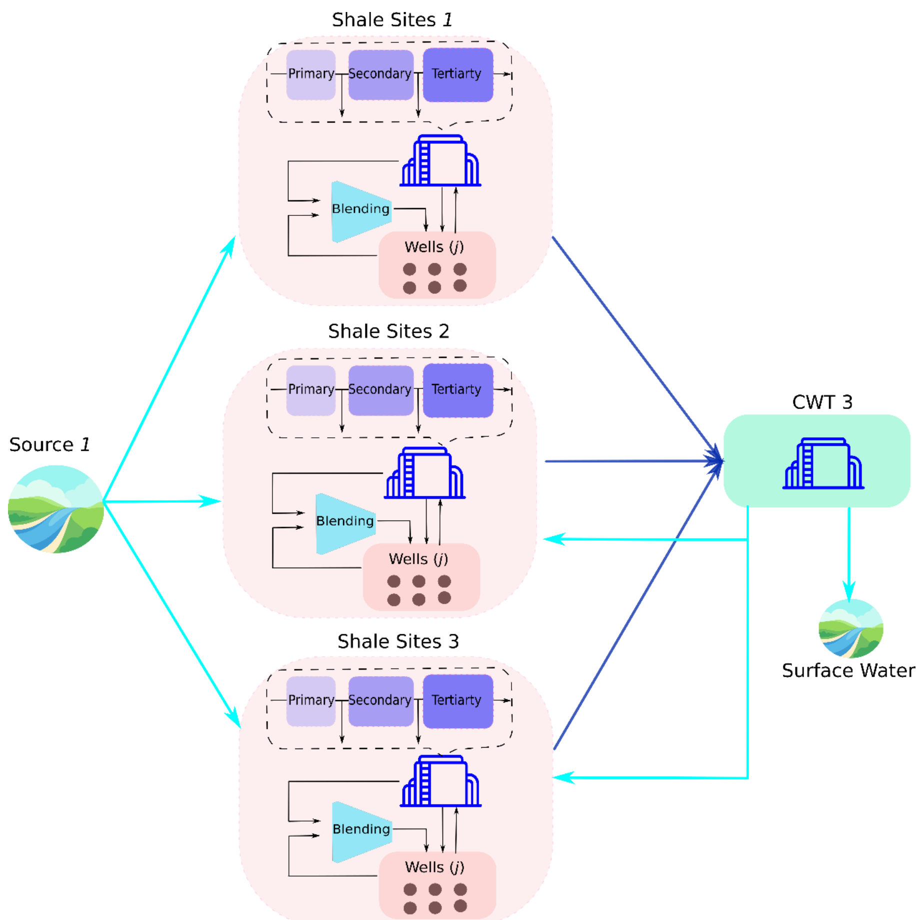

Fig. 5.11. Water supply chain network for the *2nd-ELECTRE-IV* solution (model (*MOP)).*

For this case, the profit obtained while consuming one barrel of freshwater is of $15.054. In this design due to the budget limitations for the transport and treatment investments, the associated cost for freshwater supply tasks, including acquisition and transportation, is higher than the double in comparison with the Fractional design ($559,836). This value represents a 19% of the overall distribution and management (treatment and disposal) cost (14% higher than in the *Fractional* solution). Despite the increment in the freshwater consumption, the total treatment cost was significantly reduced up to $3,029,316 (around 40% less than in the *Fractional* solution). Such a reduction was obtained due to the substitution of regenerated water (coming from onsite treatment plants) with freshwater, thus, imitating the operations of onsite treatment plants. Alike in the previous design, all the freshwater distribution is achieved through pipelines, since the required investment is compensated for its lower transportation cost during the 10 years period.

Due to the benefits of using onsite treatments, they contribute in almost 4 times more than the CWT facilities to the wastewater management. In any case, CWT was used in the final design and the small amount of recovered water from shale sites1 and 2 is still considerably larger than the one obtained with the Fractional solution (<1500 bbl/year).

5.7.2. Non-cooperative environment

NC-solution design

The optimal water supply chain network obtained through the solution of the bi-level model *(NC)* is shown in Fig. 5.12. As commented before, this solution matches with the solution that produces the best global $Profit$ performance. Notice that in this case and unlike the above designs, all the shale sites acquire freshwater from two sources due to the considerable low price for freshwater. The above is logic since only the economic benefit was considered as objective and thus the system environmental impact was neglected. In the case of the water management options, the design is quite simple since the onsite treatment is not used while the CWT is barely used. Remarkably, even if the operation/installation cost of the CWT is considerably high and goes against the economic optimization, the CWT was used in order to promote the follower operations and increase its individual benefits.

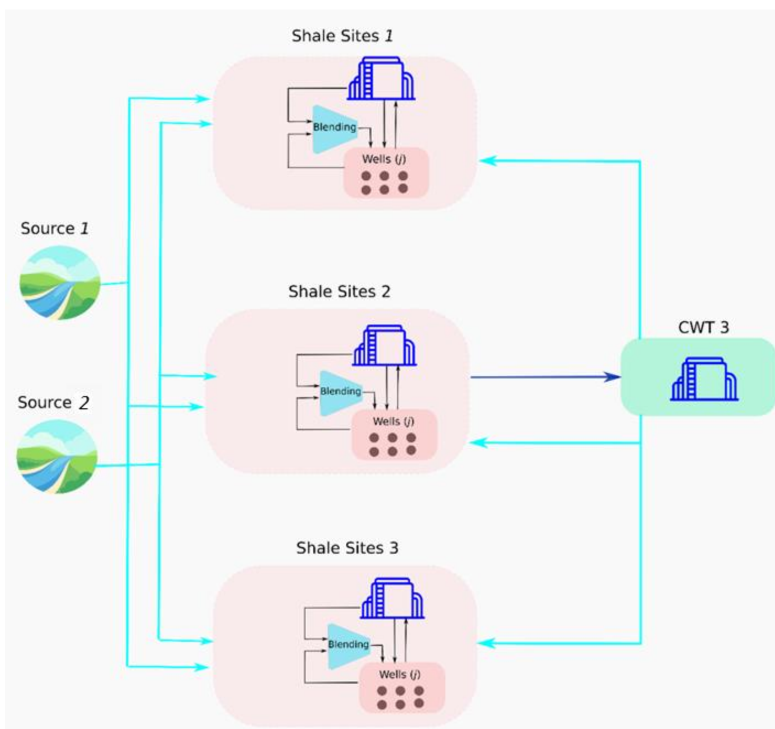

Fig. 5.12. Water supply chain network for *NC-Solution*.

The global profit obtained while consuming one barrel of freshwater is of $13.337. Notice that the leader total cost, including acquisition, transportation and operation ones, is $294,315 while the follower is of \$534. The design in Fig. 5.12 is considerably simple and in fact, the highest part of the cost for both entities is associated with transportation tasks (higher than 80%). Similarly, the benefits for the leader and follower part are \$83,459,920 and \$1,062.159 respectively. Even if the leader benefit is considerably high, this comes from the shale gas sales while the follower benefit is associated with the wastewater treatment services. Thus, such a small benefit is due to the small amount of wastewater treated (<500bbl/year). Consequently, even if mathematically the above is a feasible solution, the follower performance is too small to consider it feasible in a real-life process.

These results were obtained mainly for two reasons: (i) The small number of constraints associated to the follower part of the system; (ii) the definition of a purely economic objective for a sustainability problem. However, these issues were overcome in the solution identified by ELECTRE-IV method as described in the next section.

<u>NC-ELECTRE-Solution Design</u>

The optimal water supply chain network associated with the identified solution for the model (*NC)* using the ELECTRE-IV method is shown in Fig. 5.13. Similarly to the *Fractional* and *2nd-ELECTRE-IV* designs, in this case only one source was used to supply freshwater to all the shale sites. Also, the obtained water management strategy uses a combination of onsite and CWT units as a regeneration/reuse purposes for all the shale sites. Similarly than in the *NC-solution* design, in this case, CWT plants were used to promote the follower operations. Consequently, this option controls the consumption of freshwater and uses the onsite treatments, proving a more balanced solution in comparison with the *NC-Solution* design.

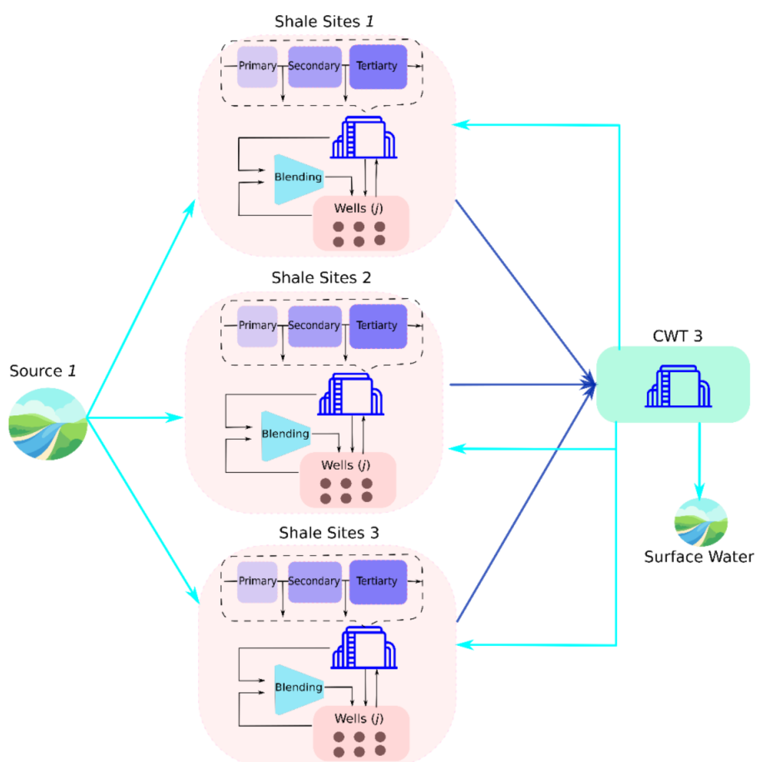

Fig. 5.13. Water supply chain network for *NC-ELECTRE-Solution*.

The global relation between profit and water consumption reaches a value of 14.67\$/bbl proving that this option takes best economic profit for a barrel of freshwater. Leader and follower, costs are \$653,275 and \$175,541 respectively while the benefits reach a value of \$81,283,000 and \$204,544 respectively. Notice that in comparison with the *NC-Solution* design, a small increment in the leader cost leads to an increase of three orders of magnitude in the follower benefits. The above clearly represents a more realistic solution for both entities.

Notice that the *NC-ELECTRE-Solution* design leads to a clearly better win-win situation compared with the design associated with the *NC-Solution*. Therefore, from these results it can be concluded that depending on the formulation of a non-cooperative problem the optimal solution may lead to non-desirable conditions. However, by applying the ELECTRE-IV method a feasible solution for non-cooperative environments can be identified from the pool of solutions produced under cooperative environments.

5.8.Final remarks

In this chapter, a systematic strategy to support decision-making processes for multi-objective multi-criteria problems has been proposed. The methodology consists of a combination of the traditional ε-constraint method to solve multi-objective problems and the ELECTRE-IV method as preference oriented multi-criteria decision-making tool to select the best one. The capabilities of this strategy have been successfully proved using as a test bed a multi-objective design and planning problem associated to a water network system within a shale gas production SC. Numerical results show that the proposed strategy is flexible enough to consider many objective/criteria's while facilitating decision making tasks, ensuring quality and avoiding subjectivity in the selection of the final solution. Additionally, a comparison against a fractional optimization strategy has been performed in terms of robustness and reliability.

Numerical results have proved that the ELECTRE-IV method is useful enough to identify a solution that better satisfies the decision maker preferences from different market situations (centralized and decentralized decision-making problems). Despite the fact that in the non-cooperative formulation several simplifications were considered and a traditional/simple solution strategy was applied, there is not a reason that hinders the application of such a methodology for larger/complex problems. Furthermore, the proposed strategy is a promising alternative to assess different challenges in the field of process systems engineering (such as sustainability, negotiation, etc.). In order to expedite the strategy performance, there is a need for a novel integrated strategy that allows defining a set of decision criteria.

In the future, the combination of the ELECTRE-IV method with other optimization strategies (such as fractional or fuzzy optimization) should be explored to expedite the generation of attractive and feasible solution from the optimization stages rather than be limited to select from a defined pool reducing the computational effort.

Despite the presented benefits of the ELECTRE-IV method to address decentralized schemes, a significant opportunity area to extend the proposed strategy is the explicit consideration of uncertainty for the third parties within an integrated framework. Chapter 9 shows such an extended formulation.

Finally, another important opportunity area is the assessment of the impact of the defined threshold over the final solution. The above becomes even more challenging if considering that the process conditions may constantly change, thus, the definition of these thresholds is critical. All these issues represent an important gap in the literature and such a limitation can be considered as one of the key future research topics.

5.9.Nomenclature

Abbreviations

MOO	Multi-objective optimization
MO	Multi-objective problems
SC	Supply chain
MILFP	Mixed integer linear fractional programming
MILP	Mixed integer linear programming
PSE	Process system engineering
ELECTRE	Elimination Et Choix Traduisant la Realité (Elimination and Choice Expressing Reality).
CWT	Centralized wastewater treatment plant
SO	Simple Objective
AHP	Analytical hierarchical processes
WSA	Weighted Sum approaches

Indexes

a	Number of solutions to be evaluated in the ELECTRE method $(a\|a = 1, \ldots, A)$
b	Number of solutions to be evaluated in the ELECTRE method$(b\|b = 1, \ldots, B)$
c	Centralized wastewater treatment site $(c\|c = 1, \ldots, C)$
cr	Number of decision criteria $(cr\|cr = 1, \ldots, CR)$
d	Disposal wells $(d\|d = 1, \ldots, D)$
e	Number of points to evaluate for the multi-objective $(e\|e = 1, \ldots, E)$
i	Shale sites $(i\|i = 1, \ldots, I)$
j	Wellbore $(j\|j = 1, \ldots, J)$
m	Transportation modes $(m\|m = 1, \ldots, M)$
n	Counter for the parametric approach
o	Onsite treatment level $(o\|o = 1, \ldots, O)$
ob	Objectives under analysis $(ob\|ob = 1, \ldots, OB)$
q	Onsite treatment unit capacities $(q\|q = 1, \ldots, Q)$
r	Transportation unit capacity $(r\|r = 1, \ldots, R)$
s	Freshwater suppliers $(s\|s = 1, \ldots, S)$
st	Storage tanks $(st\|st = 1, \ldots, ST)$
t	Time periods $(t\|t = 1, \ldots, T)$

Parameters

$Dem_{i,j}$	Total demand for well *j* in the shale site *i*
LB_{ob}	Lower feasible bound for the objective *ob*
$LC_{i,t}$	Recovery factor for the CWT treating wastewater from shale site *i*
NP	Total net present profit gained by shale gas production excluding the water management.
pt	Preference threshold
qt	Indifference threshold
Sol_a	Value for the solution *a*
Sol_b	Value for the solution *b*
UB_{ob}	Upper feasible bound for the objective *ob*
vt	Veto threshold
$VC_{i,c,t}$	Cost for treat wastewater coming from shale site *i* to CWT *c* at time *t*
Ω	Parametric approach parameter.
δ	Optimality gap
ε_o	Constraint value required for the ε-constraint method

Variables

cw	Total net present cost for the water management in the supply chain
$Frac$	Ratio of economic performance per unit of freshwater consumed.
$f_u(x,y)$	Upper-level objective function for bi-level problem
$F(\Omega)$	Fractional function.
$g_l(x,y)$	Lower-level objective function for bi-level problem
$h(x,y)$	Upper-level constraints for bi-level problem
$k(x,y)$	Lower-level constraints for bi-level problem
$m_p(a,b)$	Number of criteria for which *a* is strictly preferred to *b*
$m_p(b,a)$	Number of criteria for which *b* is strictly preferred to *a*
$m_q(a,b)$	Number of criteria for which *a* is weakly preferred to *b*
$m_q(b,a)$	Number of criteria for which *b* is weakly preferred to *a*
$m_i(a,b)$	Number of criteria for which *a* is considered indifferent to *b* but such that *a* has a better criterion value than *b*
$m_i(b,a)$	Number of criteria for which *b* is considered indifferent to *a* but such that *b* has a better criterion value than *a*
$m_o(a,b)$	Number of equal criterion values of a and b
nfw	Net freshwater consumption
$Profit$	Global system profit
$Profit_L$	Leader profit for the non-cooperative problem
$Profit_F$	Follower profit for the non-cooperative problem
$x^*_{e,ob}$	Optimal solution for each point e and each objective *ob*
x	Upper-level variables for bi-level problem
y	Lower-level variables for bi-level problem

Part III:

Uncertainty treatment strategies

Chapter 6

Efficient representation of uncertain parameters for energy generation

Besides the efficient operation management, the process sustainability highly depends on environmental factors, which are subject to different variations, for example, quality/quantity conditions for raw material resources. Analyzing and controlling the effect of these uncertain conditions is particularly challenging, which has to be addressed along with a multi-objective analysis seeking for the process sustainability. Thus, there is a need for integrated strategies that consider both, MO and uncertainty management approaches. Nevertheless, prior to the development of that holistic approach, the individual challenges associated to the uncertainty management should be addressed. Particularly, the core of this chapter addresses the efficient definition of the number of scenarios required to represent the unknown conditions; however, for continuity of this chapter a solution identification method will be used together with a scenario reduction one. The details and validation of the integrated framework will be addressed in the Part IV of this Thesis.

Thus, a solution strategy that combines a scenario reduction algorithm within the framework of a multi-objective formulation is proposed and explained in this chapter. Such a strategy is able to produce a fast and robust multi-objective optimization (MOO) while considering raw material uncertainties (more precisely quality and availability). The result consists of a set of dominant and feasible solutions, which are sorted using the ELECTRE-IV method as a way to identify the best overall solution.

6.1.Representation of uncertain process conditions

The fast environmental deterioration has motivated the scientific community to consider sustainability issues (such as water resources, atmosphere issues and alternative energy production) as the key challenges to be faced. In addition to the scientific motivation, the development and application of sustainable industrial processes have been strongly stimulated by government subsidies. Particularly, sustainability problems present multidisciplinary challenges at multiple scientific levels, which lead to the necessity of an integrated solution strategy. In fact, mathematical programming and, specifically, Process Systems Engineering (PSE) researchers are in a privileged position to address these issues. PSE community agrees that, in order to meet the highest sustainability standards, the optimization strategies should be improved within the framework of industrial symbiosis systems (IS) *(Cecelja et al., 2015)*. As commented in Chapter 2, there are two main challenges while addressing sustainability problems. First, the limitation inherent to any multi-objective (MO) problem *(Rojas-Torres et al., 2015)*, and second, the high complexity associated to the uncertainty assessment *(Grossmann et al., 2015)*. A lack of a framework capable to systematically address these challenges together introduces a significant bias in the solutions identified by current strategies; therefore, there is a necessity to develop strategies leading to robust and transparent methods to address them.

Studies regarding uncertainty approaches are vast in the PSE literature, focusing on the representation of the effect of uncertainty conditions over a process. They include reactive approaches, in which the knowledge of uncertainty is not explicitly taken into account, but most of them rely on the basic concept of proactive approaches where the robustness of the solution is guaranteed due to the in advance uncertainty description. The main advantages and disadvantages of those strategies to address SCM problems are clearly identified in Chapter 3 and the recent contribution of *Elluru et al., (2017)*. Among the most critical challenges, finding the optimal size of the uncertainty set so as to get an accurate forecasting of the uncertain parameters is the most important ones *(Moret et al., 2016, 2017)*.

Strategies such as two-stage stochastic programming *(You et al., 2009)*, robust optimization *(Deb and Gupta, 2006; Ben-Tal et al., 2009)* and chance constraint optimization *(Shapiro et al., 2009)* are commonly used as a way to model the effect of uncertain parameters over a process. However, in most of these strategies it is assumed that the larger the number of scenarios the better the uncertainty representation. This ideal approach very often leads to intractable situations due to computational limitations, which becomes a serious problem when addressing also a sustainability problem (or any other kind of MO problem). Thus, the amount of scenarios describing the uncertainty space remains as one of the main drawbacks for uncertainty management approaches. In this line, the use of scenario reduction approaches is a promising alternative.

As indicated in the broad description in section 3.4.1, scenario reduction methods allow selecting a small and representative amount of scenarios from a larger set (the original set). In spite of their relevance on uncertainty management approaches, these methods have been seldom studied until now. In fact, the most effective method to face such an open issue is the transportation distance-based method initially proposed by *Heitsch and Römisch, (2003)*. Recently, *Li and Floudas (2014a)* applied this strategy to minimize the Kantorovich distance among scenarios to find the optimal subset of scenarios that better represents the original set. This strategy was extended to introduce a sequential reduction framework with which a significant reduction in the computational effort was achieved *(Li and Floudas, 2016)*. In such a study, the selected set of scenarios is evaluated as a function of both, the input space (i.e. the values of uncertain parameters) and the output space (i.e. the objective value of optimization problem).

Despite their efficiency, most of the solution procedures based on scenario reduction techniques presented in PSE literature are applied to tailor-made approaches rather than developing a general framework. For example, *Costa et al. (2006)* use a discretization technique to reduce the scenario specification problem in a hydrothermal scheduling case. *Karuppiah et al., (2010)* presented a heuristic strategy for selecting scenarios based on an additive criterion to calculate the probabilities of the new scenarios and applied it to chemical planning problems. In very recent contributions, *Jeihoonian et al, (2017)* use the L-shaped method to design closed-loop supply, while *Alipour et al., (2017)* stress the importance of a proper scenario reduction tool for the management of energy uncertainties. Despite the efficient application of scenario reduction methods, systematic scenario reduction strategies have been never used in large-scale MO SC design and planning problems.

In this chapter, a scenario reduction method is applied within an optimization framework for the design and planning of a bio-based energy distribution network. For this purpose the study presented by *Pérez-Fortes et al., (2012)* has been modified to consider raw material availability and quality as uncertain parameters.

6.1.1. Background on the management of alternative energy sources

Energy management is a challenging sustainability issue addressed by the PSE community worldwide. Particularly, the development of processes that contribute to reduce fossil-fuels-based energy dependence *(Nie et al., 2016)* has gained attention, being biomass-based energy processes the most widely studied alternative *(Saxena et al., 2009; Dias et al., 2009)*. Since these processes rely on the energetic valorization of the biomass, literature focuses on studying/developing these techniques/strategies. Valorization techniques are based on either the reduction of the water content through a drying treatment or the reduction of particle size (thus reducing energy losses in further steps) by a chipping treatment. The definition of the conditions for biomass pre-treatment represents a key step for the efficient application of this processes at large scale. In fact, multiple strategies have been proposed, for example, *Panichelli and Gnansounou, (2008)* use torrefied wood (from forest wood residues) to produce energy by means of gasification. Later, *Magalhăes et al. (2009)* extend the evaluation of torrefaction and fast pyrolysis for the use of biomass in real processes. Such an evaluation considers prices, yields and operation costs of these pretreatment operations. In a recent literature review, *Madanayake et al., (2017)* presented a detailed description of the advantages and disadvantages of the most used pre-treatment strategies (i.e. mechanical, thermal, chemical, biological, or a combination of these). This review emphasizes the pre-treatment technical challenges, which become more difficult if considering the inherent uncertainties associated to raw material conditions, risk of equipment's failure, price fluctuations, demand variability, and weather conditions, among others.

Strategies addressing process management for MO problems under uncertainty have been already proposed in the literature. For example, *Guillén et al., (2005)* combine the standard ε-constraint method and branch and bound techniques to address the optimal design and retrofit problem of a SC, ensuring the maximum economic benefit and demand satisfaction. Later, *Gebreslassie et al., (2012)* use a mathematical model to minimize both, the annual cost and the financial risk for the design of a bio-refinery under supply and demand uncertainties; in such a work, they use a multi-cut L-shaped approach to circumvent the computational burden of solving large-scale problems. A similar strategy was used by *Ruíz-Femenia et al., (2013)* for the multi-objective optimization of environmentally conscious chemical SC under demand uncertainty; in such study, the variability of the Global Warming Potential (GWP) was accounted and represented using scenarios with given probability of occurrence. More recently, *Sabio et al., (2014)* propose a novel mathematical programming strategy to combine MOO tools and take advantages of the LCA modeling within an optimization under uncertainty. Despite the significant number of studies in this area, all the above strategies consider only bi-objective problems. Therefore, the application of these strategies for MO problems under uncertainty is considerably limited when more than two objectives are considered.

6.2.Problem statement

The design and planning problem of a centralized multi-echelon bio-based energy production SC subject to raw material uncertainties, as schematized in Fig. 6.1, is used as a paradigmatic example of the problem to be addressed.

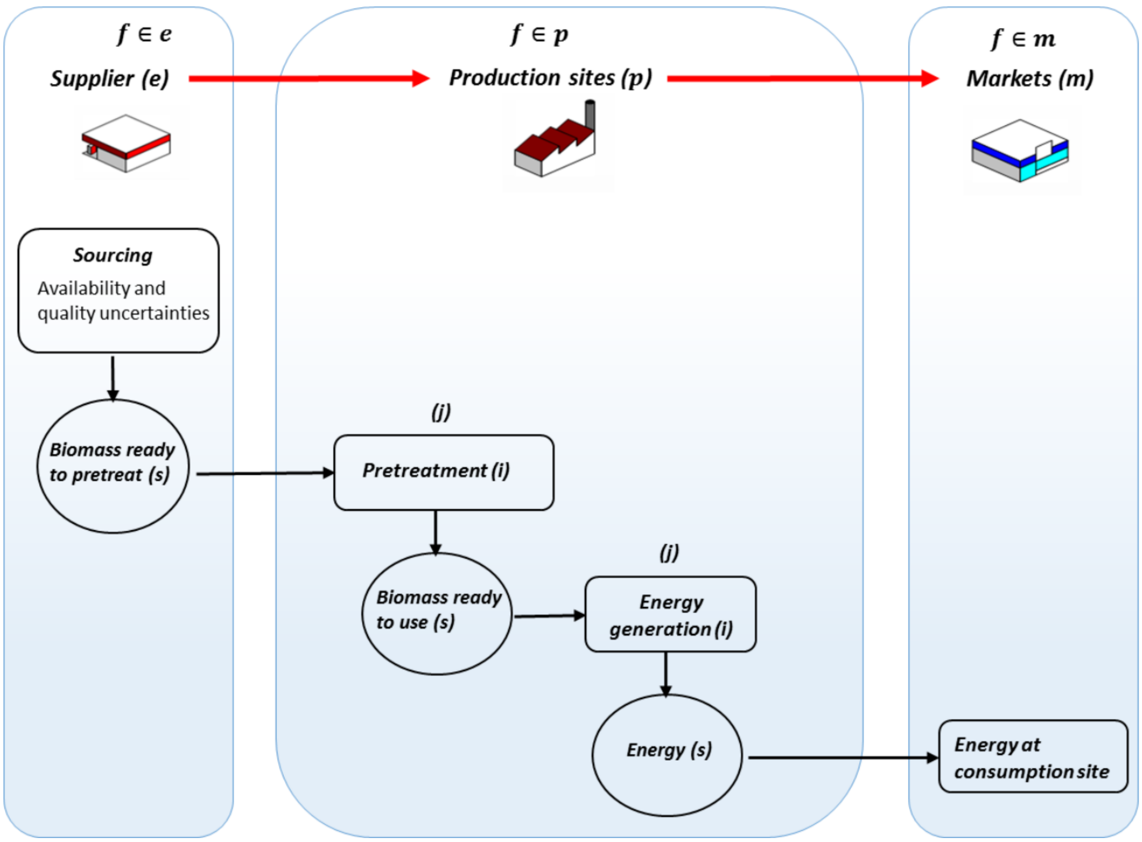

Fig. 6.1. General scheme for bio-based Supply Chain (Inspired on (Laínez-Aguirre et al., 2011).

Multiple types of uncertainty sources exist in bio-based energy generation systems. As commented, there is a major interest on determining a small subset of scenarios such that it can approximate the system behavior as close as the original set. The bio-based energy system used in this chapter has two main actors considered as the supplier (*e*) and the producer (*p*). Both actors are modeled in a unique supply chain management (SCM) problem, in which resource exchange is allowed. The exchangeable resources include raw material, and the energy generated which satisfies the demands (including the supplier requirements). Raw material availability and quality are considered uncertain parameters. The proposed approach is tested using a modified version of the case study presented by Pérez-Fortes et al. (2012). The raw material availability is modeled defining a given expected profile for each short-term period and supplier. The goal is to optimize the traditional design and planning decisions, such as the installation and capacity of the technologies (*j*) performing tasks (*i*) at locations (*f*); the distribution links among facilities; the biomass utilization at different conditions (*s*) and the expected storage levels at any period *(t)*. The objectives considered here include the expected net present value as an economic metric, the expected environmental impact of the entire SC, and the expected social performance, quantified via the opportunities of job creation. Remarkably, the most relevant mass and energy balances, as well as the associated constraints that describe the technologies involved are detailed in the following subsection while further information about the process data, equipment description and available capacities are described in ***Appendix B.4***.

6.2.1. Mathematical formulation

The following mathematical formulation follows a state task network (STN) form in which each activity is represented by a node and all the information is centralized in a single variable set. Such a variable ($P_{ijff'tc}$) must represent the specific activity i performed, using technology j receiving materials from site f and delivering to site f' at time t for scenario c. It is important to highlight that facilities f and f' are the same for treatment and pre-treatment activities, while for distribution activities f and f' must be different.

Material balances for material s must be satisfied at each network node as expressed in Eq. (6.1). A material conversion factor is used (represented by α_{sij} and $\bar{\alpha}_{sij}$). In order to facilitate the model development and further solution, predefined subsets of tasks that consume and produce material s are used ($\bar{T}_s$ and $T_s$respectively).

$$S_{sftc} - S_{sft-1c} = \sum_{f'} \sum_{i \in T_s} \sum_{j \in (j_i \cap \bar{J}_{f'})} \alpha_{sij} P_{ijf'ftc} - \sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in (j_i \cap \bar{J}_f)} \bar{\alpha}_{sij} P_{ijff'tc} \qquad \forall s,f,t,c \qquad (6.1)$$

For those activities in which the input is composed by a mixture of streams, the Eq. (6.2) should be used.

$$S_{sftc} - S_{sft-1c} = \sum_{f'} \sum_{i \in T_s} \sum_{j \in (j_i \cap \bar{J}_{f'})} \alpha_{sij} P_{ijf'ftc} - \sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in (j_i \cap \bar{J}_f)} \bar{\alpha}_{sij} P_{ijff'tc} + \sum_{i \in (T_s \cap \bar{I})} \sum_{j \in (j_i \cap \bar{J}_{f'})} Pv_{sijftc} - \sum_{i \in (\bar{T}_s \cap \bar{I})} \sum_{j \in (j_i \cap \bar{J}_{f'})} Pv_{sijftc} \qquad \forall s,f,t,c \qquad (6.2)$$

Eq. (6.3) was used in order to enforce the energy balance in which changes in the biomass heating value (HV_{sc}) are allowed due to pretreatment activities or the mixture of different biomass sources.

$$\sum_{s \in T_s} HV_{sc} * Pv_{sijftc} = \sum_{s \in \bar{T}_s} HV_{sc} * Pv_{sijftc} \qquad \forall i \in \bar{I}, f, t, c \qquad (6.3)$$

Since the biomass heating value highly depends on the feedstock moisture content ($Water_{sc}$), Eq. (6.4) is used to guarantee a $Water_{sc}$ value lower than its maximum ($Water_{ij}^{max}$).

$$\sum_{s \in S_i} Water_{sc} * Pv_{sijftc} \leq Water_{ij}^{max} \sum_{s \in \bar{S}_i} Pv_{sijftc} \qquad \forall i \in \bar{I}, j, f, t, c \qquad (6.4)$$

Together, Eqs. (6.3) and (6.4) model the energy required to achieve a certain degree of moisture content in the processed biomass. Thus, by allowing biomass mixture, these equations might affect the SCs design decisions.

Eqs. (6.5) and (6.6) represent equipment installation as well as capacity expansion, while the use of the well-known SOS2 variable (ξ_{jfktc}) is used to bypass non-linearities. Eq. (6.7) describes the total capacity F_{jftc} including its increment during the planning period t (FE_{jftc}).

$$\sum_{k} \xi_{jfktc} * FE_{jfk}^{limit} = FE_{jftc} \qquad \forall\, j \in \bar{J}_f, f, t, c \tag{6.5}$$

$$\sum_{k} \xi_{jfktc} = V_{jftc} \qquad \forall\, j \in \tilde{J}_f, f, t, c \tag{6.6}$$

$$F_{jftc} = F_{jft-1c} + FE_{jftc} \qquad \forall\, j \in \tilde{J}_f, f, t, c \tag{6.7}$$

Production rates are constrained by a minimum level (β_{jf}) and the available capacity, as described in Eq. (6.8). Similarly, Eq. (6.9) ensures the maximum biomass purchased from site f according to the availability uncertainty A_{sftc}. The electrical network is built through Eqs. (6.10) and (6.11) by using the binary variable $Z_{f'fc}$ for the energetic links. It is important to comment that the model allows a partially unsatisfied demand.

$$\beta_{jf} F_{jft-1c} \leq \sum_{f'} \sum_{i \in I_j} \theta_{ijff'} * P_{ijff'tc} \leq F_{jft-1c} \qquad \forall\, j \in \tilde{J}_f, f, t, c \tag{6.8}$$

$$\sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in \bar{J}_i} P_{ijff'tc} \leq A_{sftc} \qquad \forall\, s \in RM, f \in Sup, t, c \tag{6.9}$$

$$P_{ijff'tc} \leq M * Z_{f'fc} \qquad \forall\, s \in FP, i \in Mkt, f' \notin Mkt, t, c \tag{6.10}$$

$$\sum_{f'} \sum_{i \in T_s} \sum_{j \in \bar{J}_i} P_{ijf'ft,c} \leq Dem_{sft} \qquad \forall\, s \in FP, f \in Mkt, t, c \tag{6.11}$$

Without loss of generality, the total expected revenue was modeled using product sales in period t as stated in Eq. (6.12).

$$ESales_{ftc} = \sum_{s \in FP} \sum_{f' \in Mkt} Sales_{sff'tc} * Price_{sf't} \qquad \forall\, f \notin (Mkt \cup Sup), t, c \tag{6.12}$$

Overall operating costs are estimated by means of indirect and direct costs. Direct costs include fixed operating costs represented by Eq. (6.13), where $FCFJ_{jft}$ is the fixed unitary capacity cost of using technology j at site f. Indirect costs include the purchases from suppliers e, considering raw material purchases, transportation, and production resources at any scenario c (Eq. (6.14)).

$$FCost_{ftc} = \sum_{j \in \bar{J}_f} FCFJ_{jft} * F_{jftc} \qquad \forall\, f \notin (Mkt \cup Sup), t, c \tag{6.13}$$

$$EPurch_{etc} = Purch_{et}^{rm} + Purch_{et}^{tr} + Purch_{et}^{pr} \qquad \forall\, e, t, c \tag{6.14}$$

Raw materials acquisition ($Purch_{etc}^{rm}$) from suppliers e are accounted in Eq. (6.15). The associated cost is described by the variable X_{est} while Eq. (6.16) and Eq. (6.17) determine transportation and production costs, respectively. τ_{ijfet}^{ut1} represents the unitary production cost associated with performing task i using technology j, whereas τ_{ijfet}^{ut2} represents the unitary inventory costs of material s storage at site f. The parameters τ_{ijfet}^{ut1} and τ_{ijfet}^{ut2} entail similar assumptions to the ones considered regarding to α_{sij} and $\bar{\alpha}_{sij}$, since the amount of utilities and labor required by an activity are proportional to the amount of material processed.

$$Purch^{rm}_{etc} = \sum_{s \in RM} \sum_{f \in F_e} \sum_{i \in \bar{T}_s} \sum_{j \in J_i} P_{ijfftc} * X_{est} \qquad \forall\, f \in E_{rm}, t, c \qquad (6.15)$$

$$Purch^{tr}_{etc} = \sum_{i \in Tr} \sum_{j \in (J_i \cap \bar{J}_e)} \sum_{f} \sum_{f\prime} P_{ijfftc} * \rho^{tr}_{eff\prime t} \qquad \forall\, e \in \bar{E}_{tr}, t, c \qquad (6.16)$$

$$\begin{aligned} Purch^{pr}_{etc} = & \sum_{f} \sum_{i \notin Tr} \sum_{i \in \bar{T}_s} \sum_{j \in (J_i \cap \bar{J}_e)} P_{ijfftc} * \tau^{ut1}_{ijfet} \\ & + \sum_{s} \sum_{f \notin (Sup \cup Mkt)} S_{sftc} * \tau^{ut2}_{ijfet} \end{aligned} \qquad \forall\, e \in \tilde{E}_{prod}, t, c \qquad (6.17)$$

The required investment is calculated in Eqs. (6.18) and (6.19).

$$FAsset_{tc} = \sum_{j} \sum_{f} \sum_{k} Price^{limit}_{jft} * \xi_{jfktc} + \sum_{f} \sum_{f\prime} Invest^{MV} Distance_{ff\prime} Z_{ff\prime c} \qquad \forall\, t = 0, c \qquad (6.18)$$

$$FAsset_{tc} = \sum_{j} \sum_{f} \sum_{k} Price^{limit}_{jft} * \xi_{jfkt} c \qquad \forall\, t > 0, c \qquad (6.19)$$

Eq. (6.20) represents the calculation of profit at each period. Finally, the rate of return used in a discounted cash flow analysis to determine the *NPV* is computed by means of Eq. (6.21).

$$Profit_{ftc} = ESales_{ftc} - \left(FCost_{ftc} + \sum_{e} EPurch_{eftc} \right) * X_{est} \qquad \forall\, f, t, c \qquad (6.20)$$

$$NPV_c = \sum_{f} \sum_{t} \left(\frac{Profit_{ftc} - FAsset_{ftc}}{(1 + rate)^t} \right) \qquad (6.21)$$

All the environmental interventions are quantified through characterization factors (Eq. (6.22)). The environmental impact of site f, due to the activities *i*, is calculated through the variable IC_{aftc}. Variable $\psi_{ijff\prime a}$ is used to characterize the environmental impact factor for a specific task i performed using technology j, receiving materials from node f and delivering them at node f' for each environmental category a.

$$IC_{aftc} = \sum_{j \in \tilde{J}_f} \sum_{i \in I_j} \sum_{f\prime} \psi_{ijff\prime a} * P_{ijff\prime tc} \qquad \forall\, a, f, t, c \qquad (6.22)$$

The value of the environmental impact factor $\psi_{ijff\prime a}$ is linked to transport as stated in Eq. (6.23). Here, ψ^{T}_{ija} represents the a environmental impact factor associated to the material transported over a given distance. It is important to emphasize that the environmental impact in distribution activities is assigned to the origin node.

$$\psi_{ijff'a} = \psi^{T}_{ija} * Distance_{ff'} * Tortuosity \qquad \forall\, i \in Tr, j \in J_i, a, f, f' \qquad (6.23)$$

Eq. (6.24) introduces $DamC_{gftc}$ variable, which is a weighted sum of all environmental interventions. They are combined using g endpoint damage factors ζ_{ag}, normalized with $NormF_g$ factors, as states the LCA method (Bojarski et al., 2009). Moreover, Eq. (6.25) calculates g normalised endpoint damage along the SC ($DamC^{SC}_{gc}$).

$$DamC_{gftc} = \sum_{a \in A_g} NormF_g * \zeta_{ag} * IC_{aftc} \qquad \forall g, f, t, c \qquad (6.24)$$

$$DamC_{gc}^{SC} = \sum_f \sum_t DamC_{gftc} \qquad \forall g, c \qquad (6.25)$$

Eq. (6.26) sums the endpoint environmental damages for each site f,

$$Impact_{fc}^{2002} = \sum_g \sum_t DamC_{gftc} \qquad \forall f, c \qquad (6.26)$$

For further details regarding the operational and environmental formulation, the interested reader is addressed to (Pérez-Fortes et al., 2012; Laínez-Aguirre et al., 2009).

Objective function.

The expected NPV is defined as in Eq. (6.27)

$$ENPV = \sum_c NPV_c * prob_c \qquad (6.27)$$

Where $prob_c$ represents the probability of occurrence of scenario c. Eq. (6.28) calculates the expected environmental impact as a function of the probability of occurrence of scenario c.

$$Impact_{overall}^{SC} = \sum_f \sum_t \sum_g \sum_c DamC_{gftc} * prob_c \qquad (6.28)$$

Without loss of generality, the social impact is associated with the number of required working places, which promote the economic activation and will lead to an improvement in the lifestyle of the community around the industry. Therefore, the social criterion employed is the number of sites that have a treatment or pre-treatment system installed as shown in Eq. (6.29). V_{jftc} is a binary variable that characterizes the number of units installed per site so this criterion assigns a value of 1 to each unit installed per site f.

$$SoC_c = \sum_j \sum_f \sum_t V_{jftc} \qquad \forall c \qquad (6.29)$$

It is worth noticing that in order to ease the formulation of the MO problem Eq. (6.30) introduces the expected SoC impact as a function of the probability of occurrence $prob_c$.

$$ESoC = \sum_c SoC_c * prob_c \qquad (6.30)$$

It is important to highlight that the proposed social performance calculation is less efficient than other methods, such as social life cycle assessment. However, here the social performance it is used as a crude assessment to illustrate its effect on the solution selection in the proposed method.

6.3. Methodology

The proposed solution strategy consists of four steps: deterministic optimization, scenario reduction, stochastic optimization and solution selection. A detailed description of each step, including the specific methods/algorithms used, is provided in the following subsections. Additionally, the general algorithm of the presented solution strategy is shown in Fig. 6.2.

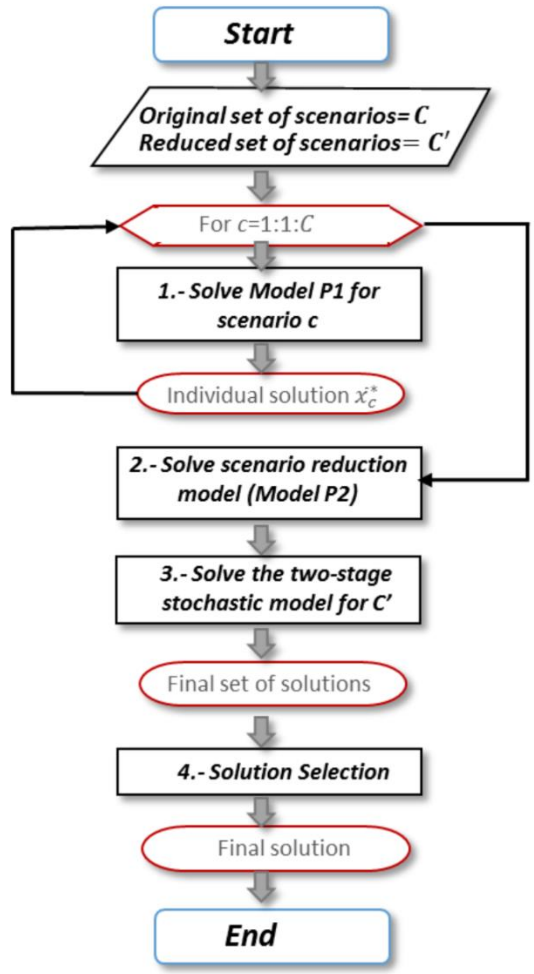

Fig. 6.2. A detailed description of the solution strategy proposed.

6.3.1. Deterministic optimization.

The first step of the proposed strategy consists in an iterative procedure for the deterministic optimization for each scenario in the original set of them. Such an optimization is required, since the results of each scenario are later used for the scenario reduction part of this strategy.

The based model has the following general form (see Eq. (6.31)), and will henceforth know as *Model P1*:

$$\begin{aligned} &Model\ P1 \quad \max_{x\ y_c} \{fo_1(x,y_c), fo_2(x,y_c), fo_3(x,y_c)\} \\ &s.t. \\ &\qquad h(x,y_c) = 0 \qquad \forall c \in C \\ &\qquad g(x,y_c) < 0 \qquad \forall c \in C \\ &\qquad x \in X, y_c \in Y \end{aligned} \tag{6.31}$$

Notice that even if this model is a MO, multi-scenario two-stage stochastic one, according to the proposed solution strategy (see Fig. 6.2) the same model has to be solved twice. At stage 1, for each one of the elements within the entire original set of uncertain parameters (deterministic MILP optimization) and at stage 3 for the entire reduced set of the uncertain parameters (two-stage stochastic MILP optimization). Additionally, note that during the deterministic optimization the only objective function considered is the economic one (i.e., environmental and social impacts are calculated in parallel during the process, but they never act as objective functions). It is important to comment that a complex objective function that accounts for more than one objective can be applied, however in order to facilitate the result reproduction and comparison a single economic objective was used.

From *Model P1*, $fo_{ob \epsilon OB}$ represents the different objective functions considered in the problem (in this particular case $fo_1 = ENPV$, $fo_2 = -Impact^{2002}_{overall}$, $fo_3 = ESoC$). x represents the first-stage decision variables, $\mathrm{y_c}$ the second-stage decision variables and c the uncertain parameters values that belong to the uncertain parameters space ϕ. $h(x_c, y_c)$ and $g(x, y_c)$ are vectors of equality and inequality constraints representing the constraints described in the model (Eqs 6.1-6.30).

Notice that in both, deterministic and stochastic model, the decision variables for the design and planning are the same. Since the reduced set of scenarios is expected to "mimic" the performances of the original set. Thus, the performance of the reduced set of scenarios is compared against the expected performance considering the whole set.

6.3.2. Scenario reduction algorithm.

The second step of the proposed strategy consists of a scenario reduction method, able to produce a reduced set of scenarios that properly represents the original distribution.

In order to apply such an algorithm the following elements are required:

- A general set of scenarios/samples *C* with their associated probability (summation equals one). It is important to highlight that the scenario probabilities may not necessarily be the same for all the samples.
- A reduced set of scenarios *C'*. All the elements in the reduced set are part of the main set of scenarios *C*. The probabilities associated with the preserved scenarios have to be updated (so that their summation is 1).

The scenario reduction strategy is inspired in the clustering-based algorithm proposed by *Li and Li (2016)*. Such a strategy considers that the subset of elements represents the cluster centers while the nearest scenarios compose the clusters themselves.

The scenario reduction process compromises four sequential steps, being the cluster centers initialization, the clusters generation associating the remaining scenarios to each cluster center, the evaluation of the cluster centers performance, and the cluster centers updating. This process has to be repeated until a defined tolerance is achieved. A graphical representation of the scenario reduction algorithm is displayed in Fig. 6.3.

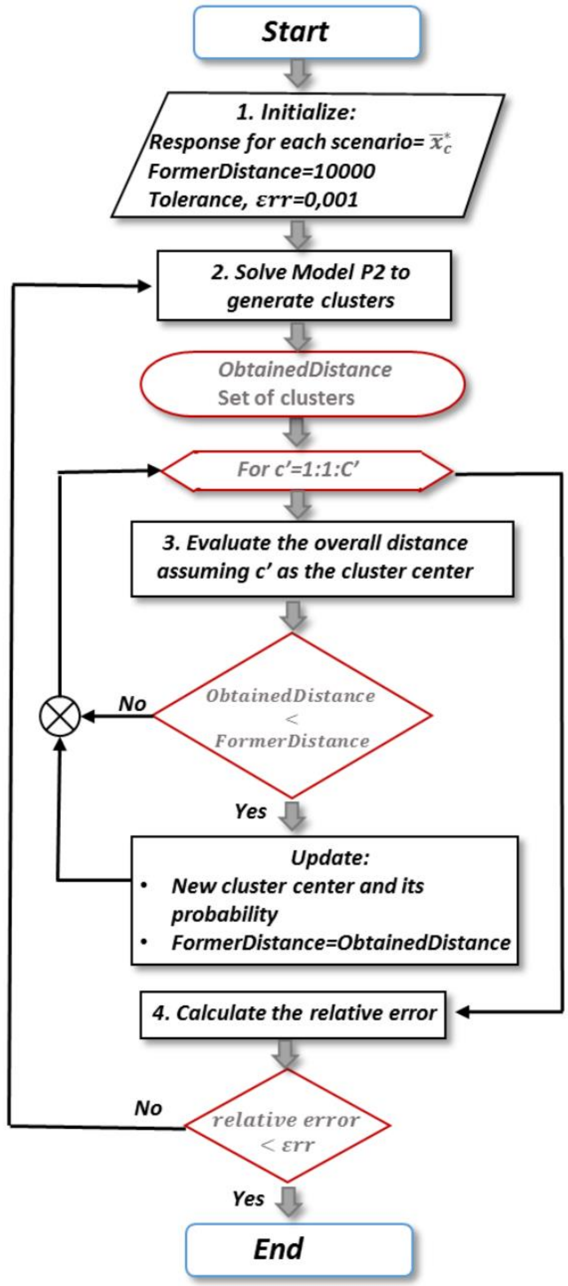

Fig. 6.3 The scenario reduction algorithm.

During initialization step, a set of cluster centers are generated. Here, a random selection among the already existing scenarios was used; however, this selection may be performed using a more sophisticated sampling technique such as k-means clustering method. Since further cluster centers updates will be required, the set of initial samples does not compromise the global performance of the proposed strategy (Li and Floudas, 2016).

In step 2, the *Model P2* has to be generated and solved. *Model P2* adopts the form of a general mixed integer programming-based scenario reduction model described by Li and Floudas (2014a). A brief description of such a formulation is next presented.

$$Model\ P2 \qquad \min\ Distance = \sum_{c \in C} \sum_{c' \in C'} n_{c,c'}\, cd_{c,c'} + funct_{err}^{exp}$$

s.t.

$$\sum_{c \in C} yy_c = N \tag{6.32}$$

$$\sum_{c' \in C} v_{c,c'} = yy_c \qquad \forall c \in C \tag{6.33}$$

$$0 \leq v_{c,c'} \leq 1 - yy_c \qquad \forall c, c' \in C \tag{6.34}$$

$$\sum_{c \in C} n_{c,c'} = p_{c'}^{new} \qquad \forall c' \in C' \tag{6.35}$$

$$\sum_{c' \in C'} n_{c,c'} = p_c^{orig} \qquad \forall c \in C \tag{6.36}$$

$$funct_{err}^{exp} \geq -\sum_{c' \in C'} p_{c'}^{new} funct_{c'} + \sum_{c \in C} p_c^{orig} funct_c \tag{6.37}$$

$$funct_{err}^{exp} \geq \sum_{c' \in C'} p_{c'}^{new} funct_{c'} - \sum_{c \in C} p_c^{orig} funct_c \tag{6.38}$$

$$cd_{c,c'} = \sum_{t=1}^{T} |\lambda_c^t - \lambda_{c'}^t| \tag{6.39}$$

$$p_{c'}^{new} = (1 - yy_{c'}) p_{c'}^{orig} + \sum_{c \in C} v_{c,c'} p_c^{orig} \qquad \forall c' \in C' \tag{6.40}$$

$$n_{c,c'} \geq 0, \qquad \forall c \in C, \forall c' \in C' \tag{6.41}$$

$$yy_c \in \{0,1\}, \qquad \forall c \in C \tag{6.42}$$

From the above formulation *c* and *c'* represent scenarios in the superset (*C*) and the subset (*C'*) respectively. The associated probability for each scenario in the original superset is represented by p_c^{orig} while $v_{c,c'}$ express the probability of scenario *c* to be associated to scenario *c'*. yy_c is the key binary variable that denotes whether a scenario is "transported" ($yy_c = 1$) or a preserved one ($yy_c = 0$). The probability of scenario *c'* is expressed through the variable $p_{c'}^{new}$ ($p_c^{new} = 0$ if scenario *c* is removed). In the formulation, one of the key parameters is $cd_{c,c'}$ which defines the distance between two scenarios. Here, such a distance is modeled using the Manhattan distance (Eq. 6.39) in which the realization of the *t* uncertain parameter associated to each scenario is represented by λ_c^t.

One of the most important features of the above model is that it minimizes the probabilistic distance in both the parameter space and the output space (i.e. the expected performance of the objective value). In order to model such a feature, the difference between the expected objective value obtained by the original and by the reduced set of scenarios has to be explicitly included in the main objective function of the scenario reduction algorithm ($funct_{err}^{exp} = \left|funct_{orig}^{exp} - funct_{new}^{exp}\right|$). At this point is where the deterministic optimization performed in the step 1 becomes relevant. Here, $funct_c$ is the objective value obtained by scenario *c*, $funct_{orig}^{exp} = \sum_{c \in C} p_c^{orig} funct_c$ is the expected value of the objective value of c the original scenario set, and $funct_{new}^{exp} = \sum_{c' \in C'} p_{c'}^{new} funct_{c'}$ is the one for the c*'* preserved scenario set. More details about the scenario reduction algorithm can be found in *Li and Floudas, (2014a)*.

From the *Model P2* (step 2), the clusters are defined using as a basic idea that a scenario belongs to a specific cluster when the distance between the scenario location and the cluster center is minimum (compared with the rest of cluster centers). The above is justified assuming that the lower the distance between *c* and *c'*, the smaller the difference in the uncertainty realization. Parallel to the definition of the clusters, *Model P2* allows the calculation of scenario probabilities for the reduced subset. These probabilities are obtained through the summation of the individual probabilities of all the scenarios belonging to the cluster.

Even if by introducing an initialization step, the clusters centers can be identified faster, this do not affects the strategy performance, thus, the cluster initialization has been neglected. The third step of the scenario reduction strategy consists on a dynamic evaluation of the clusters in order to update the cluster centers according to the obtained distances associated to the value of the uncertainty parameters. This evaluation consists of defining each scenario as the center of the cluster and calculates the associated displacement (i.e. Manhattan distance). This procedure has to be repeated until all the scenarios in the cluster were evaluated. The scenario with the lower overall distance to the rest of scenarios in the same cluster is defined as the new cluster center since it better represents the whole cluster. The probability associated with the new center is the same since the group remains equal.

At the end of the evaluation step procedure (step 3), the elements in the reduced set of scenarios are the best possible representation of the original distribution for the initially defined clusters. However, since the cluster centers were moved, there is a chance that some of the scenarios belonging to one cluster would be better allocated to another cluster. In order to avoid such an issue and to ensure the representativeness of the subset of scenarios within the global original superset (*C*), a relative error has to be calculated and compared with a defined tolerance value (typically *err*=0.001). Such a relative error is calculated following the general form, which can be represented as:

$$relative\ error = \frac{Distance_{n-1} - Distance_n}{Distance_{n-1}} \tag{6.43}$$

Where $Distance_n$ represents the displacement (i.e. Manhattan distance) obtained after solving the overall procedure for iteration n. Therefore, until the relative error is lower than the tolerance value, the entire process has to be repeated iteratively for the new cluster centers generated in the step 3.

6.3.3. General two-stage stochastic programming model.

As commented before, the *Model P1* has to be solved for this section as well (Stage 3 of the proposed strategy (Fig. 6.2)). In this section, the reduced set of uncertain parameters was considered (two-stage stochastic MILP optimization). Note that this set (as well as the probabilities of occurrence of each member of this set) differ from those used at the beginning of the scenario reduction approach. In addition, for this part of the solution strategy all the SC decisions were taken by the simultaneous optimization of the three objectives.

As commented before, the typical design and planning decision variables are considered in this step. In addition, the variables that are subject to uncertainties includes exchange of materials (raw material, treated mass or energy), fraction of materials blended to produce energy, amount of water extracted from the raw material, total revenues as well as location and amount of treatment/pretreatment units installed.

6.3.4. Solution selection procedure (ELECTRE-IV algorithm)

Because of the second step in the proposed solution strategy (scenario reduction), a reduced set of scenarios is obtained. However, even if such a reduction significantly expedites the uncertainty representation task, the decision-making task associated with the MO part of the problem remains unsolved. Therefore, a method that systematically selects a unique and robust solution is needed (step 4 of the proposed solution strategy). The use of the well-known ELECTRE-IV method is again a promising alternative to overcome this limitation.

6.4. Case study

A real-life case study previously studied by *Pérez-Fortes et al. (2012)* has been used to illustrate the application of the proposed procedures. Particularly, nine communities in a rural area of Ghana, Africa (Atebubu-Amantin district) may play simultaneously the role of biomass producers, energy generators and consumers. For this case study, 40 different biomass states (s) have been identified as the input/output conditions for the six available transformation technologies (j) considered, which include treatment, pre-treatment and transportation tasks, resulting in 79 activities (i) each one consisting on a pair of biomass state-processing or biomass state-transportation combinations. These activities, if required, should be developed in one or more of the 31 considered sites (f): nine suppliers, nine potential pre-treatment and/or treatment sites, nine markets and four additional sites in which a treatment unit can be installed. Detailed data regarding the situation considered in this study can be found in Appendix B.4. A planning horizon of 10 years with an annual interest rate of 15% is used which is a typical time horizon in this type of SC`s *(Seider et al., 2009)*.

The scope of this chapter is limited to provide an effective strategy to address the challenges associated with the use of a large set of scenarios to represent process uncertainties within a MOO problem. Consequently, technical challenges such as temporal electricity supply (e.g., electricity storage, switching on/off the transfer grid, availability of power supply in certain hours of a day etc.) are out of this scope. Additional studies, extending this formulation and addressing electricity supply challenges, are also required to explore the differences in the solution in terms of economic, environmental and social performances.

Cassava Rhizome (CR) was considered as raw material for energy production, mainly for the abundance of Cassava crop in the region under study. The raw material properties considered as uncertain parameters in the analysis include Cassava availability, Lower Heating Value and Moisture Content (LHV and MC respectively). From historical data, their average values per community are used to generate an initial set of 100 scenarios assuming a normal distribution and a variance of 30% (see Table 6.1).

The drying and chipping processes were considered as potential pre-treatments, since they are more suitable for rural areas in developing countries. Cassava Rhizome is pre-processed before gasification to obtain the required shape and MC for further processing steps. As commented before, each community represents a unique supplier-production-consumer site. All the communities could be connected to a specific-built low voltage (energetic self-sufficiency) or medium voltage micro grid in order to export energy to other communities and/or receive energy from the grid (LV and MV respectively).

Table 6.1 Average values for biomass properties at each community in Atebubu-Amantin district.

	*Water**	*LHV(MJ/kg)*	*Availability (Tons)*
Senso	0.425	10.61	12.74
Old Konkrompe	0.426	10.56	24.39
Fakwasi	0.427	10.51	81.10
Kunfia	0.429	10.46	122.18
Trohye	0.431	10.40	16.22
Bompa	0.432	10.34	22.07
Nwunwom	0.434	10.28	5.272
Boniafo	0.436	10.22	21.08
Abamba	0.438	10.15	28.15

* This values are expressed as a weight fraction

As well as in the originally proposed case study, a LCA was performed using the Impact 2002+ indicator and the Ecoinvent database as a way to quantify the environmental impact *(Ecoinvent, 2008; Simapro, 2008*), in order to maintain coherence with previous results). The LCA analysis considers the same traditional 15 mid-point categories associated to biomass production (Cassava waste), transportation, pre-treatment (chipper and dryer) and generation of electricity through biomass gasification. Detailed information about the environmental analysis of this case study can be found in *Pérez-Fortes et al., (2012)*.

The objective is to select the most suitable processing units (including their capacities and locations), the best way to interconnect the various elements of the supply chain (i.e., providers, intermediates and consumers), and the adequate biomass storage/transport flows in order to make the best use of biomass as feedstock. The solution obtained will be compared with the originally presented results, in order to highlight the effects of the reduction of scenarios over the overall solution space.

6.4.1. Scenario reduction solution. First case.

Deterministic solution analysis and Scenario reduction

For this study, 100 scenarios have been randomly generated using as a mean value the average values for the uncertain parameters (biomass availability and properties) as shown in Table 6.1. Without loss of generality, such a set was used for two reasons. On the one hand, ensuring a sufficiently large set of scenarios stresses the capabilities of proposed methodology to handle a large number of scenarios in the original set, and thus, evaluating the computational effort required (evaluating the methodology time efficiency). On the other hand and since in this case the model uncertainties were assumed independent (alike in previous works) by considering a larger set of scenarios it is ensured that the original set is representative enough. Besides, in order to ensure the representativeness of the original set, an additional analysis was carried on varying the size of the set of scenarios between 25 and 150. Using these results, the plot below (Fig. 6.4) demonstrates that any increment in the original set of scenarios (<100) leads to a small variation in the final solution (less than 1%), while lowering the number of scenarios exponentially increases such a difference.

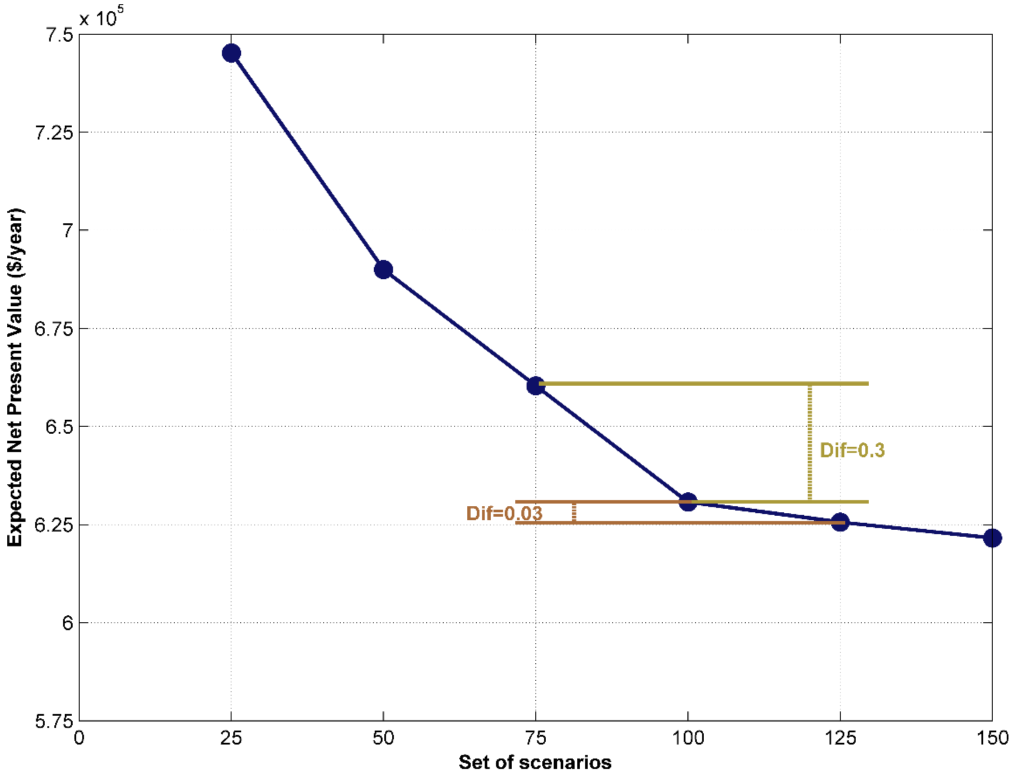

Fig. 6.4. ENPV performance for each set of scenarios

The mathematical model has been written in GAMS and the problem has been solved using CPLEX 11.0 on a PC Intel(R) Core(TM) i7-2600M CPU 2.70 GHz and 16.00 GB of RAM. The deterministic model contains 17,328 equations, 144,703 continuous variables and 186 binary variables and the whole optimization process entails a CPU time of approximately 10,000 seconds.

Deterministic optimizations were performed using the economic performance (NPV) as unique objective, although a MO analysis will be performed in the following steps of the strategy. After the optimization procedure, 100 solutions were obtained. Individually, they represent a poor approximation for the global problem; however, they may be used to evaluate the "similarity" among sets of scenarios of different dimensions. Thus, using the NPV values for the complete set of 100 solutions, a reduced set of 10 scenarios with their probability of occurrence can be obtained following the algorithm described in Section 6.4.2. The scenarios are strategically allocated in order to represent better both, the input (uncertain conditions) and output (expected economic performance) data. Fig. 6.5 compares the original scenario distribution against the reduced set of scenarios, while Table 6.2 shows the probability of occurrence for the new set of scenarios.

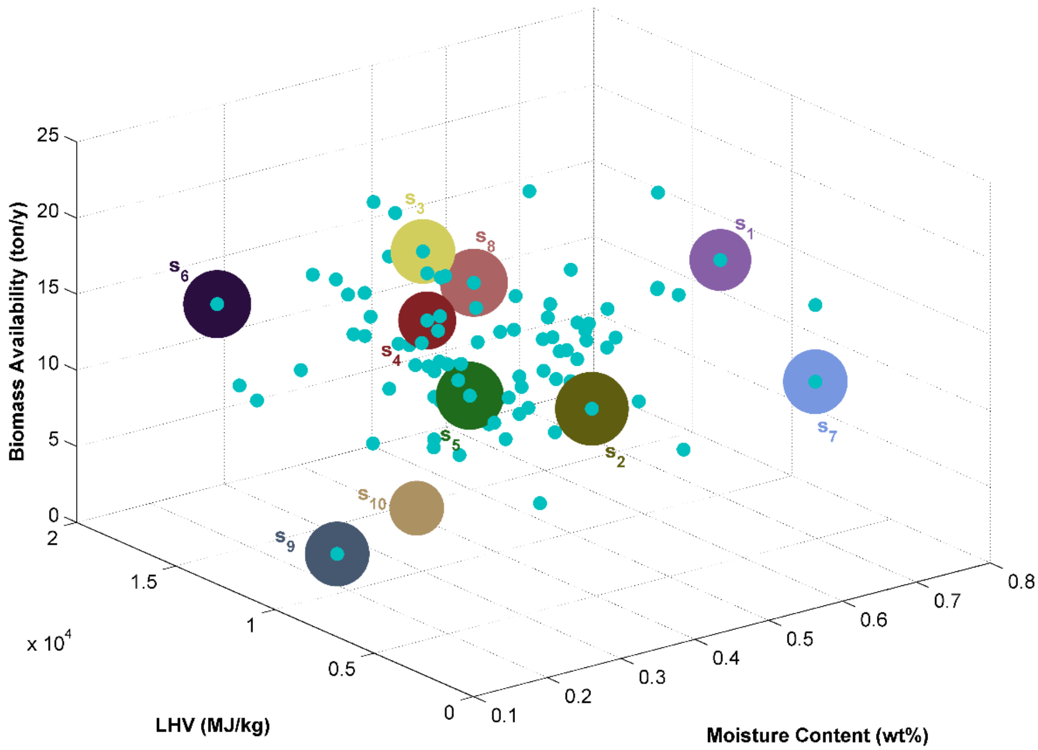

Fig. 6.5 Input uncertainty representation for the original and reduced set of scenarios for the Senso community (the diameter of each scenario represents the probability of occurrence).

Fig. 6.5 was used as a way to visualize the relationships between the original and the reduced sets of scenarios for the three uncertain conditions (LHV, Biomass availability and MC). Notice that the reduced set produces a well-balanced distribution considering simultaneously the three uncertain parameters.

Remarkably, the strategy has the capacity to adjust the probability of occurrence as a function of the number of scenarios belonging to the new subset. Such an adjustable probability provides the required flexibility to mimic accurately the original uncertainty distribution. Notice that s_2, s_5, s_6 and s_8 are the scenarios with higher probability compared with the mean value (*probability >> 0.1*). On the contrary, s_1, s_4 and s_{10} can be considered as "minor" scenarios since their probability is lower than the mean (*probability << 0.1*) suggesting that a further scenario reduction is still feasible (for example, from 10 to 7). For example, s_4 may be merged with one of the closest and "more important" scenarios (such as s_3, s_5 and s_8). Nevertheless, the selection of these scenarios is conditioned to both, the third uncertain condition as well as the output criteria in order to reduce the gap between sets.

Table 6.2 Probability of occurrence for each set within the reduced set of scenarios.

	Scenario									
	s_1	s_2	s_3	s_4	s_5	s_6	s_7	s_8	s_9	s_{10}
Probability	0.09	0.13	0.1	0.08	0.11	0.11	0.1	0.11	0.1	0.07

As commented before, the economic objective was used as the single “similarity” criteria in order to evaluate the output performances. Therefore, the economic behavior between the original and reduced set of scenarios was compared, obtaining a difference of less than 0.0005%. In other words, the reduced set of scenarios reaches an optimal value of $ 636,143.5, while the best economic performance for the original set was $ 636,146.4. A comparison between both designs is next presented.

Design and Planning comparison for different sets of scenarios

In order to validate the reduced set representativeness, a comparison of the designs obtained after solving the *Model P1* for both, original and reduced sets was performed. Note that even if *Model P1* is a MO model, the *ENPV* value was considered as the only objective function for comparison purposes. The reason for this is that the application of any MOO approach for a large number of scenarios leads to a computationally intractable problem.

Table 6.3 Equipment capacity for the optimum networks configurations obtained for the different sets of scenarios.

	Reduced Set of Scenarios			*Original Set of Scenarios*		
	Dryer (t/h)	*Chipper (t/h)*	*G-ICE (kWe)*	*Dryer (t/h)*	*Chipper (t/h)*	*G-ICE (kWe)*
Senso	-	-	-	-	-	-
Old Konkrompe	0.126	0.1	168.97	0.17	0.1	168.98
Fakwasi	0.218	0.1	243.30	0.24	0.1	241.74
Kumfia	0.302	0.135	360.00	0.31	0.12	316.93
Trohye	0.1	0.1	90.88	-	-	-
Bompa	-	-	-	-	-	-
Nwunwom	-	-	-	-	-	-
Boniafo	-	-	-	-	-	-
Abamba	0.1	-	-	0.1	0.1	97.48
Extrasite1	-	-	-	-	-	-
Extrasite2	-	-	-	-	-	-
Extrasite3	-	-	-	-	-	-
Extrasite4	-	-	-	-	-	-

For the reduced set of 10 scenarios, a direct two-stage stochastic programming strategy was applied while for the case of 100 scenarios, the *Model P1* was solved following a sample average approximation (SAA) strategy described in Chapter 3: first only one scenario at a time is considered and only a single-objective (*NPV*) optimization is addressed; after this, the obtained first-stage variables (i.e., the design of the supply chain) are fixed and the optimization of the *ENPV* in *Model P1* considering all the |C| scenarios simultaneously is addressed. Table 6.3 shows the technologies to be installed at each specific site as well as their capacities, according to the results obtained using this is strategy.

Table 6.3 shows that the final design is different for each set of scenarios, being the location of the treatment/pretreatment units their main difference. Remarkably, these units were installed as a group (Dryer, chipper and G-ICE together). Note that the fact that the set of 100 scenarios was solved using an approximation technique may explain the small differences in both designs. The SAA procedure, although reliable, does not guarantee a globally optimal solution, as does the stochastic programming. Therefore, since the difference in the expected economic objective is lower than 0.001% and the design is partially the same, the solution for the reduced set of scenarios should be considered accurate and at least equally reliable as the full-space solution.

<u>Traditional MO analysis. Design and Planning</u>

For the completeness of the work, after the validation of the reduced set of scenarios, a MOO is carried out in order to identify the best solution. In this case, the economic, environmental and social performances ($ENPV, EImpact_{overall}^{2002}$ and $ESoC$ respectively) were considered, and the optimization was implemented through the well-known ε-constraint method. The two-stage MO-MILP model was written in GAMS and solved using CPLEX 11.0 on a PC Intel(R) Core(TM) i7-2600M CPU 2.70 GHz and 16.00 GB of RAM. A total of 172,020 equations, 1,505,017 continuous variables and 204 binary variables were obtained and each iteration entails a CPU time of approximately 6,500 seconds.

Resulting from the individual optimization of each objective, the boundaries (i.e. anchor points) were identified and collected in Table 6.4. The best expected economic performance is $\$5.83 \text{x} 10^5$, which becomes zero for the best environmental and socially friendly networks respectively. In environmental network due to the best environmental choice, do not operate at all, while in the socially friendly network due to unnecessary expenses (installation and transportation costs for instance) that reduces the benefit to zero. Logically, this result is highly economically undesirable, but provides a feasible lower bound on the process performance.

Table 6.4 Individual performances at each single objective optimization

	Economic optimization	*Environmental optimization*	*Social optimization*
$ENPV$ ($)	583917.4	0	0
$EImpact_{overall}^{2002}$	1.2864	0	1.4054
$ESoC$	13	0	27

While optimizing $ENPV$, the $EImpact_{overall}^{2002}$ indicator keeps a considerably high value since it is reduced only by 9%, compared with its worst performance ($ESoC$ optimization). The best expected environmental performance is "reached" when the process is stopped at all. Logically, this situation is undesirable; however, it is in fact a feasible extreme solution. The highest environmental impact was found while considering a single $ESoC$ optimization, mainly due to the large amount of transported material and production emissions. It is important to notice that $ESoC$ maximum value was considered as 27 since it was assumed that all the pretreatments/treatments options were installed at all the feasible locations.

Without loss of generality, the three objectives were analyzed simultaneously using the well-known ε-constraint method. Such a method provides as a result a set of feasible solutions that belong to the Pareto surface of $ENPV$ vs $EImpact_{overall}^{2002}$vs $ESoC$ (see Fig. 6.6). From Fig. 6.6, it can be inferred that for lower value of $ESoC$ the economic objective ($ENPV$) increases, at the expense of the depletion in the environmental objective function ($Impact_{overall}^{2002}$), which demonstrates the conflict between the objectives. As commented before, one of the extreme solutions is highly undesirable (i.e. lower $Impact_{overall}^{2002}$) and may be removed beforehand. However, although in Fig. 6.6 that point has been removed, these easily identified undesirable solutions will be maintained in further steps of the solution selection strategy in order to prove its sensitivity. From Fig. 6.6, it can be also noticed that Pareto solutions with high environmental impact (high expected environmental indicators) lead to the same $ENPV$ and $EImpact_{overall}^{2002}$ performances. Additionally, when the social criteria range goes below 16, there is no significant change in the economic and environmental performance. On the contrary, for social criteria values greater than 16, the performance of the others gradually decreases. It is worth mentioning that these values range from \$5.6x10^5 to \$5.44x10^4 and from 0.2 to 1.0 for the economic and environmental performance, respectively. As can be seen from Fig. 6.6 the system is slightly sensitive to the social indicator. For instance, a change in the social indicator (iso-lines) has a small impact in the performance for the other two indicators. The above is evident since the social impact represents the number of treatment/pretreatment units installed, however the location is not fixed and in fact such a location depends on the rest of objectives. Conversely, for a defined/fixed social value, the other two objectives have a significant impact over each other.

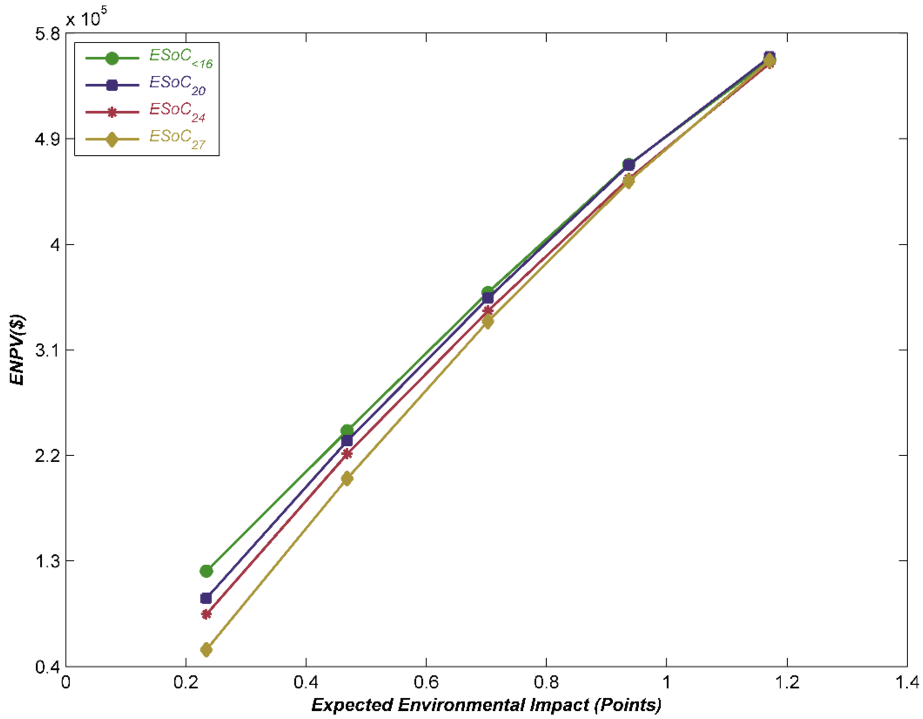

Fig. 6.6 Pareto frontier for each set of solutions.

Although the solution obtained by optimizing environmental criteria is highly undesirable, optimization under social criteria also achieves poor economic performance. The above can be explained since the optimal social solution leads to install pre-treatment/treatment units at any site, which reduces to zero the transportation loads (i.e. zero emissions). This is clearly illustrated in

Table 6.5, which shows the technologies installed at each specific site as well as their capacities. Consequently, the installation cost is significantly increased affecting the economic performance.

From Table 6.5 it can be also concluded that the best designs (installed capacity at every site) are completely different for each objective and thus representing extreme solutions. So far, a reduced set of solutions were obtained expediting the solution of the stochastic problem. However, from the above Pareto surface analysis it is evident the necessity of a robust solution selection strategy that enhances the decision-making procedure. Therefore, a solution selection based on ELECTRE-IV methods was applied.

Table 6.5 - Equipment capacity for the optimum networks configurations obtained for the three selected criteria.

	Economic Optimization			*Environmental Optimization*			*Social Optimization*		
	Dryer (t/h)	*Chipper (t/h)*	*G-ICE (kW_e)*	*Dryer (t/h)*	*Chipper (t/h)*	*G-ICE (kW_e)*	*Dryer (t/h)*	*Chipper (t/h)*	*G-ICE (kW_e)*
Senso	-	-	-	-	-	-	0.1	0.1	18.0
Old Konkrompe	0.126	0.1	168.98	-	-	-	0.141	0.1	75.0
Fakwasi	0.218	0.1	243.30	-	-	-	0.116	0.1	360.0
Kumfia	0.302	0.135	360.00	-	-	-	0.1	0.1	132.0
Trohye	0.1	0.1	90.88	-	-	-	0.1	0.1	75.0
Bompa	-	-	-	-	-	-	0.1	0.1	189.0
Nwunwom	-	-	-	-	-	-	0.1	0.1	38.08
Boniafo	-	-	-	-	-	-	0.1	0.1	148.16
Abamba	0.1	-	-	-	-	-	0.425	0.1	246.0
Extrasite1	-	-	-	-	-	-	-	-	-
Extrasite2	-	-	-	-	-	-	-	-	-
Extrasite3	-	-	-	-	-	-	-	-	-
Extrasite4	-	-	-	-	-	-	-	-	-

Solution selection (ELECTRE-IV)

The decision maker interests are represented using a set of thresholds defined for each objective. Table 6.6 shows the particular preference, indifference and infeasible thresholds used.

Table 6.6 Thresholds values for the three objectives considered in this case study.

Thresholds	*Criteria*		
	$ENPV$ ($)	$EImpact_{overall}^{2002}$	$ESoC$
Indifference (q)	408742.18	0	18.00
Preference (p)	525525.66	0.5	24.00
Veto (v)	613113.27	1.0	28.00

Here, the indifference threshold for the $ENPV$ has been set as 30% lower than the best possible performance while the preference threshold is set by reducing in 10% the upper bound. For the case of the veto thresholds, a slightly higher value than its maximum is defined (5% higher) since no higher $ENPV$ performance is expected. Similar assumptions were used for the $ESoC$ since both are objectives to be maximized. For the case of $EImpact_{overall}^{2002}$ (objective to be minimized) a different thresholds definition was followed. Particularly, the indifference threshold is defined at the lower bound (i.e. zero emissions) since no lower values can be reached. A preference threshold 0.5 was defined since it is preferable to have values as low as possible. Finally, according with the previous to analysis of the Pareto frontier, a veto threshold of 1.0 was defined (even if there are solutions with higher environmental impact, these solutions are undesirable for the other defined criteria). Using these thresholds, ELECTRE-IV method is applied in order to evaluate and rank a total of 45 feasible optimal solutions as a function of their desirability (see Fig. 6.7).

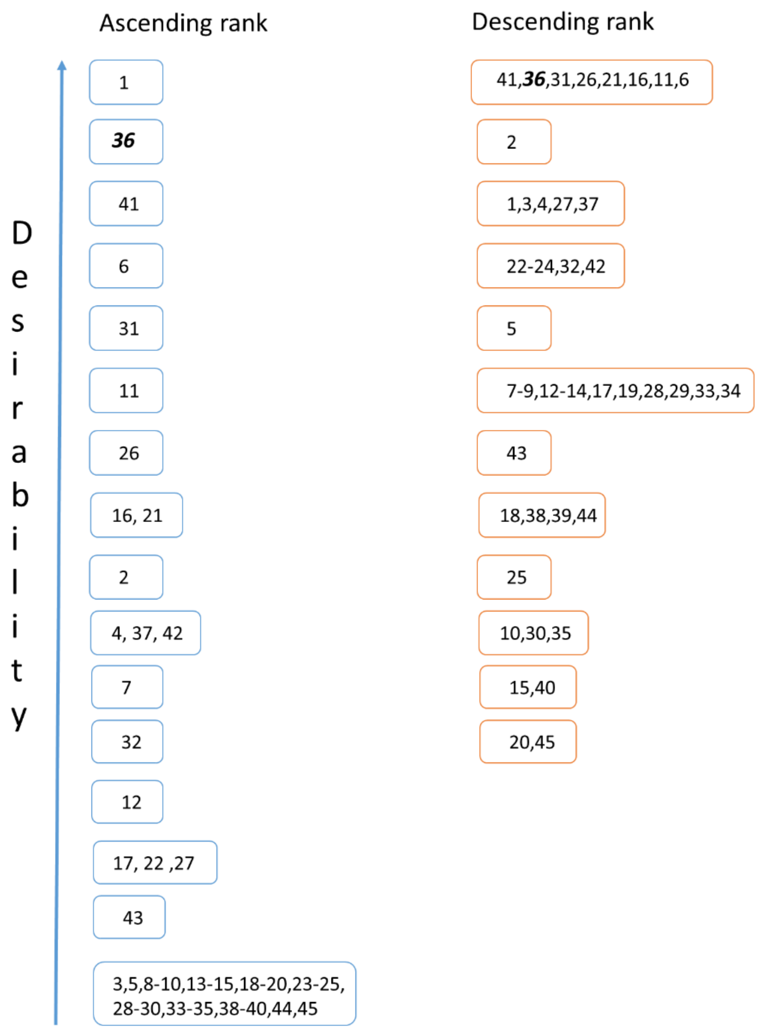

Fig. 6.7 Solution rank for both ascending and descending order.

Resulting from the solution ranking (Fig. 6.7), the “direct” definition of a dominant solution was not possible since for both lists there is not a single solution at the first level of desirability. Even if at this point the ELECTRE-IV method was unable to produce directly an overall optimal solution, the hierarchically ordered reduced set of solutions obtained expedites the decision maker tasks. Therefore, by making a visual comparison of these lists, solutions, 1 and 41 show a good performance, representing interesting alternatives to be explored. Nevertheless, solution 36 was selected as the overall dominant solution since it is the one with the highest rank in both lists. For this solution, the $ENPV$ value is \$ 2.21x10^5, and the environmental and social impact is 0.46847 and 24, respectively. The above solution entails a reduction of approximately 60%, 65% and 10% form the best possible economic, environmental and social performance values (utopia point), respectively. Fig. 6.8 shows the selected solution within the solution space. Additionally, Table 6.7 shows equipment units installed as well as their capacities for the SC network associated to solution 36.

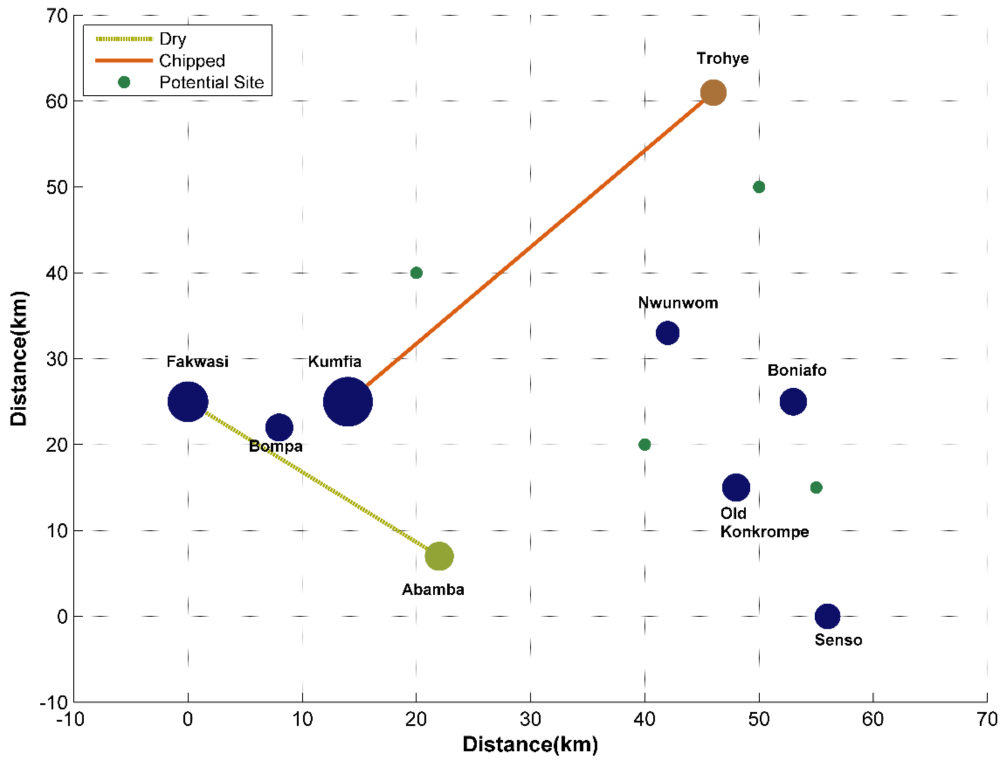

Fig. 6.8. Selected solution within the Pareto frontier space. Golden dots represent the communities in which external dry material is required (only one in this case) while Orange dots identify the use of external chipped material.

It is important to highlight that these decisions highly depend on the definition of the thresholds for each criterion. Therefore, another solution might be selected using different thresholds.

From Fig. 6.8 it can be noticed that the final network needs a significantly low amount of material distribution (raw and chipped) at the expense of treating that material at each particular site. The above highly affects the final profit due to the installation costs that also penalize the energetic self-sufficiency of the community. Table 6.7 shows the capacities of each installed technology required to provide a robust structure for the complete uncertain solution space. This solution considers the installation of energy generators at all the sites. Even if there are only two communities in which pretreatment units (Dryer/chipper) are not installed, the rest of them have them at their lower capacity (0.1 t/h). On the other hand, the capacity of G-ICE systems installed varies according to its localization. For example, gasifiers with low capacity are installed near the smallest communities, while the two gasifiers with the highest capacity are located close to the largest communities in order to properly satisfy the energy demand and minimize at the same time the transportation tasks. It is important to remember that the material flows highly depend on the conditions of each scenario.

The proposed strategy allows exploring a large number of uncertainty scenarios in a small amount of time (and computational effort). The above allows not only to expedite the solution for problems under uncertainty but also to solve problems that may be under multiple and/or independent sources of uncertainty. This point represents an important improvement in the current PSE literature. Additionally, it has been also proven that ELECTRE-IV method can be applied in a systematic decision support strategy that considers a significantly large amount of objectives/criteria.

Table 6.7. Equipment capacity for the configuration of the robust network.

	Dryer (t/h)	*Chipper (t/h)*	*G-ICE (kW$_e$)*
Senso	0.1	0.1	18
Old Konkrompe	0.1	0.1	18
Fakwasi	0.1	0.1	75
Kumfia	0.1	0.1	85.33
Trohye	-	-	18
Bompa	0.1	0.1	18
Nwunwom	0.1	0.1	18
Boniafo	0.1	0.1	18
Abamba	-	0.1	18
Extrasite1	-	-	-
Extrasite2	-	-	-
Extrasite3	-	-	-
Extrasite4	-	-	-

Computational effort comparison.

In order to evaluate the required computational effort, the same case study has been solved using a decomposition-based formulation (particularly a SAA explained in Chapter 3). Such a description is for a single objective problem under uncertainty. However here the same approach is used for a MO problem and combined with ELECTRE-IV method to overcome the solution identification issue.

The computational effort required at each step of the solution strategy to solve the above-presented case study using both the decomposition-based formulation and the scenario reduction formulation presented are displayed in Table 6.8. It is important to notice that the complete stochastic Single Objective model, that includes 100 scenarios and maximizes the expected profit as unique criterion cannot be solved in less than 48h (172,800s) due to CPU limitations (i.e., after this CPU time, CPLEX is unable to close the optimality gap below 5%); consequently, larger CPU times are expected when dealing with multiple objectives. Thus, the decomposition-based strategy was solved for the same number of scenarios and a comparison of the computational effort obtained with the proposed scenario-reduction strategy using the same amount of scenarios is performed. Notice that the analysis in computational time is centered in the application of the strategies and the algorithms used. It is important to highlight that the computational efforts associated with different problem formulations and/or optimization issues are out of the scope of this analysis.

From Table 6.8 notice that both approaches provide very different values for the objective functions, which suggest that the considered decision criteria/objectives have a significant effect over the results obtained with a reduced set of scenarios. Thus, further research lines should address this issue. Table 6.8 also displays the time consumed for both solution strategies, which were evaluated for five different conditions. Remarkably, each solution strategy presents its highest computational effort at different points. Particularly, for the decomposition-based strategy the stochastic optimization requires more effort, while for the scenario-reduction strategy the highest computational effort was due to the deterministic optimization. It is important to comment that even for this case (100 scenarios) the difference in the computational effort is already significant (>900 seconds), such a difference becomes bigger when a larger amount of scenarios is considered (Fig. 6.9).

Table 6.8 Computational effort associated with the compared solution strategies.

	Computational effort (CPU seconds/scenario)	
	Decomposition-based	*Scenario reduction*
Solve optimization model deterministically	1000	1000
Scenario reduction model	N/A	300
Fix binary variables	0	N/A
Solve stochastic optimization model	1700	540*
Solution selection strategy	0,6	0,6
Total	2700.06	1870.06
$ENPV$ ($)	359,873	221,453
$EImpact_{overall}^{2002}$	0.9	0.46847
$ESoC$	17	24

* This value is for 10 scenarios (the size of the reduced set)

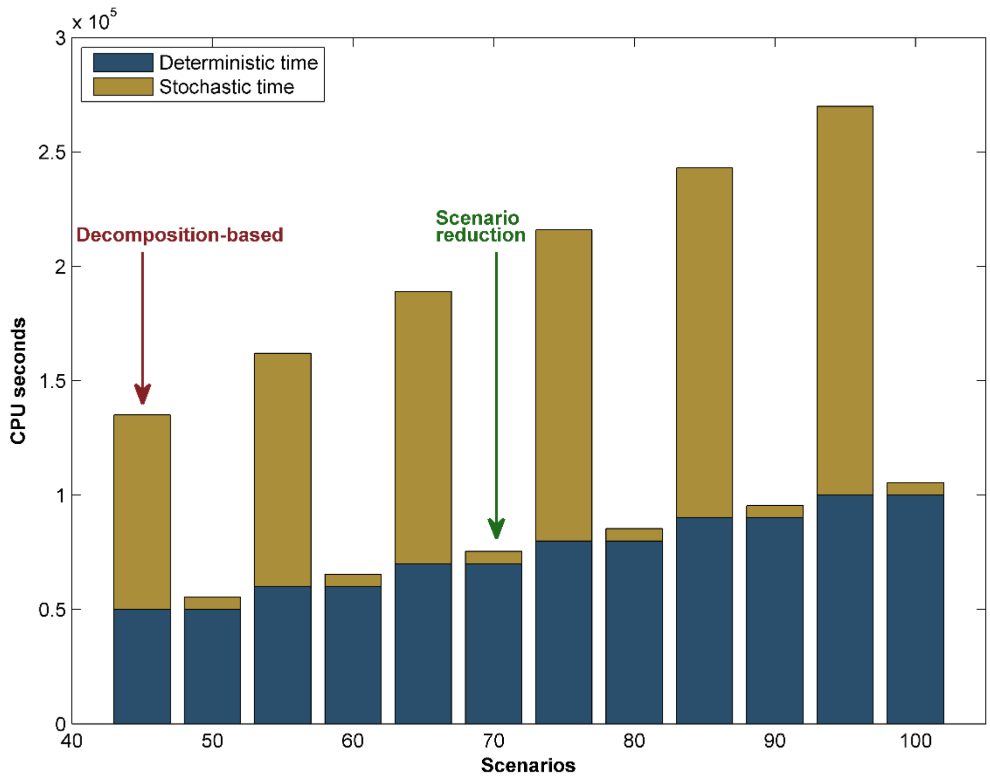

Fig. 6.9- Time-consuming comparison for decomposition-based and scenario reduction strategies.

From Fig. 6.9 it is clear that the solution for the deterministic model shows the highest CPU time in the proposed strategy. Thus, one possible way to reduce this time consumption could be to determine the size of the original set in a systematic way. Particularly the use of sophisticated sampling techniques such as Sobol sampling or polynomial-based methods (cubature formula) is a promising alternative. Notice that since these techniques seek for a sufficiently large set of scenarios (i.e. original set) they only affect the first two steps of the proposed strategy. However, the rest of the steps in the scenario reduction strategy will remain and will end up with a reduced set (like in this case). In other words, these techniques may expedite the solution of the deterministic problem but their use does not affect the usefulness of the proposed scenario reduction strategy and in fact, such a combination is possible due to the strategy robustness.

6.5. Conclusions

A strategy to efficient reduce the number of scenarios used to represent the complete uncertainty space was presented. This strategy reduced the number of uncertainty parameter realizations required to maintaining the best representation for both, input and output values. Numerical results express that this strategy significantly contributes to the reduction of the computational effort associated to the solution of problems under different uncertainty sources. For completeness of this work, the proposed strategy combines a scenario reduction based formulation with a solution selection algorithm to produce a flexible and robust formulation while reducing the computational effort required for solving the problem. Such a strategy promotes the application of a stochastic multi-objective approach to solve design-planning problems when the quality of the feed streams is uncertain, facilitating decision-making tasks while avoiding subjectivity in the selection of the final solution.

The capabilities of this approach have been successfully demonstrated using, as test-bed, the multi-scenario and multi-objective design and planning problem of an energy distribution network using biomass as raw material. It has been found that this method allows managing different material flows with independent uncertain properties in a sustainable way, ensuring the energy availability and reducing operational costs. Thus, the proposed strategy represents a step forward to overcome problems such as long period forecasting of uncertainty conditions.

Additionally, it has been proven that this solution strategy is useful to solve sustainability problems under uncertain conditions by explicitly considering multiple objectives. Such a solution strategy is a promising alternative that fills in an important PSE gap. Besides, different lines have been identified that need further research:

(i) Increase the robustness of the final solution in real life energy supply chains;
(ii) Enhance the systematically identification of the elements and the size of the reduced set of scenarios;
(iii) Identify the most important uncertainty sources as a function of their effect over the process performance
(iv) Evaluate the effect of additional criteria/objectives over the definition of the reduced set of scenarios.

6.6. Nomenclature

Abbreviations

CR	Cassava Rhizome
ELECTRE	Elimination and Choice Expressing Reality for its abbreviation in French.
G-ICE	Gasifier internal combustion engine
GWP	Global Warming Potential
IS	Industrial Symbiosis
LCA	Life Cycle Assessment
LHV	Lower heating value
LV	Low voltage
MC	Moisture content
MILP	Mixed integer linear programming

MO	Multi-objective
MOO	Multi-objective optimization
MV	Medium voltage
PSE	Process system engineering
SAA	Sample average approximation
SC	Supply chain
SCM	Supply chain management
STN	State Task Network

Indices

a	Midpoint environmental category
c	Scenarios
e	Supplier site
f	Origin sites
f'	Destination sites
g	Endpoint damage category
i	Task
j	Technology (Treatment/Pre-treatment equipment's)
k	Interval for Piecewise approximation (Economies of scale)
m	Market site
p	Producer
s	Material state
t	Time period

Sets

C	Set of scenarios
E_{rm}	Suppliers *e* that provide raw materials
$\hat{E}_{prod}$	Suppliers *e* that provide production services
$\bar{E}_{tr}$	Suppliers *e* that provide transportation services
FP	Materials *s* that are final products
$\bar{I}$	Task *i* with variable input
I_j	Tasks *i* that can be performed in technology *j*
$\bar{J}_e$	Technology *j* that is available at supplier *e*
$\bar{J}_f$	Technology that can be installed at location *f*
J_i	Technology that can perform task *i*
J_{Stor}	Technologies to perform storage activities
Mkt	Market locations
Ntr	Not transport tasks
RM	Materials *s* that are raw materials
Sup	Supplier locations
T_s	Task that produces material *s*
$\bar{T}_s$	Task that consumes material *s*
Tr	Distribution tasks
$\bar{x}_c^*$	Optimal set of solutions for scenario c
Φ	Space of uncertain parameters

Parameters

A_{sftc}	Maximum availability of raw material *s* in period *t* in location *f* and for scenario *c*
Dem_{sft}	Demand of product *s* at market *f* in period *t*
$Distance_{ff'}$	Distance from location *f* to location *f'*
err	Tolerance value
$FCFJ_{jft}$	Fixed cost per unit of technology *j* capacity at location *f* in period *t*

FE_{jfk}^{limit}	Increment of capacity equal to the upper limit in interval *k* for technology *j* in facility *f*
$Invest^{MV}$	Investment required for medium voltage
M	Big positive number
N	Number of scenarios to be removed
$NormF_g$	Normalizing factor of damage category *g*
p	Preference thresholds
$p_{c'}^{new}$	New probability of occurrence for the scenario c'
$p_{c'}^{orig}$	Original probability of occurrence for the scenario c'
$Price_{sft}$	Price of product *s* at market *f* in period *t*
$Price_{jfk}^{limit}$	Investment required for an increment of capacity equal to the upper limit of interval *k* for technology *j* in facility *f*
$Prob_c$	Probability of occurrence of scenario *c*
q	Indifference thresholds
$rate$	Discount rate
$Tortuosity$	Tortuosity factor
v	Veto thresholds
$Water_{sc}$	Moisture for material *s* and scenario *c*
$Water_{ij}^{max}$	Maximum moisture for task *i* performed in equipment *j*
α_{sij}	Mass fraction of task *i* for production of material *s* in equipment *j*
$\bar{\alpha}_{sij}$	Mass fraction of task *i* for consumption of material *s* in equipment *j*
β_{jf}	Minimum utilization rate of technology *j* capacity that is allowed at location *j*
ζ_{ag}	*g* endpoint damage characterization factor for environmental intervention *a*
$\theta_{ijff'}$	Capacity utilization rate of technology *j* by task *i* whose origin is location *f* and destination location *f'*
$\rho_{eff't}^{tr}$	Unitary transportation costs from location *f* to location *f'* during period *t*
τ_{sfet}^{ut1}	Unitary cost associated with task *i* performed in equipment *j* from location *f* and payable to external supplier *e* during period *t*
τ_{sfet}^{ut2}	Unitary cost associated with handling the inventory of material *s* in location *f* and payable to external supplier *e* during period *t*
χ_{est}	Unitary cost of raw material *s* offered by external supplier *e* in period *t*
$\psi_{ijff'a}$	*a* environmental category impact CF for task *i* performed using technology *j* receiving materials from node *f* and delivering it at node *f'*
ψ_{ija}^{T}	*a* environmental category impact CF for the transportation of a mass unit of material over a length unit
λ_c	Uncertain parameters vale

Variables

$cd_{c,c'}$	Represents the "displacement cost" from scenario c to c'
$DamC_{\mathrm{gftc}}$	Normalized endpoint damage *g* for location *f* in period *t* and scenario *c*
$DamC_{gc}^{SC}$	Normalized endpoint damage *g* along the whole SC for scenario *c*
$Distance_n$	Displacement distance (i.e. Manhattan distance) at iteration *n*
$ENPV$	Expected net present value
$EPurch_{etc}$	Economic value of sales executed in period *t* during scenario *c*
$ESales_{tc}$	Economic value of sales executed in period *t* and scenario *c*
$ESoC$	Expected social performance
$FAsset_{ft}$	Investment on fixed assets in period *t*
$FCost_{ft}$	Fixed cost in facility *f* for period *t*
F_{jft}	Total capacity technology *j* during period *t* at location *f*
FE_{jft}	Capacity increment of technology *j* at location *f* during period *t*
$funct_{err}^{exp}$	Absolute difference among the objective function obtained using the original and the reduced set of scenarios (c and c', respectively).
$funct_c$	Objective function obtained using one scenario ($c \epsilon C$)
$funct_{c'}$	Objective function obtained using one scenario ($c' \epsilon C'$)

$funct_{orig}^{exp}$	Expected objective function obtained using the original set of scenarios
$funct_{new}^{exp}$	Expected objective function obtained using the reduced set of scenarios
IC_{aftc}	Mid-point *a* environmental impact associated to site *f* which rises from activities in period *t* and scenario *c*
$Impact_{fc}^{2002}$	Total environmental impact for site *f* and scenario *c*
$Impact_{overall}^{2002}$	Total environmental impact for the whole SC
$n_{c,c'}$	Probability displacement between scenarios
NPV_c	Economic metric for a deterministic case (just one scenario *c*)
$P_{ijff'tc}$	Specific activity of task *i*, by using technology *j* during period *t*, whose origin is location *f* and destination is location *f'* and scenario *c*
$Profit_{ftc}$	Profit achieved in period for each facility *f* at time period *t* and scenario *c*
Pv_{sijftc}	Input/output material of material *s* for activity of task *i* with variable input/output, by using technology *j* during period *t* in location *f* and scenario *c*
$Purch_{et}^{pr}$	Amount of money payable to supplier *e* in period *t* associated with production activities
$Purch_{et}^{rm}$	Amount of money payable to supplier *e* in period *t* associated with consumption of raw materials
$Purch_{et}^{tr}$	Amount of money payable to supplier *e* in period *t* associated with consumption of transport services
$relative\ error$	Relative error for the iterative procedure.
$Sales_{sff'tc}$	Amount of product *s* sold from location *f* in market *f'* in period *t* and scenario *c*
S_{sftc}	Amount of stock material *s* at location *f* in period *t* and scenario *c*
SoC_c	Surrogate social metric at scenario *c*
$v_{c,c'}$	Dual variable representing the clustering. It defines whether scenario *c* is removed and assigned to scenario *c'*
x	First stage decision variables
y_c	Second stage decision variables

Binary Variables

V_{jf}	Technology installed at location *f* in period *t*
yy_c	Binary variable that denote whether a scenario is "transported" ($y_c = 1$) to a preserved one ($y_c = 0$).
$Z_{ff'}$	Facilities *f* and *f'* interconnected by a medium voltage line

SOS2 variable

ξ_{jfkt}	Variable to model the economies of scale (technology *j* in facility *f* at period *t*) as a piecewise linear function

Chapter 7

A decision support framework based on data-driven strategies.

In this chapter, a data-driven decision-making framework is applied to the problem addressed in the previous chapter considering multiple uncertainty sources during the MO decision making process within a bio-based energy generation supply chain.. The proposed framework exploits machine-learning techniques as a way to approximate the optimal management decisions as a function of the input uncertainties such as the energy demand or the environmental, social and economic scenario that continuously influence the process behavior. A design of computer experiments technique is also part of the integrated framework, generating representative information about the optimal management values as a function of the uncertain parameters.

For applying the proposed framework, any conventional optimization method can be used to determine the optimal decision values and an Ordinary Kriging meta-model is built to describe the resulting data-driven relations (i.e. mapping the relationship between the optimal decision variables and the uncertain parameters themselves). Then, the proposed framework uses this constructed meta-model to predict the optimal decisions considering uncertain parameters as input data. The above is challenging for two reasons: (i) The accuracy required by the parametric meta-models; (ii) The significant computational effort usually needed to generate and validate the required samples as well as running the optimization of the design of experiments in front of the effort required to optimize the process when the uncertainty is unveiled.

7.1.Data-driven decision making

The limited availability of fossil fuels, together with the dependence on these non-renewable resources and the hard environmental regulations has exposed the need for alternative energy generation technologies. However, it was after the apparition of large government subsidies to eco-friendly processes when the development and application of green energy generation technologies were actually promoted. One of the most significant initiatives is the use of agro-industrial wastes (e.g., biomass) as a fuel for power generation systems. The proper and systematic management of a bio-based energy production supply chain brings once again the two major challenges associated to sustainability problems as already stressed along this Thesis. Particularly, the necessity of efficient decision-making strategies to address multi-objective problems and highly complex uncertainty assessment simultaneously is needed *(Silvente et al., 2013; Guillén-Gosálbez and Grossmann, 2009)*.

Regarding MO problems, many approaches are available in the Process Systems Engineering (PSE) literature addressing decision-making issues. From these studies, two main challenges/limitations can be identified: (i) The reliance on the quality of the final solution most of the times are not guaranteed and; (ii) the large computational effort required applying the decision making task and/or running the optimization procedures. These limitations increase in complexity when the problem is subject to single and/or multiple types/sources of uncertainty *(Kopanos and Pistikopoulos, 2014)*. Therefore, the enhancement of currently available decision-support systems for the systematic identification of the optimal solution under uncertain conditions is still an open issue and represents a significant step forward in uncertainty management *(Greco et al., 2016)*. Addressing this issue is the core of this chapter.

Until now, different methods and tools have been proposed to address the system uncertainties while addressing the optimization of industrial problems (such as multi-hierarchical SC's). In general, uncertainty approaches are classified into reactive and proactive being the second ones the most widely used. Studies for proactive approaches are vast in the PSE literature describing mainly robust optimization (RO) *(Ning and You, 2017)* and scenario-based formulations (such as stochastic optimization). In general, these approaches produce a conservative solution at the expense of assuming a financial/performance risk against uncertain conditions. On the contrary, a risk-averse attitude against uncertainties promotes the use of reactive approaches. Nowadays reactive approaches are gaining interest since their right management guarantees a better overall performance even under uncertain conditions. Within reactive approaches, the well-known model predictive control (MPC) *(Perea-López et al., 2003)*, rolling horizon *(Kopanos and Pistikopoulous, 2014; Silvente et al., 2015)* and multiparametric programming (MP) *(Pistikopoulous et al., 2011)* can be highlighted. Notice that even if most of these methods can handle multiple uncertainty sources, MP surpass the capabilities of the others, due to its capacity to solve problems in which the uncertainty affects the process conditions as well as the optimization parameters (including decision-maker preferences and/or objectives hierarchy).

Particularly, MP aims to obtain a set of equations that reproduce the optimal solution as a function of multiple uncertain/varying parameters *(Charitopoulos and Papageorgiou, 2017)*. In addition, the specific regions in which these equations remain feasible within the solution space are identified/bounded. Besides the commented advantage of using MP, the significant reduction in computational effort obtained by avoiding the repetitive optimization procedure when the uncertainty is unveiled is currently its most interesting feature *(Pistikopoulos et al., 2002)*. The first record of MP is vague; however, its use has increased after being combined with MPC *(Bemporad et al. 2002; Kouramas et al., 2011)*. In such an integrated (MP-MPC) framework, a model is used to control the process in a finite time horizon. However, two major conditions are required to be successfully applied: first, a complex mathematical knowledge associated to the development of the MP framework *(Shokry and Espuña, 2015)* and, second, the availability of a clear discrete-time linear state space model of the process *(Bemporad et al. 2002; Pistikopoulos et al., 2002; Kouramas et al., 2011)*. These requirements hinder the application of MP analysis to problems in which a highly nonlinear, high dimensional, complex structure (sequential simulation models), and/or non-transparent mathematical model must be considered.

To address these MP limitations, the use of sophisticated data-driven optimization techniques has been proposed, including data-driven robust optimization *(Ning and You, 2017)* and meta-multiparametric analysis (M-MP) *(Shokry and Espuña, 2015a; 2015b)*. In the recent past, M-MP has been successfully applied to several industrial cases including the optimal management of a utility plant *(Shokry and Espuña, 2015b)* and energy production process *(Shokry and Espuña, 2017)*. Additionally, M-MP has been used for the control of batch processes *(Shokry et al. 2016)*, emission control in scheduling systems *(Lupera et al., 2016)* and the dynamic optimization of batch processes *(Shokry and Espuña, 2017)*. However, all these applications address continuous variables and the use of this framework in Mixed-Integer optimization problems is dramatically compromised. Even if recently in the works of *Shokry et al., (2017)* and *Lupera et al., (2017)* a combination of M-MP with classification techniques have been successfully applied to simple small-scale problems (i.e. managing continuous plus discrete variables), the applicability of M-MP approaches to manage large-scale problems still requires a systematic definition of the most significant decision variables.

The use of M-MP methodology to address SCM problems has been scarcely explored due to the high dimensionality and complexity of these problems and the existence of different sources of uncertainty that often interrupt the supply chain dynamics. The work presented in this chapter has a special interest in the evaluation of data-driven strategy capabilities and its impact on the decision-making process. The analysis aims to highlight the practical advantages of the M-MP as an optimization approach and evaluate the time effectiveness and reliability of the obtained solution.

7.2. Problem Statement

Here, a centralized multi-objective multi-echelon bio-based energy production SC under raw material uncertainties (the same one presented in Chapter 6) was used as case study. Fig. 7.1 provides an overview of the whole SC in terms of the potential equipment's to be installed and the distance between communities. The biomass availability is the primary source of variability in bio-based energy generation systems and it addressed through a tailor-made approach (see section 7.4.1). Alike in Chapter 6, the main objectives considered are the net present value (NPV), the environmental impact of the entire SC and the creation of job opportunities (social performance). Through the simultaneous optimization of these objectives, the system sustainability is promoted. Notice that even if in the previous section ELECTRE IV shows outstanding capabilities to aid the decision-making process, for simplicity and in aim of highlighting the capabilities of the data-driven framework to handle uncertainty problem, in this Chapter the resulting MO problem was assessed using the weighted sum approach (WS). A set of weighting factors were defined for the environmental and social performances to scalarize them into a single economic result.

The detailed description of the case study can be found in Chapter 6; however, for completeness of this section the main elements that describe the problem are now commented.

- The set of states/materials $s \in S$, which includes raw, intermediates and final products.
- The set of tasks $i \in I$, which include on-site treatments, pre-treatments, and transportation.
- The set of economic weights allowing normalize the environmental and social objectives ($WeightSoc_c$ and $WeghtEnv_c$ respectively).
- The set of locations $f \in F$, fixed in the initialization step.
- A time horizon $t \in T$.

- A given expected energy demand profile for each short-term period and market. Different (uncertain) target values are considered.
- Product and consumable prices.
- Environmental uncertainty, which influences expected raw material production, process, and transportation systems performance.
- The social impact as a function of the size of the different installed processes, although again, the future importance of this assessment on the decision-making procedure is uncertain.

Furthermore, the goal is to maximize the economic vector by modifying the following decisions concerning the tactical management of the resulting SC:

- All the amounts of materials processed by task *i* using equipment *j* during period *t*, at site *f*.
- Storage levels at each site and time.

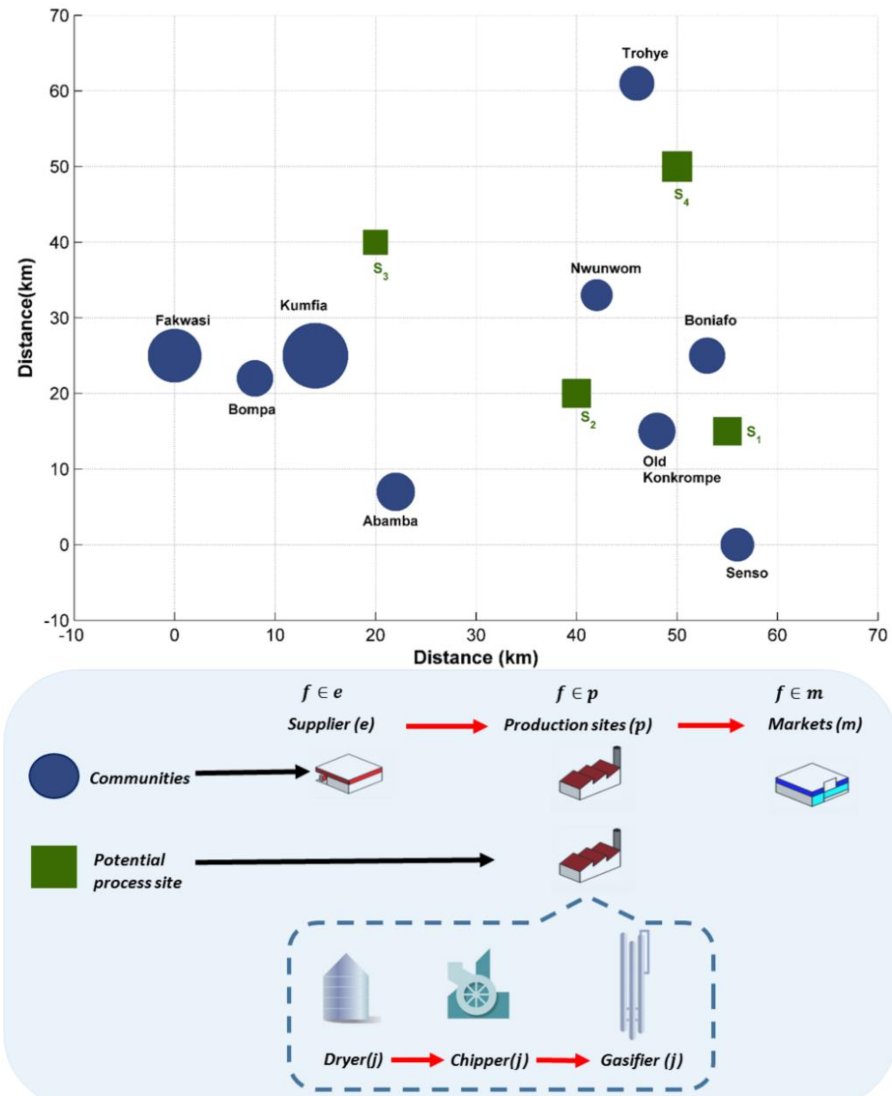

Fig. 7.1. The general scheme for bio-based energy supply chain.

In the next section, the main and basic mathematical constraints that model the case study are presented. Further details about the process data, equipment description, and nominal capacities, can be found in Chapter 6.

7.3. Basic mathematical formulation

The description of the main equations from the mathematical formulation is presented as follows. Notice that, even if the solution strategy eases the process management under uncertainty, an explicitly multi-scenario solution approach is not used. Therefore, unlike in Chapter 6, here, the mathematical model used adopts a deterministic form (i.e. without a scenario index).

The material balance is represented in Eq. (7.1), in which the states not consumed ($P_{ijf'ft}$) with a defined efficiency (α_{sij} and $\bar{\alpha}_{sij}$ for consumable or product states respectively) can be stored (S_{sft}) at any time.

$$S_{sft} = S_{sft-1} + \sum_{f'} \sum_{i \in T_s} \sum_{j \in (J_i \cap \bar{J}_{f'})} \alpha_{sij} P_{ijf'ft} - \sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in (J_i \cap \bar{J}_f)} \bar{\alpha}_{sij} P_{ijff't} \qquad \forall s, f, t \qquad (7.1)$$

Similarly, Eq. (7.2) represents the energy balance of the system, in which the latent heat values (HV_s) of the materials (Pv_{sijft}) are considered at all the input and output states ($s \in T_s$ and $s \in \bar{T}_s$, respectively) of all the tasks across the entire system.

$$\sum_{s \in T_s} HV_s \cdot Pv_{sijft} = \sum_{s \in \bar{T}_s} HV_s \cdot Pv_{sijft} \qquad \forall i \in \bar{I}, f, t \qquad (7.2)$$

A minimum energy and treated/pretreated material production level is guaranteed using β_{jf}, which represents the minimal proportion of the total available capacity used in technology j at site f and it is defined by the decision maker. Similarly, Eq. (7.3) limits the production to the respective equipment capacities.

$$\beta_{jf} \cdot F_{jft-1} \leq \sum_{f'} \sum_{i \in I_j} P_{ijff't} \leq F_{jft} \qquad \forall j \in \tilde{J}_f, f, t \qquad (7.3)$$

In a similar way, Eq. (7.4) ensures that the raw material s purchased at site f and delivered to location f' at time t satisfies the physical availability, while Eq. (7.5) limits the sales to a specified demand. The above represents the assumption that the energy produced using biomass never exceeds the forecasted demand.

$$\sum_{f'} \sum_{i \in \bar{T}_s} \sum_{j \in J_i} P_{ijff't} \leq A_{sft} \qquad \forall s \in RM, f \in Sup, t \qquad (7.4)$$

$$\sum_{f' \in M} Sales_{sf'ft} \leq Dem_{sft} \qquad \forall s \in FP, f \in Mkt, t \qquad (7.5)$$

The economic performance (NPV) represents the net present value of the entire SC. Without loss of generality, NPV is obtained considering the traditional incomes ($Sales_t$) and costs function annualized considering a defined interest rate ($rate$) as stated in Eq. (7.6). Note that process costs considers the fixed/investment ($FCost_t$) and variable ones including transportation, acquisition and production costs ($Purch_{et}$).

$$NPV = \sum_t \left(\frac{Sales_{tc} - (FCost_t + \sum_e Purch_{etc})}{(1 + rate)^t} \right) \qquad \forall t \tag{7.6}$$

As well as in the base case study, a Life Cycle Impact Analysis (LCIA) is performed using the well-known Impact 2002+ methodology. Thereby, a useful assessment of the process environmental impact may be obtained by combining midpoint/damage approaches *(Jolliet et al., 2003)*. Impact 2002+ needs a database to assess the system impact, which for this case is the Ecoinvent database *(Ecoinvent, 2008)*. Thus, the environmental impact quantification considers the traditional 14 mid-point categories associated with biomass production (e.g., cassava waste), transportation, pre-treatment (chipping and drying) and generation of electricity through biomass gasification. Eq. (7.7) displays the resulting equation. For more details about the life cycle analysis and the implementation of Impact 2002+ methodology readers are referred to *Pérez-Fortes et al., (2012)* and *Jolliet et al., (2003)*. Notice that it is possible to use alternative databases and methodologies; however, the analysis of the effect of these elements over the strategy performance is out of the scope of this Thesis.

$$Impact^{2002}_{overall} = \sum_f \sum_g \sum_t \sum_{a \epsilon A_g} NormF_g \zeta_{ag} IC_{aft} \tag{7.7}$$

Finally, Eq. (7.8) calculates the social impact and represents the number of treatment/pre-treatment sites installed/used. Here, the binary variable V_{jft} represents the use or not of a particular unit.

$$SoC = \sum_j \sum_f \sum_t V_{jft} \tag{7.8}$$

In order to evaluate the effect of the proposed strategy in comparison with traditional decision-support strategies, a fixed superstructure is assumed, thus, the number of units installed will be the same for further comparisons. As commented, the non-economic criteria are scalarized into an economic one to formulate the main objective. Such a scalarization is achieved by applying a defined factor ($WeightSoc$ and $WeghtEnv$, respectively) as described in Eq. (7.9).

$$OF = NPV + \left(WeightEnv * Impact^{2002}_{overall}\right) + (WeightSoc * SoC) \tag{7.9}$$

Notice that the value of these factors directly affects the OF value, compromising the solution reliability. For this reason, the creation of a meta-model facilitates future optimization for different economic factors.

7.3.1. Methodology: Meta-Multiparametric framework (M-MP)

The general idea of the M-MP is to replace complex functions with simpler approximations that require less computational effort. These approximations are created by the training of a set of meta-models (in this work, based on Ordinary Kriging as machine learning technique) using input-output information *(Shokry and Espuña, 2015a; 2015b; Lupera et al., 2016)*. In particular, the uncertain parameters are considered input information while the corresponding optimal SC decision variables and objectives are the outputs obtained through a multiparametric approach. The resulting meta-models represent the multiparametric black box relations that describe the behavior of the decision variables and objectives over the entire uncertainty space. Thus, for any future change in the uncertain parameters, the meta-models can be used to perform simple interpolations and predict the values of the new optimal decision variables and objectives. The M-MP method comprises three main tasks (and five steps) as shown in Fig. 7.2. A detailed description of each step (including the specific methods/algorithms used) is provided in the following subsections.

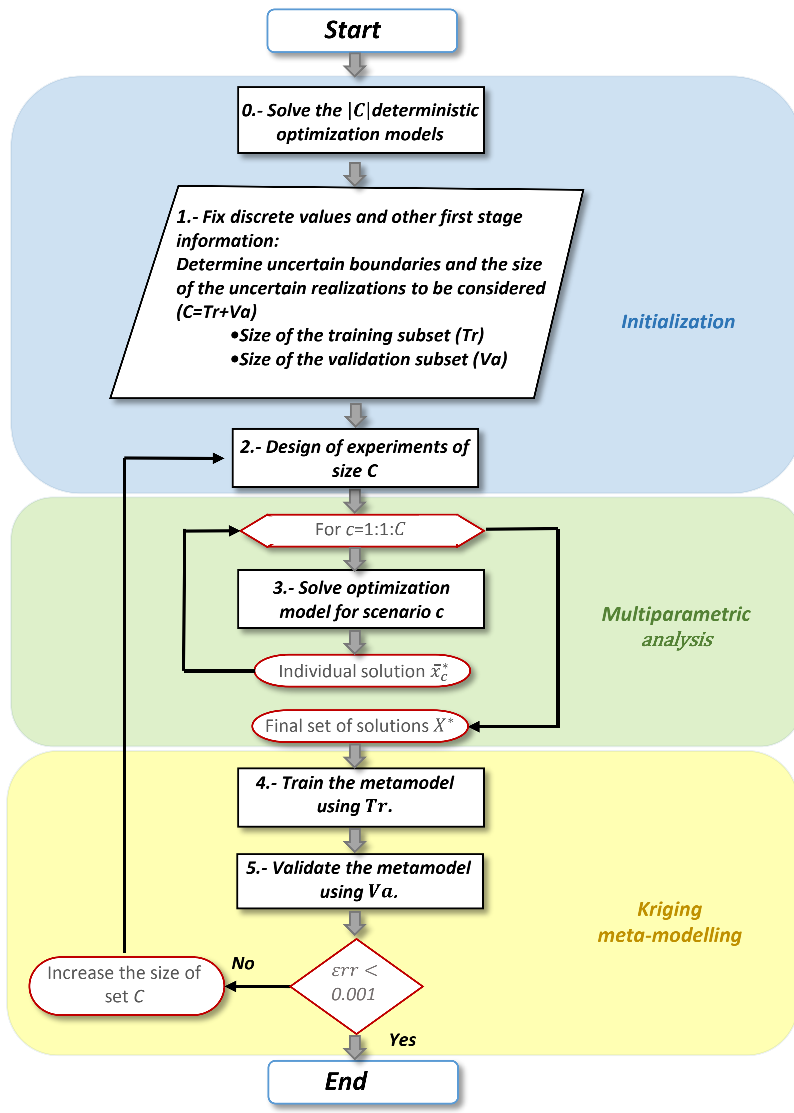

Fig. 7.2. The detailed description of the solution strategy proposed.

Initialization

During initialization step, the original MILP problem is solved under deterministic conditions (i.e., for specific pre-defined values of the uncertain information). Using the results from the MILP solution, the discrete variables are fixed. Thus, the original MILP is transformed into a Linear Programming (LP) problem.

Design of computer experiments and data generation

To obtain accurate meta-model predictions, the training step requires as much information as possible of the output behavior over the input domain (uncertainty space). Thus, to ensure the reliability and feasibility of such a data, the main issue to be addressed is the identification of a reasonable number of input combinations (i.e., sample points or sampling plan) well-distributed through the input domain (uniformity) *(Shokry and Espuña, 2014)*.

Within the different existing techniques for the design of computer experiments that generate well-distributed sampling plans, in this work Hammersley sampling technique is used. The analysis of the effect of the sampling technique over the final solution is out of the scope of this Thesis. Therefore, interested readers are referred to *Forrester and Keane, (2009)* and *Fang et al., (2006)* for more details.

The resulting sampling plan has the form of $[XP]_{c'\cdot k}$, where *c'* is the size of the training data set (number of equiprobable generated scenarios), and *k* represents the number of uncertain parameters affecting the system (i.e. input dimensionality). After designing the sampling plan, the optimization problem has to be solved for each sample point (i.e. *c* times) to obtain the associated outputs$[YP]_{c'\cdot u}$ where, *u* is the number of output variables including the main objective function and the decision variables under control (*u−1*). In addition to the training set, a different validation set must be generated in the same way, in order to assess the prediction accuracy of the meta-models. Notice that the size uncertainty realizations must be augmented if the meta-model accuracy is below a tolerance value.

Multiparametric analysis step

After fixing the superstructure during initialization steps, the mathematical formulation of the problem follows the general form described next (*Model P*).

$$Model\ P \qquad \max_{x\ y_c} \left\{ \sum_c NPV_c - \left(WeightEnv_c * Impact^{2002}_{overall\,c} \right) + \left(WeightSoc_c * SoC_c \right) \right\}$$

$$s.t.$$

$$h(x, y_c) = 0 \qquad \forall c \in \mathrm{C}$$
$$g(x, y_c) < 0 \qquad \forall c \in \mathrm{C}$$

$$x \in \mathrm{X}\,, y_c \in \mathrm{Y}$$

From such a formulation, *x* represents the first stage decision variables while y_c are the second stage ones, which are directly affected by the uncertain parameters *c* belonging to the uncertain space ϕ while $h(x_c, y_c)$ and $g(x, y_c)$ are vectors of equality and inequality constraints representing the constraints described in the model (see Chapter 6). According to the proposed solution strategy (see Fig. 7.2), *Model P* has to be solved iteratively for each sampling point within the design of experiments. Therefore, first the LP model is solved and then, the values obtained are collected (e.g. production, storage and flow levels across the supply chain). By replacing the values of the uncertain parameters used in the solution of the deterministic model by those associated with another sampling point an iterative procedure is performed in order to obtain the optimal supply chain plan for each of the remaining |*C*|-1 scenarios so that, at the end, |*C*| different solutions are generated. It is important to highlight that, *Model P* is never solved for multiple scenarios simultaneously, and the addition of index *c* is included only for informative purposes.

The results of all the scenarios represent a very inefficient approximation of the global problem. However, the meta-model is built using the whole set of solutions for all the sub-problems. The following subsection describes such a meta-model construction.

Meta-model training and validation

In many engineering applications, the well-known Kriging modeling *(Krige, 1951; Cressi, 1993)* has exhibited two main outperforming features: (i) a high prediction accuracy using a relatively small number of training data points; (ii) a transparent way to adjunt the required parameters to obtain the best fit. Thus, Kriging models offer high flexibility for parameters tuning while measuring the effect of each input variable over the output. The Kriging method is particularly useful for the approximation of nonlinear models *(Caballero and Grossmann, 2008; Shokry and España, 2014)*. Moreover, the Ordinary Kriging meta-model is generally used as the machine learning technique *(Fang et al., 2006; Forrester and Keane, 2009)*.

For this strategy, the result from steps one and two (Fig. 7.2) leads to a set of uncertain parameters combinations $[XP]_{c\prime\cdot k}$ and their corresponding optimal solutions $[YP]_{c\prime\cdot u}$. Thus, a set of u Kriging meta-models are constructed, each of them representing a data-driven multiparametric relation that identifies the underlying mapping between the uncertain parameters and the optimal behavior of each output. Notice that the Kriging meta-model assumes a stochastic process, where the error in the predicted value is also a function of the input variables x_c. The Kriging predictor $\hat{y}(x_c)$ is composed by two main parts: a constant term μ, and a residual $Z(x_c)$ form that constant, leading to the following equation *(Forrester and Keane, 2009)*.

$$\hat{y}(x_c) = \mu + Z(x_c) \tag{7.10}$$

The residual $Z(x_c)$ is considered as a stochastic Gaussian process with expected value zero $E(Z(x_c)) = 0$, and a covariance between two points (in this case scenarios) x_c, x_{c^*} calculated as: $cov(Z(x_c), Z(x_{c^*})) = \sigma^2 R(x_c, x_{c^*})$, where σ^2 is the process variance, and $R(x_c, x_{c^*})$ is a spatial correlation function which is usually selected exponential, see Eq. (7.11). The parameter Υ_l represents a measure of the degree of correlation among the data along the l^{th} input dimension, and p_l is a smoothness parameter that is usually fired at the value of 2.0 *(Forrester and Keane, 2009)*.

$$R(x_c, x_{c^*}) = exp\left(-\sum_{l=1}^{k} \Upsilon_l \left|x_c - x_{c^*,l}\right|^{p_l}\right) \qquad l = 1,2,\dots,k \tag{7.11}$$

Maximizing the likelihood function (Eq. (7.12)) of the observed data $[YP]_{c\prime\cdot l}$ yields the optimal expressions of the parameters μ, σ^2 that depend on *l*. This task is accomplished through differentiating the natural logarithm of the likelihood function concerning μ and σ^2, and after some mathematical derivations, their optimal formulas are obtained and displayed in Eq. (7.13), and Eq. (7.14) *(Jones et al., 1998)*. Being **1** in Eqs. (7.12-7.13), the column vector of ones with length *c*. Substituting by the optimal values of $\hat{\mu}$ and $\hat{\sigma}^2$ in the likelihood function leads to obtaining a concentrated log-likelihood function (Eq. (7.15)).

$$Lik = \frac{1}{(2\pi\sigma^2)^{c/2}|R|^{1/2}} exp\left(\frac{-(Y - \mathbf{1}\mu)^T R^{-1}(Y - \mathbf{1}\mu)}{2\sigma^2}\right) \quad (7.12)$$

$$\hat{\mu} = \frac{\mathbf{1}^T R^{-1} Y}{\mathbf{1}^T R^{-1}\mathbf{1}} \quad (7.13)$$

$$\hat{\sigma}^2 = \frac{(Y - \mathbf{1}\mu)^T R^{-1}(Y - \mathbf{1}\mu)}{n} \quad (7.14)$$

$$Max_{\ (\Upsilon_l, p_l)}\left[-\frac{n}{2}\ln(\hat{\sigma}^2) - \frac{1}{2}\ln(|R|)\right] \quad (7.15)$$

The Kriging final predictor in Eq. (7.16) is obtained through deriving the augmented likelihood function of the original training data set and a new interpolating point (x_{c-new}, y_{c-new}). Where: r is the $c \times 1$ vector of correlations between the predicted $\hat{y}_{c-new}$ and the sample design points (i.e., $R(x_{c-new}, x_c)$). Detailed information about the required mathematical development can be found in *(Caballero and Grossmann, 2008)*.

$$\hat{y}(x_{c-new}) = \mu + r^T R^{-1}(Y - \mathbf{1}\mu)^T \quad (7.16)$$

The optimal parameters of the Kriging meta-model [Υ_l, p_l, $\hat{\mu}$, $\hat{\sigma}^2$] were obtained by the optimization of the concentrated log-likelihood function. In this work, the Matlab "*fmincon*" algorithm is used to solve this nonlinear optimization problem, while Cholesky factorization is used to find the inverse of $R_{c\cdot n}$to avoid the ill-conditioning. After fitting, the Kriging meta-models should be assessed to verify that they show a range of accuracy for the intended application as recently used in *(Shokry and España, 2014)*. Hence, the Kriging meta-model is used to estimate the outputs of the previously generated validation set, and an accuracy measure can be then calculated via comparing the outputs and their corresponding real values. The Normalized Root Mean Square Error (NRMSE %) is used in the work as an accuracy measure, see Eq. (7.17). where $y_{c\text{-}new}$, $\hat{y}_{c-new}$ are the real and the estimated outputs, and c is the number of validation data points.

$$NRMSE = 100 \times \frac{\left[\frac{1}{c}\cdot\sum_{c=1}^{c}(\hat{y}_{c-new} - y_{c-new})^2\right]^{0.5}}{(y_{max} - y_{min})} \quad (7.17)$$

As commented before, if the accuracy measure is not satisfactory enough (NRMSE<err), the training set size should be extended. Fig. 7.2 proposes an automatic sequential modeling framework in which the size of the training set automatically changes to achieve a defined satisfaction level; however, any other validation method can be used (any algorithm automation can be simply coded).

7.4.Case study

As already commented, the problem presented in Chapter 6 has been used as a Case Study to test the performance of the proposed method. Thus, the problem description and details can be found in such a chapter and Appendix B.4. The scope of this chapter is limited to provide an effective management strategy to support the decision-making processes under multiple types of uncertainties. In particular, in this section the effect of the changes in the electricity demand and weighting criteria over the planning decisions is evaluated. Thus, Table 7.1 shows the considered range for the uncertain parameters.

Table 7.1. The range of the input data.

DATA	TYPE	Ranges	
		Lower	*Upper*
Environmental Cost (€/unit)	Input	10	100
Social Benefit (€/unit)	Input	100	10,000
Electricity demand t_1 (kWh/month)	Input	49,916	61,009
Electricity demand t_3 (kWh/month)	Input	50,536	61,767
Electricity demand t_3 (kWh/month)	Input	51,156	62,524
Profit (€/year)	Output		
Energy production level at each facility (kWh/month)	Output		

For comparison purposes, in this example, a significantly high variation in the energy demand for the three time periods was assumed. Thus, a total of36 output variables were obtained after each optimization (the detailed energy production and economic benefit of the nine plants at each period ((9*3) + (9*1))). Remarkably, even if the study considers the energy demand as one of the principal uncertainty sources, addressing the challenges associated to the technical electricity supply is out of the scope of this Thesis; previous studies address these issues, like the convenience of switching on/off the transfer grid or the availability of the power supply during certain hours of the day *(Silvente and Papageorgiou, 2017)*.

7.4.1. SC superstructure

The fixed SC superstructure has been identified by optimizing the deterministic MILP problem assuming the same energy demand (θ_1= *Demand*) for the three time periods (50,000 kWh/month) as well as the nominal values of 50 €/Unit and 1000 €/Unit for the other two uncertain parameters (θ_2=*WeightEnv*$_c$ and θ_3=*WeightSoC*, respectively). The mathematical model has been written in GAMS 23.8.2 and the problem was solved using CPLEX 11.0 on a PC Intel Core i7-2600M CPU 2.70 GHz and 16.00 GB of RAM. The model contains 27,015 equations, 830,554 continuous and 1,106 binary variables and it entails a CPU time of approximately 300 seconds. The result is displayed in Fig. 7.3.

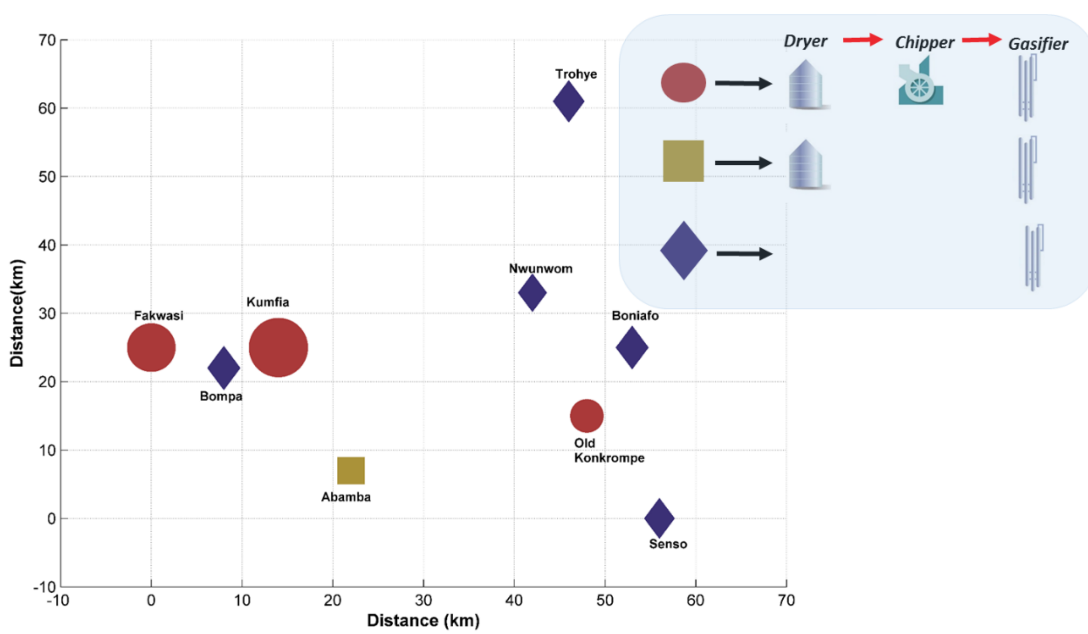

Fig. 7.3. Optimal deterministic bio-based energy production superstructure.

Fig. 7.3 shows that the communities with the highest population and biomass availability (Kumfia and Fakwasi) use all the pre-treatment/treatment available equipments. The above is logical considering that it is cheaper to treat the raw material onsite rather than distribute it to communities with a more convenient allocation (closer to the others). Similarly, for the case of Old Konkrompe all the pre-treatment/treatment equipment were installed, to work as a central plant treating the biomass for the closest communities. The above results match with the design found in the original paper for the economic optimization *(Pérez-Fortes et al., 2012)* which justifies the use of such a fixed structure for the following planning decisions.

Notice that the planning decisions are not displayed here, since these decisions will change according to the realization of the uncertain parameters. At this point, all the binary variables are fixed, thus, the model is transformed from MILP into an LP. Such as LP model reduces the computational effort required to take the planning decisions, including raw material flows, production levels and equipment/storage capacities, among others.

7.4.2. Meta-modeling training and evaluation

For this part of the method, 150 sample points were considered. Particularly, 50 points were used for validation while the rest of them were divided into four sets with different sizes (being 25, 50, 75 and 100 sampling points) and used as training points as described during the design of experiments. The above avoids the use of common points between the training and validation data. Remarkably, the use of such an increasingly sampling size allows exploring its effect on the accuracy of the performance prediction. Fig. 7.4 displays the sampling point's distribution for the four sets within the ranges proving the uniform representation of the complete uncertainty space. Logically, the bigger the number of sampling points is, the better the representation will be.

The LP optimization problem is deterministically solved for each one of these points. In this case, the mathematical model contains 27,015 equations and 830,554 continuous variables. The optimization process entails a CPU time of approximately 33 seconds for each iteration.

The optimization procedure produces sets of 25, 50, 75 and 100 solutions, which individually, represent a poor approximation for the global stochastic problem; however, they assist in the evaluation of the obtained meta-model. The uneven behavior of the economic performance as a function of uncertain parameters is demonstrated in Fig. 7.5. It is important to comment that such a figure relates the *ENPV*, total demand and total *WeightEnv*. For simplicity, the other parameter under evaluation *WeightSoC* is not represented in the figure; however, the resulting surface is clearly irregular, confirming that the parametric function may be nonlinear although the basic problem formulation is linear.

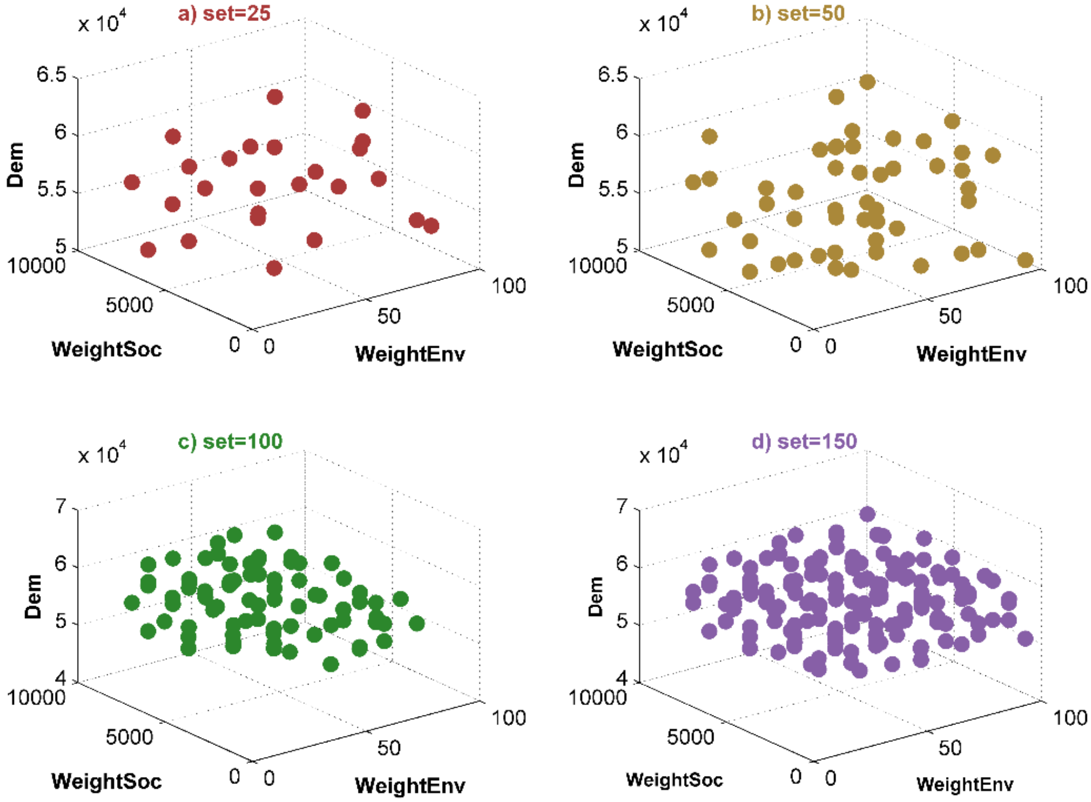

Fig. 7.4. Representation of the uncertainty space for different training set size. a) 25 sample points; b) 50 sample points; c) 100 sample points and d) 150 sample points.

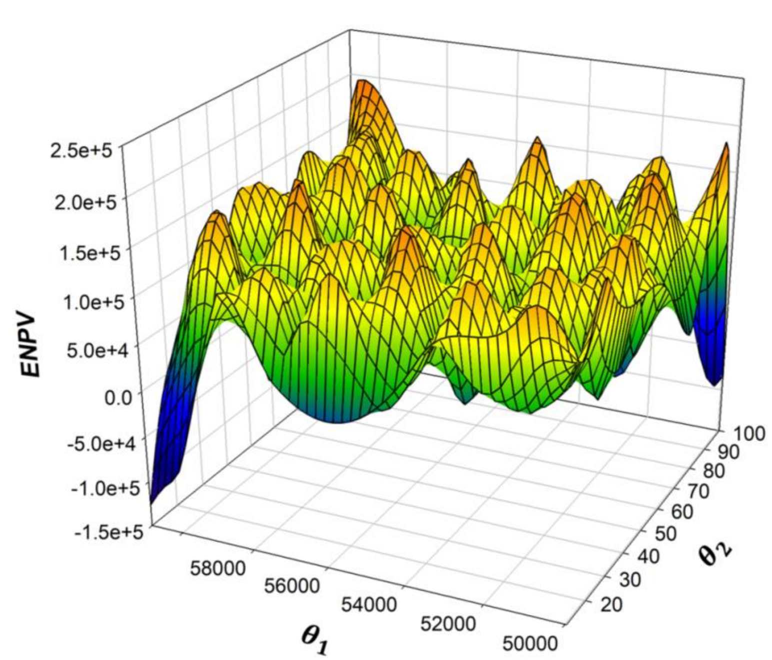

Fig. 7.5. The behavior of the optimal objective functions for different values in *WeightEnv* (θ_2) and total demand (θ_1) parameters.

From Fig. 7.5 it is clear that there is a messy behavior across the meta-model space, which compromises the reliable prediction of system performance. Thus, the accuracy of the resulting Kriging meta-model (for ENPV and global energy production) for all the training sets is estimated using the relationship between the values obtained by the surrogate model (estimation) and the traditional optimization values (real values) as shown in Fig. 7.6.

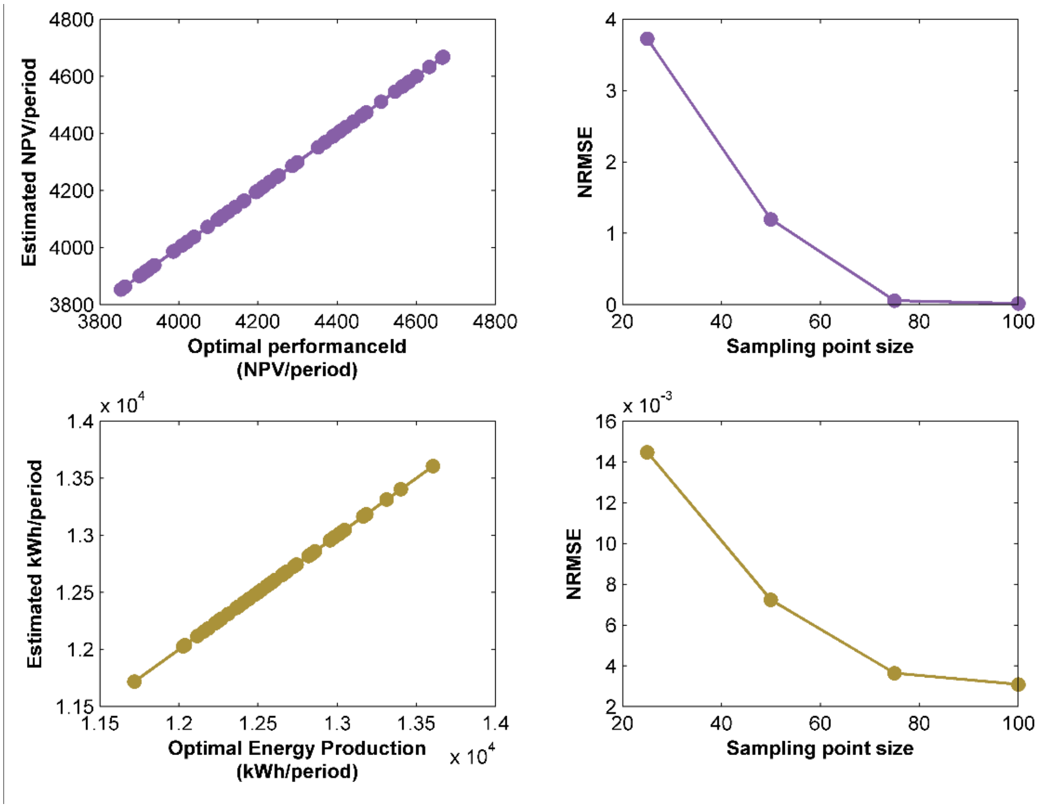

Fig. 7.6. Direct meta-model validation (Left) and Meta-model performance assessment as a function of the training set size (Right). In the top, the ENPV is considered while the bottom plots represent the global energy production.

Fig. 7.6 clearly demonstrates the high accuracy obtained. In particular, Fig. 7.6(left) shows a 45 degrees line suggesting an accurate prediction of the optimization results. Nevertheless, in order to stress the strategy benefits, an analysis of the quality of the meta-model as a function of the size of the training set was performed in Fig. 7.6(right). Such a figure proves that the accuracy of the obtained solution increases as a function of the size of the training set. Notice that even if a better accuracy is obtained with large training size sets, Fig. 7.6 proves and justifies the use of the surrogate model even for small training sets (NRMSE<0.01).

In summary, we can conclude that, for this case, a design of experiments with 75 sampling points is large enough to produce an accurate prediction of the objective function performance. Notice that the methodology allows finding the minimum number of sampling points to obtain representative results. The above has a significant impact on the computational effort, which represents a significant step forward for the current state of the art in decision-making literature for PSE.

The meta-models analysis has been focused on the objective function (*ENPV*) and the global energy production function, however, the detailed analysis of the rest of the decision variables is presented as follows.

7.4.3. Deeper meta-model analysis

In this section, a detailed analysis of the results for each meta-model is performed. In particular, the effort (time) required to validate and train/fit the meta-model (See Fig. 7.7) is of significant interest.

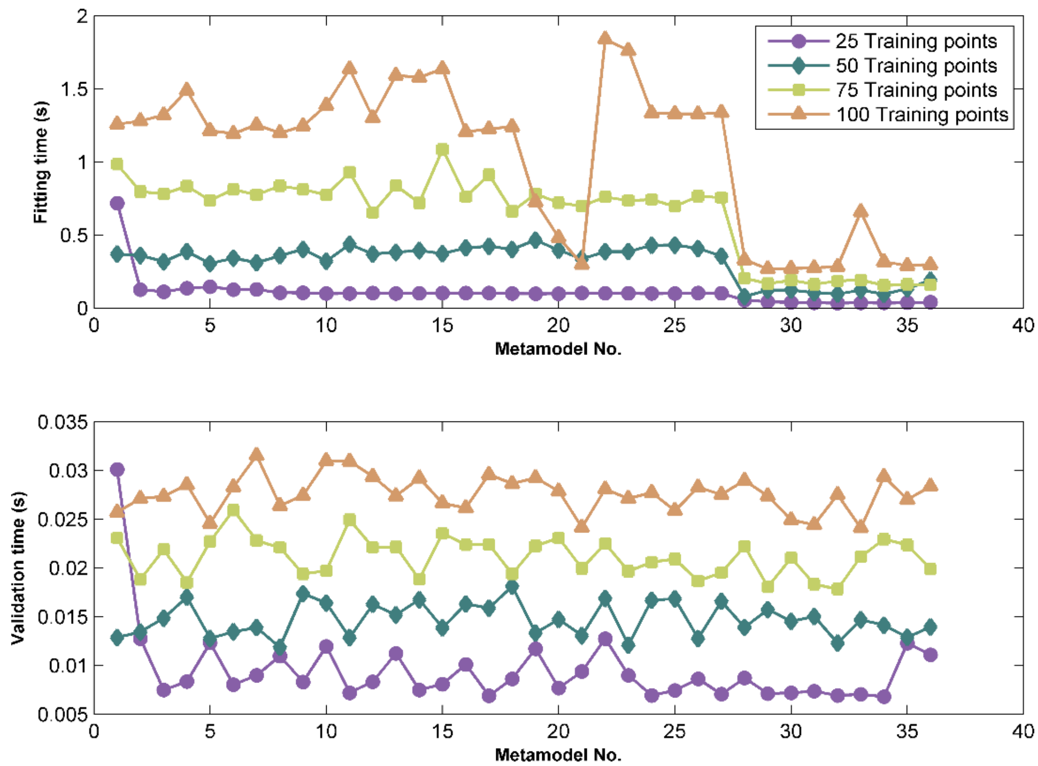

Fig. 7.7. The computational behavior of meta-model training and validation.

It can be noticed from Fig. 7.7 that, even if the time required for both, meta-model fitting and validation highly depends on the number of training points, it can be negligible due to its small value (1.5s and 0.03s for training and validation respectively). In addition, it is important to notice that for the energy production meta-models (metamodels 1 to 27) a significantly fitting time is required if compared with the Profit ones (above 27).. Logically, such a difference is not observed in the validation step since for this part the meta-model has been already produced. The validation of these meta-models guarantees the quality of the results obtained through the meta-model. Fig. 7.8 shows the relation of the results obtained by both, the traditional optimization ("Real values") against the M-MP optimization ("Estimated").

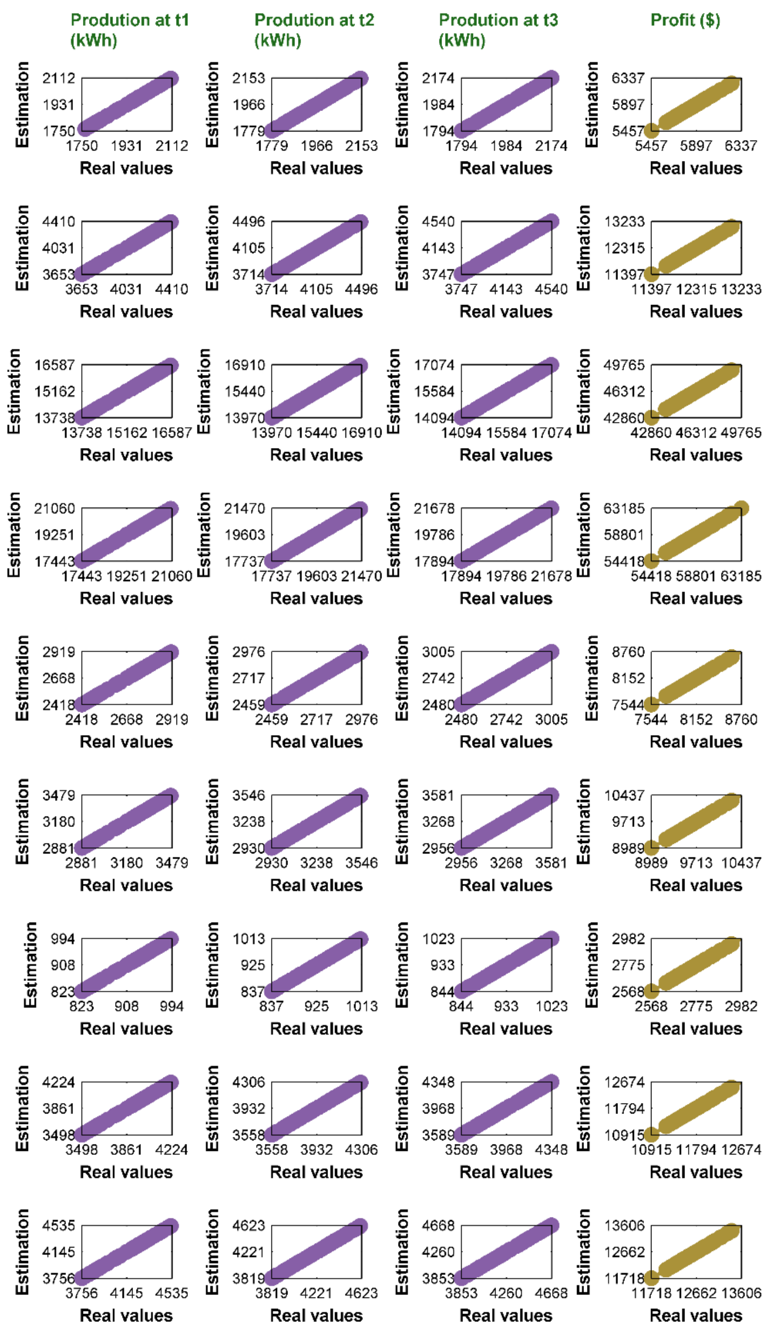

Fig. 7.8. The validation of the meta-models for each variable.

Currently, several studies of data-driven strategies suggest that the variables (meta-models) may be jointed in clusters to improve the estimation of traditional optimization behaviors *(Shokry et al., 2017)*. Such a clustering strategy is particularly interesting when dealing with MI problems (due to the presence of binary variables). Nevertheless, the benefits of such a strategy are limited if only continuous variables are addressed (which is the case under study). Thus, Fig. 7.9 shows the performance of the resulting meta-models using different clusters (from two to ten). Such a figure proves that in this case the use of clustering strategies does not provide any significant improvement.

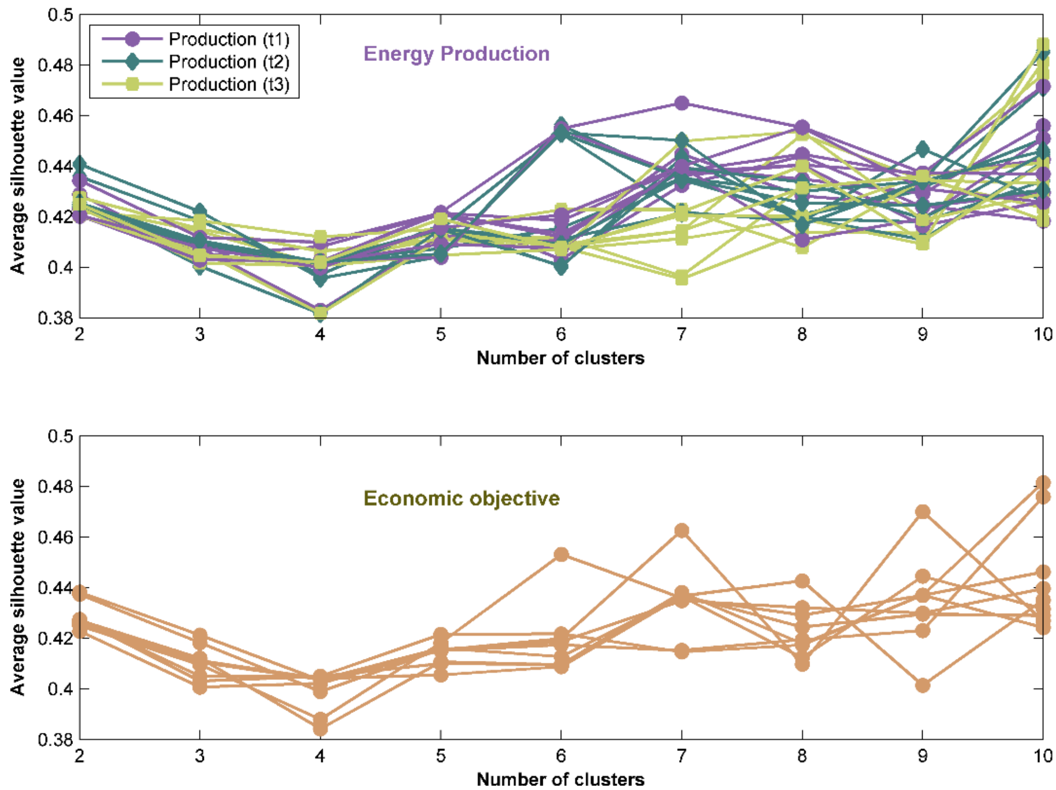

Fig. 7.9. Parallel coordinated plot for different defined clusters.

7.4.4. Computational effort analysis

This section describes the strategy performance in terms of the computational effort stressing the advantages of using the meta-model strategy. Table 7.2 compares the computational effort required to solve the problem using both, the traditional optimization formulation and the one based on Kriging meta-modeling. In order to provide a better understanding of the presented values, it is important to mention that the mathematical model contains 24,515 equations and 820,350 continuous variables. Also, notice that, since the stochastic MILP model that includes 100 scenarios and maximizes the *ENPV* as a unique criterion cannot be solved in less than 48h (172,800 s), the information of solving the LP problem deterministically are used instead (the difference may be significantly higher).

Table 7.2 shows the time consumed for each solution approach in five different categories. Each solution strategy presents its highest computational effort at a defined step. For the traditional mathematical programming, the optimization step requires the largest effort, while for the Kriging meta-modeling this is associated with the training/building one. For this case (i.e. 150 sampling points), the difference in the computational effort is relatively low. However, a bigger difference can be expected for a complex model. From Table 7.2 it is clear that training part requires the highest CPU effort (time) in the proposed strategy.

Table 7.2. Computational effort required.

	Computational effort (CPU seconds/scenario)	
	Math. Programming	*Kriging meta-model*
Model building	Variable	Variable
Solve optimization model (MILP)*	3,300	N/A
Training*	N/A	3,300
Validation*	N/A	70
Re-Optimization (LP)*	33**	0.00466**
Total	4,322	4,370

* (CPU s)   ** This value is for a single sample point

Additionally, the last category (re-optimization) emphasizes the most important quality of the meta-multiparametric strategy presented here. Although the solution of the 150 problems used for training and validation requires a relatively high computational effort, after the definition of the surrogate model the optimization time drops to irrelevant values. For this example, the time to obtain the solution is more than three orders of magnitude lower (1/7,085) and, certainly, larger reductions are expected for more complex optimization problems.

7.4.5. Optimal planning strategies

Until this point, the meta-models high accuracy and low computational effort have been discussed. Moreover, this section describes the real effect of the meta-models results in the supply chain operation and production management. For this purpose, two particular sampling points were considered as case studies (Table 7.3).

Table 7.3. Input data for the two considered case studies.

Case Study	$\boldsymbol{\theta_2}$ (€/unit)	$\boldsymbol{\theta_3}$ (€/unit)	$\boldsymbol{\theta_1}$ (kWh/month)		
			t1	*t2*	*t3*
1	27.4	7215.63	57448.71	59610.78	53708.64
2	67.6	332.03	52838.21	54849.14	60701.91

Table 7.4 shows the associated production levels of each plant/location and period obtained from the traditional optimization. Plants from one to nine represent Senso, Old Konkrompe, Fakwasi, Kumfia, Trohye, Bompa, Nwunwom, Boniafo, and Abamba respectively. Table 7.4 also shows the deviation of the results obtained through meta-model in comparison with the traditional optimization results.

Notice that there is a significantly small difference in the quality of the solution, being the largest differences below 0.0014% (highlighted in Table 7.4). Remarkably, even if these differences are sufficiently small, all of them appear at the third period. The above shows the individual effect of each uncertainty parameter/source to the process performance and stress the need for further sensitivity analysis to identify the most significant ones.

It is also worth noting that planning decisions (such as production levels) are different for each case study and that disregarding the different total productions, , the demand is ultimately satisfied through different paths. For instance, plants two and three (Old Konkrompe and Fakwasi, respectively) have the largest energy productions at time one and two for the first case while for the second case the period with the largest production is achieved at time three. Similar behaviors were found for different sampling points. These results show that M-MP strategy is significantly sensitive and thus, the effects of even the smallest changes in the uncertainty values can be addressed.

In addition to the sensitiveness of the strategy, it is important to illustrate that the M-MP allows also to completely emulating the system behavior across the entire uncertainty space. For example Fig. 7.7 shows the energy production at locations 2, 4 and 7 (Old Konkrompe, Kumfia, and Nwunwom respectively) for the whole uncertainty solution space. Notice that the obtained meta-models were generated using five different uncertainty sources (inputs in Table 7.1), however, in order to illustrate the process behavior, only two out of these five uncertainty values were plotted against the output variable (energy production).

Table 7.4. Output data for the two considered case studies.

Case Study	*Plant*	*Mathematical optimization*					*Meta-model deviation*				
		Production (kWh/month)				*OF*	*Production(kWh/month) (x 10^{-3})*				*OF (x 10^{-3})*
		t1	*t2*	*t3*	*Total*		*t1*	*t2*	*t3*	*Total*	
1	1	2,011	2,087	1,880	5,978	170,768	-1.3	-1.1	+0.2	-2.1	+8.2
	2	4,201	4,358	3,927	12,486		-2.0	-1.8	+0.6	-3.2	
	3	15,796	16,391	14,768	46,955		+10.8	-7.5	+2.1	+5.4	
	4	20,056	20,811	18,751	59,618		+14.3	-9.5	+2.2	+6.9	
	5	2,780	2,885	2,599	8,264		-0.9	-1.2	+0.8	-1.3	
	6	3,313	3,437	3,097	9,847		+2.1	-1.6	+0.5	+1.1	
	7	946	982	885	2,813		+0.2	-0.8	+0.6	+0.1	
	8	4,023	4,174	3,761	11,958		-1.3	-1.4	+0.9	-1.7	
	9	4,319	4,481	4,037	12,837		-1.5	-2.1	+0.2	-3.4	
2	1	1,850	1,920	**2,125**	5,896	14,908	+1.2	-1.1	**+3.1**	+3.2	-5.2
	2	3,863	4,010	**4,438**	12,312		+1.6	-2.1	**+5.5**	+5.0	
	3	14,529	15,082	16,691	46,302		-4.4	-7.4	+12.5	+0.6	
	4	18,447	19,149	21,192	58,788		-5.7	+10.0	+15.2	+19.5	
	5	2,557	2,654	**2,938**	8,150		+0.5	-1.8	**+4. 1**	+2.7	
	6	3,047	3,163	**3,500**	9,711		-0.8	-1.5	**+4.2**	+1.9	
	7	870	903	1,000	2,774		-1.0	-0.9	0.0	-1.9	
	8	3,700	3,841	4,251	11,792		+1.1	-2.4	+4.6	+3.2	
	9	3,972	4,123	4,563	12,659		+0.7	-2.4	+5.0	+3.3	

From Fig. 7.7 it can be seen that the three displayed locations show a different energy production performance (first row). The above suggests that using this strategy a particular process control can be obtained. Particularly:

- For locations, Kumfia and Nwunwom, the uncertain parameters θ_2 and θ_3 have a significant effect over the energy production while for Old Konkrompe the effect of *WeightSoc* can be neglected.
- Similarly, for the second row, it is clear that for Old Konkrompe and Kumfia both uncertain parameters ($\theta_{1,(t1)}$ and θ_2) affect the energy production performance in completely different ways.
- Finally, the third row represents the energy demand at two different time periods, showing that there is not a significant effect in that combination of parameters at any energy production site.

Remarkably, disregarding the application, the detailed process behavior (i.e. the effect of each variation over the system performance) can be extracted. In this particular case, it is important to highlight that the system behaviors shown in Fig. 7.7 represent only few outputs for few locations, although similar conclusions may be obtained from different output variables. Traditional stochastic optimization produces a single robust solution (i.e. one main plan works for any uncertainty realization) while for the M-MP the plan changes as a function of the uncertainty realization. Even if the M-MP optimization results may be challenging due to the highly dynamic process obtained (i.e. challenging logistic problem), the detailed system behavior is useful for the accurate assessment of the uncertainty parameters even if they are evolving across the time.

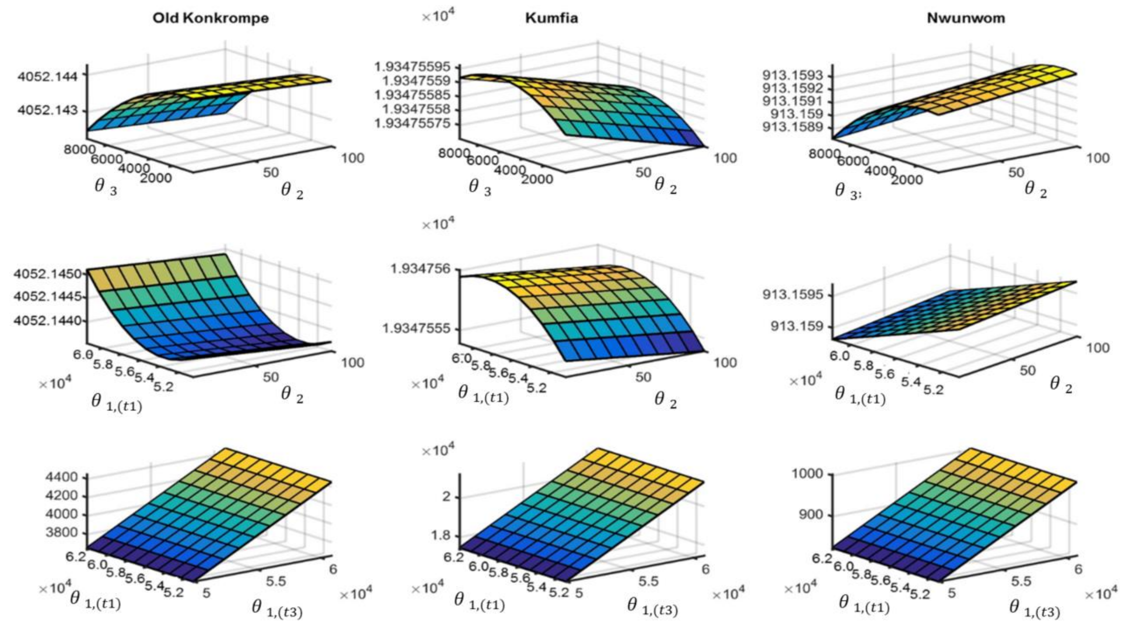

Fig. 7.7. Energy production behavior for Old Konkrompe, Kumfia and Nwunwom and uncertainty parameters variations in in θ_1, θ_2 and θ_3.

Additionally, using such detailed information, the data-driven decision-making strategies may significantly enhance, addressing the following issues:

(i) Systematic definition of the uncertainty parameters hierarchies over the objective function.

(ii) Optimal solution identification for multi-criteria problems (i.e. selecting an alternative solution that performs better in the overall perspective even if it is a sub-optimal for the traditional stochastic formulation).

Finally, it is important to comment that this work focuses on the M-MP strategy capabilities evaluation to assess SC planning. The production levels were the only outputs under analysis proving the usefulness of M-MP. So, in order to detail the resulting SC plan, additional meta-models have to be built, one for each of the outputs to be detailed (such as material flows).

7.5. Concluding remarks

Here, a meta-multiparametric framework for the management of a SC production and distribution problem under different types of uncertain parameters was proposed. This framework combines the traditional optimization techniques and surrogate modeling, based on a Kriging meta-model, to estimate the expected state of the system (predictor).

Numerical results show that the resulting surrogate model predicts the system performance with high accuracy and time efficiency proving that the M-MP technique successfully addresses complex real-world problems. More importantly, M-MP can manage multiple uncertain parameters representing a step forward for the management of sustainability issues becoming a feasible/alternative to multiparametric programming since a single meta-model can cover the entire uncertainty space. Even if compared with traditional optimization approaches (such as two-stage stochastic programming), M-MP may be considered as a more challenging strategy since the detailed information on the system behavior provides additional advantages to be potentially combined with sophisticated decision-making strategies. For example, a proper evaluation of the whole set of solutions produced with M-MP may be evaluated through a multi-criteria decision-making strategies (ELECTRE-IV) and produce a systematic solution identification considering the decision-maker preferences.

The results exhibit the very high accuracy of the parametric meta-models and justify its use for predicting the optimal decision variables under process uncertainties. More importantly, a dramatic reduction of the computational effort required to obtain these optimal values in response to the change of the uncertain parameters is achieved, compared to the traditional optimization techniques. Thus, the use of the proposed data-driven decision tool promotes a time-effective optimal decision-making.

Disregarding the simplicity of the case study used, the results show that the methodology is robust and flexible enough to handle problems with large number of optimization variables as well as model complexity, including highly non-linear models formulations. It is important to emphasize that a step forward is needed to consider mixed integer problems (for example, design supply chain problems).

To wrap-up the two main advantages of applying the proposed data-driven decision strategy are:

I. It enables a detailed qualitative analysis of the effect of different uncertainty sources over the process performance (further than the qualitative value), settling the basis to combine this approach with other robust approaches (for example, scenario reduction strategies).
II. It produces a highly accurate prediction of the process performance with relatively low information.

7.6. Nomenclature

Abbreviations

ELECTRE	ELimination and Choice Expressing REality
LCIA	Life Cycle Impact Analysis
LP	Linear programming
M-MP	Meta multiparametric programming
MILP	Mixed integer linear programming
MO	Multi-objective
MP	Multiparametric programming
MPC	Model predictive control
MP-MPC	Multiparametric model predictive control
NRMSE	Normalized Root Mean Square Error
PSE	Process Systems Engineering
RO	Robust optimization

SC	Supply Chain
WS	Weighted Sum

Indices

c	Scenario/sampling point
e	Supplier site
f	Potential sites
i	Treatment/distribution tasks
j	Equipment’s
k	Input dimensionality
l	Input dimension counter
m	Market site
p	Production site
s	Material states
t	Time period

Set/Subset

FP	Biomass states associated with final products
Mkt	Market sites
n	Sampling plan size
RM	Biomass states for raw material
RSS	Raw set of solutions
Sup	Supplier sites
Tr_c	Training samples plan subset
u	Number of output variables
Va_c	Validation samples plan subset
Φ	Space of uncertain parameters

Parameters

A_{sftc}	Maximum availability of raw material *s* in period *t* in location f and for scenario *c*
Dem_{sft}	Demand for product *s* at market *f* in period *t*
err	Tolerance value for the *NRMSE*
HV_{sc}	lower heating value for material s at scenario c
$NormF_g$	Normalizing factor of damage category *g*
p_l	Smoothness parameter
$WeightEnv_c$	Economic equivalence for environmental objective
$WeightSoc_c$	Economic equivalence for social objective
x_c	Input variables for scenario *c*
$\hat{y}_{max}$	Boundary for the maximum output value
$\hat{y}_{min}$	Boundary for the minimum output value
$Z(x_c)$	Residual term
α_{sij}	Mass fraction of material *s* produced by task *i* in equipment *j*
$\bar{\alpha}_{sij}$	Mass fraction of material *s* consumed by task *i* in equipment *j*
β_{jf}	Minimum utilization rate of technology *j* capacity that is allowed at location *f*
Υ_l	Degree of correlation along the l^{th} input
μ	Constant term for meta-modeling
$\hat{\mu}$	Constant value that leads to the “optimal” values
ζ_{ag}	*g* endpoint damage characterization factor for environmental intervention *a*

Variables

F_{jft}	Total capacity of technology *j* during period *t* at location *f*
$FCost_t$	Fixed cost in facility *f* for period *t* and scenario *c*

IC_{aftc}	Mid-point *a* environmental impact associated to site *f* which rises from activities in period *t* and scenario *c*
$Impact^{2002}_{overall_c}$	Total environmental impact for the whole SC
NPV	Net present value
OF	Global objective function
$P_{ijf'ftc}$	Production level of task *i* in equipment *j* in location *f'* and delivered (if required) in location *f* at time *t* and scenario *c*
$Profit_{tc}$	Profit achieved in period for each facility *f* at time period *t* and scenario *c*
$Purch_{etc}$	Economic value of sales executed in period *t* during scenario *c*
Pv_{sijftc}	Input/output of material *s* for *i* with variable input/output, by using technology *j* during period *t* in location *f* and scenario *c*
r	Vector of correlation
S_{sftc}	Storage level of material *s* at location *f* in time *t* and scenario *c*
$Sales_{sf'ft}$	Amount of product *s* sold from location *f* in market *f'* in period *t* and scenario *c*
SoC_c	Social performance at scenario *c*
x	First stage decision variables
x_c	Input variables for scenario *c*
x_{c-new}	Point to be predicted at a particular time
$\bar{x}^*$	Optimal set of solutions for scenario *c*
y_c	Second stage decision variables
$\hat{y}(x_c)$	Kriging prediction for specific input values
σ^2	Process variance
$\hat{\sigma}^2$	Process variance that leads to the optimal values
$[XP]_{c \cdot k}$	Sampling plan
$[YP]_{c \cdot u}$	Outputs of the sampling plan

Binary Variables

V_{jft}	Technology installed at location *f* in period *t*

Part IV:

Functional integration

Chapter 8

Using decision-support tools to integrate risk management optimization

As discussed previously, process optimization under uncertainty is one of the most studied topics in the recent past by the academic process systems engineering (PSE) community. Particularly, for the proper uncertainty management, a major challenge to address is the reduction of the side-risks (either, financial or operational) by controlling more effectively the influence of the unpredictable conditions over the objective function. Traditional risk management methods focus on optimizing a single risk metric along with the expected performance. The above, combined with the increasing interest in promoting the process sustainability, leads to a necessity of a holistic approach that guarantees an economically and environmentally feasible process.

As a first attempt to satisfy such a necessity, an alternative MO approach capable of efficiently handle economic objective functions together with different risk metrics is proposed in this chapter. Such an approach consists of two main steps. First, it is necessary to formulate a multi-objective stochastic model considering a set of risk metrics besides economic performance. Such a MO model is solved efficiently using a customized decomposition strategy inspired on the Sample Average Approximation (SAA). The second part consists of an assessment of a set of feasible solutions through a solution identification procedure based on a Pareto filters approach, which select the solutions showing better performance in the uncertain parameters space. Even if a MO model under uncertainty has been used before in this Thesis, a new batch problem was introduced in this Chapter not only to illustrate the capabilities and benefits of this approach, but also to emphasize the flexibility of the proposed framework.

8.1.Risk metrics and their use to assess uncertainty problems.

Besides its clear effect on business behaviour, market globalization compromises the prediction of industrial and process trends. When analysing the decision-making processes around a typical supply chain (SC), uncertainties such as market demands and raw materials availability should be considered to capture their direct and local effects over the individual echelons as well as their indirect effects that propagate to other echelons through the existing links between them. However, these effects and especially the indirect ones have often been overlooked by the traditional mathematical models used in the industry, which are commonly built over the assumption that all the information is known with accuracy beforehand *(Zamarripa et al., 2014)*.

Stochastic programming is the most commonly used method to solve optimization problems under uncertain conditions. Particularly, such a solution strategy addresses this challenge by defining recourse actions that allow reacting against every possible uncertainty realization *(Birge and Louveaux, 2011)*. In this context, a given design might obtain different results depending on the scenario in which it is evaluated, and it is very likely that the optimal design calculated for nominal conditions might render suboptimal (or even unfeasible) under other circumstances. Commonly, stochastic programs are solved over a number of stages, being the two-stage stochastic models the most studied ones in Supply Chain Management (SCM) problems: stage-1 decisions involve the selection of the design variables for the first time period, whereas stage-2 decisions are modelled using variables that can be adjusted according to the realization of the scenarios *(Grossmann and Guillén-Gosálbez, 2010; Guillén-Gosálbez and Grossmann, 2009,2010; Ben-Tal et al., 2009)*. This allows stochastic programming models to react after a scenario materializes (corrective action). As acknowledged by different authors, the main weakness of the traditional stochastic approaches lies in the lack of control on how the information regarding uncertain parameters affects optimal decisions. *Ierapetritou et al., (1996)* emphasized the need of an information index in order to evaluate the quality of the solution associated to the uncertain input data (named Value of Perfect Information (VPI)). Both, *Bernardo et al., (2000, 2001)* and *Ahmed and Sahinidis (1998)* proposed a robustness index as a way to evaluate the confidence of the information used, and ultimately provide a robust and confident solution. The robustness index has been applied and evaluated recently in terms of computational effort and solution quality *(Li and Floudas, 2014b)*, yet, the quality of the predicted information used is out of the scope of the present work.

Standard stochastic approaches tend to optimize the expected performance of the objective function distribution as a unique criterion. This strategy provides no control over the variability of the objective function in the uncertain parameters space. One way to overcome such limitation consists of incorporating risk metrics into the model. For instance, *Cheng et al. (2003)* solved a design and planning uncertainty problem considering multiple objectives, in which one of these objectives was the Downside risk (DR) metric. Additionally, the choice of the appropriate risk metric for the problem at hand is another issue to be considered. Several types of risk metrics have been evaluated in the literature. *Barbaro and Bagajewicz (2004)* included financial risk management in the framework of two-stage stochastic programming for a planning problem using Financial risk (henceforth known as risk) and DR as risk metrics. On the other hand, *Bonfill et al. (2004) and You et al. (2009)* have used Risk, DR and Worst Case (WC) metrics as a way to handle risk management in scheduling and planning problems under uncertainty. More recently, *Sabio et al. (2014)* minimized separately the WC and DR metrics as a way to reduce the probability of not meeting some environmental targets in the multi-objective optimization (MOO) of industrial networks.

According to *Aseeri and Bagajewicz (2004)*, no single risk metric can be regarded as "complete" risk metric, since they all present at least one of the following disadvantages:

- *(i)* Lack of associated probability value, limited solution space exploration (i.e., they focus on down, middle or upper side);
- *(ii)* Lack of capability of assessing simultaneously the probability and potential level of winnings and/or losses. Indeed, in practice most metrics tend to concentrate on penalizing

the worst scenarios rather than rewarding the best ones, thereby leading to "risk-averse" solutions.

To overcome these limitations, *Aseeri and Bagajewicz (2004)* proposed a Risk area Ratio (RAR) metric to compare the potential winnings against losses for the entire risk curve using a single value. This metric is useful because it considers the full risk spectrum, yet it does not achieve a simultaneous/complete financial risk analysis. In 2004, *Barbaro and Bagajewicz (2004)* found a close relationship between DR and risk used to compute the latter without the need to define binary variables, thereby simplifying the associated calculations. Here it is important to notice that the minimum DR at a defined target profit (Ω) does not guarantee that risk is minimum at every single value of profit ($\leq \Omega$). Therefore, this relation is an indirect way of measuring financial risk, but not a simultaneous analysis of economic metrics.

In summary, there is no single risk metric capable of providing a full control of the objective function in the uncertain parameters space. Hence, ideally, several complementary risk metrics should be optimized along with the expected performance. To the best of our knowledge, however, the simultaneous optimization of several risk metrics has never been addressed in the literature, which constitutes an important gap already acknowledged by several authors *(Cheng et al., 2003; Barbaro and Bagajewicz, 2004; Aseeri and Bagajewicz, 2004; Cardoso et al., 2016)*. One possible reason why this approach has never been applied is that the incorporation of several risk metrics in optimization under uncertainty leads to MOO problems containing a large number of objectives that are difficult to solve for different reasons. First, because generating Pareto solutions of stochastic models with a large number of objectives is computationally challenging. Second, because these stochastic multi-objective models tend to contain an infinite number of Pareto solutions, so even if a representative subset of them is generated, there is still the issue of interpreting and selecting the best solution.

This chapter proposes a novel approach for the optimization under uncertainty where the risk management considers several risk metrics simultaneously during the optimization step. First, a set of solutions behaving in different ways in the uncertain parameters space are generated using an algorithm based on the SAA algorithm. Then, the "Pareto filter approach", developed by *Mattson et al., (2003, 2004)* and later used by *Pozo et al. (2012)* and *Antipova et al. (2015)* is applied to rank these solutions. In order to illustrate the capabilities of this approach, the strategic planning problem over a supply chain under uncertainty is used as a benchmark. The problem is solved considering different financial risk metrics and identifying strategic decisions that are particularly appealing for decision-makers.

8.2. Problem statement

This chapter addresses the design of a SC of multi-product batch processes as schematized in Fig. 8.1. The problem formulation is essentially the same as the one presented in *(Corsano et al., 2011, 2014)*, however, in this chapter several financial risk elements were evaluated. One of the main advantages of this framework is that using simple modifications an independent problem formulation can be adapted to address additional information to aid the decision-making process.

In order to illustrate the capabilities and limitations of the proposed methodological framework are demonstrated using the MILP model presented by *Corsano et al. (2014).* Particularly, the SC includes a set of raw material suppliers $sp \in N_{sp}$ from which supplier sp can provide one or more types of raw materials $r \in N_r$, which are delivered to the batch plants $l \in N_l$. Each multiproduct batch plant has a set of batch stages $j \in N_{jl}$, for producing a set of products $i \in N_i$. In phase and out of phase unit duplication are considered for each multiproduct batch plant. The use and allocation of intermediate storage tanks is assumed as feasible at each of the $|N_{jl}| - 1$ positions in plant l, between two batch stages (j and j+1). Final products are transported from batch plants to different warehouses $m \in N_m$, according to their capacity limitation. Products are then delivered from the warehouses to different customer zones $g \in N_g$, in order to satisfy a given product demand D_{ig}. Further details on this SC design can be found in (Corsano et al., 2011, 2014).

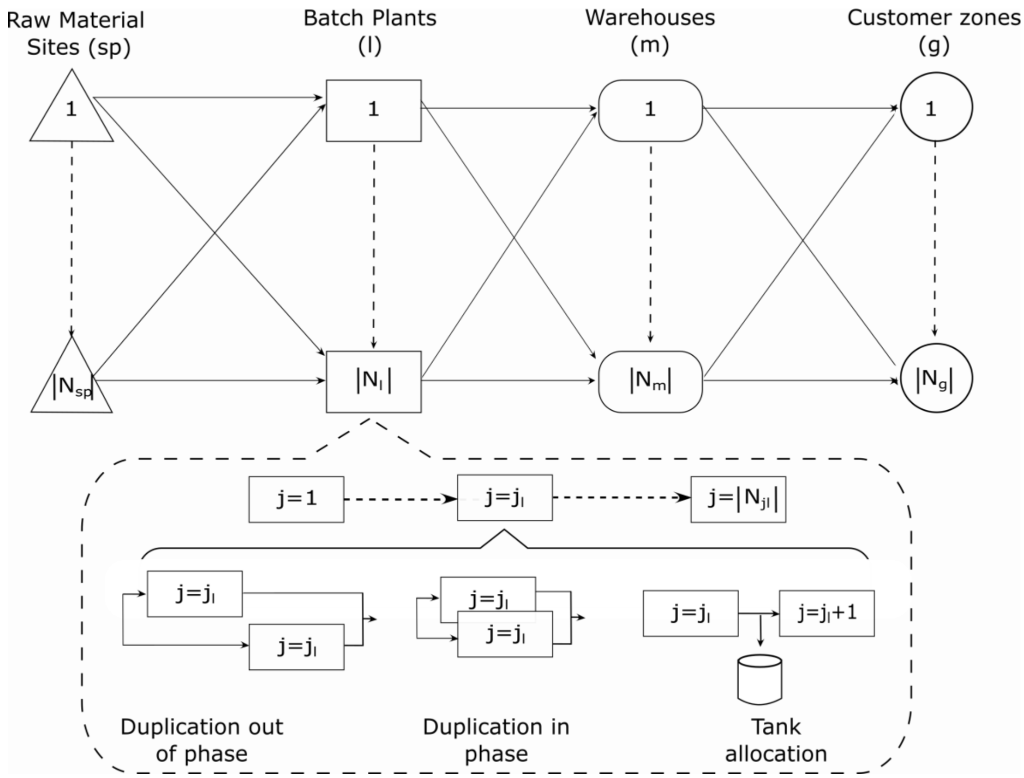

Fig. 8.1. Process scheme of the supply chain under analysis.

The goal of the analysis is to identify the best planning and design decisions (e.g. the number of plants to be installed, equipment units selected, etc.) in terms of maximum expected economic performance at the minimum risk.

To this end, the following data is required: discrete size of each batch unit to be eventually installed; set of allowable tank sizes and data concerning raw material procurements, distribution cost from-to different sites and overall batch plant parameters.

In this framework, product demands are modeled as uncertain parameters following known probability distribution patterns whose characteristic parameters are also given.

The detailed mathematical formulation that models the problem is presented as follows:

8.2.1. Mathematical formulation

The main equations that model the SC and batch plant design are following described.

Network mass balances

The produced amount of product i is quantified by Q, while $zz_{i,l}$ is the binary variable that decides whether a product i is produced in plant l (Eq. (8.1)).

$$zz_{i,l}Q_{i,l}^{LO} \le Q_{i,l,s} \le zz_{i,l}Q_{i,l}^{UP} \qquad \forall i,l,s \tag{8.1}$$

In the same way, the use of each raw material type is conditioned by its availability in each supplier site sp, as shown in Eq. (8.2). In addition, the distribution flow is restricted by Eq. (8.3).

$$\sum_{i,l} Q_{sp,r,i,l,s} \le Q_{sp,r}^{UP} \qquad \forall sp,r \tag{8.2}$$

$$Q_{sp,r,i,l,s} \le zz_{i,l}Q_{sp,r}^{UP} \qquad \forall sp,r,i,l \tag{8.3}$$

The resources required for production processes considering the conversion factor ($fl_{r,i,l}$) is calculated using Eq. (8.4).

$$\sum_{sp=1}^{Ns} Q_{sp,r,i,l,s} = fl_{r,i,l}Q_{i,l,s} \qquad \forall r,i,l,s \tag{8.4}$$

In order to avoid infeasibilities, binary variable ex_l model the installation of a particular plant, thus, forcing the production to be zero if the plant does not exist.

$$zz_{i,l} \le ex_l \qquad \forall i,l \tag{8.5}$$

The distribution links between production plants l and warehouses m are controlled by Eq.(8.6), while the use of potential warehouses is guaranteed by defining the binary variable, $yy_{m,s}$, in Eq.(8.7).

$$\sum_{m=1}^{Nm} Q_{i,l,m,s} = Q_{i,l,s} \qquad \forall i,l,s \tag{8.6}$$

$$\sum_{i,l} Q_{i,l,m,s} \le Q_m^{max}\, yy_{m,s} \qquad \forall m,s \tag{8.7}$$

Assuming a steady-state operation (i.e., lack of stock accumulation), the total amount of stored product has to be delivered to any customer zones g, as expressed in Eq. (8.8).

$$\sum_{l=1}^{Nl} Q_{i,l,m,s} = \sum_{g=1}^{Ng} Q_{i,l,g,s} \qquad \forall i,m,s \tag{8.8}$$

The amount of products to be stored is limited, as shown in Eq. (8.9). On the other hand, product demand is completely satisfied using Eq. (8.10).

$$\sum_{i,g} Q_{i,m,g,s} \le Q_m^{max}\, yy_{m,s} \qquad \forall m,s \tag{8.9}$$

$$D_{i,g} = \sum_{m=1}^{Nm} \sum_{l} Q_{i,l,m,s} \qquad \forall i,s \tag{8.10}$$

Batch units design equations

Without loss of generality, the batch unit size ($VZ_{j,l,s}$), is computed through Eq. (8.11).

$$VZ_{j,l,s} \geq \frac{Size_{i,j,l} B_{i,j,l,s}}{NP_{j,l}} \qquad \forall i,j,l,s \tag{8.11}$$

Particularly, $Size_{i,j,l}$ is the size factor (the size required at stage *j* to produce 1kg of final product *i*), $B_{i,j,l,s}$ is the batch size and $NP_{j,l}$ is the number of units working in-phase at this stage. The total amount of product *i* produced in plant *l* is defined by Eq. (8.12) assuming that $Nb_{i,j,l,s}$ is the number of batches of product *i* in stage *j* of plant *l*.

$$Q_{i,l,s} = Nb_{i,j,l,s} B_{i,j,l,s} \qquad \forall i,j,l,s \tag{8.12}$$

By combining Eq. (8.11) and Eq. (8.12), the following constraint is obtained.

$$Nb_{i,j,l,s} \geq \frac{Size_{i,j,l} Q_{i,l,s}}{VZ_{j,l,s} NP_{j,l}} \qquad \forall i,j,l,s \tag{8.13}$$

To formulate the problem as a MILP, such a non-linear constraint is rewritten using Eq. (8.14) in which $xz_{j,l,d}$ is the binary variable that represents the existence of parallel units in phase. Particularly, Eq. (8.15) states that at least one unit per stage must exist if plant *l* is allocated.

$$NP_{j,l} = \sum_{d=1}^{NP_{j,l}^{UP}} d \, xz_{j,l,d} \qquad \forall j,l \tag{8.14}$$

$$\sum_{d=1}^{NP_{jl}^{UP}} xz_{j,l,d} = ex_l \qquad \forall j,l \tag{8.15}$$

The unit size calculation was also reformulated considering a set of available discrete sizes *p* (Eq. (8.16)) while Eq. (8.17) defines both, the existence of a plant and its size.

$$VZ_{j,l,s} = \sum_{p=1}^{P_{j,l}} VZ_{j,l,p,s} VF_{j,l,p} \qquad \forall j,l,s \tag{8.16}$$

$$\sum_{p \in SV_{jl}} VZ_{j,l,p,s} = ex_l \qquad \forall j,l,s \tag{8.17}$$

Thus, using Eqs. (8.14-8.17) the Eq. (8.13) can be reformulated in terms of $NP_{j,l}$ definition, leading to Eq. (8.18).

$$Nb_{i,j,l,s} \geq \sum_{p,d} \frac{Size_{i,j,l} Q_{i,l,s}}{VF_{j,l,p} d} v_{j,l,p} xz_{j,l,d} \qquad \forall i,j,l,s \tag{8.18}$$

However, the product between $Q_{i,l,s}$, $v_{j,l,p}$ and $xz_{j,l,d}$ in Eq. (8.18) is another non-linear term. Therefore, a new nonnegative continuous variable, $ee_{i,j,l,p,d,s}$, has to be defined.

$$ee_{i,j,l,p,d,s} = \begin{Bmatrix} Q_{i,l,s} & \text{if} & v_{j,l,p} \text{ and } xz_{j,l,d} = 1 \\ 0 & & \text{otherwise} \end{Bmatrix} \qquad \forall i,j,l,p,d,s \tag{8.19}$$

And finally the following constraints (Eqs. (8.20-8.23)) are used to substitute Eq. (8.18):

$$Nb_{i,j,l,s} \geq \sum_{p,d} \frac{Size_{i,j,l}}{VF_{j,l,p}d} ee_{i,j,l,p,d,s} \qquad \forall i,j,l,s \tag{8.20}$$

$$\sum_{d} ee_{i,j,l,p,d,s} \leq Q_{i,l}^{UP} v_{j,l,p} \qquad \forall i,j,l,p,s \tag{8.21}$$

$$\sum_{p} ee_{i,j,l,p,d,s} \leq Q_{i,l}^{UP} xz_{j,l,p} \qquad \forall i,j,l,d,s \tag{8.22}$$

$$Q_{i,l,s} = \sum_{p,d} ee_{i,j,l,p,d,s} \qquad \forall i,j,l,s \tag{8.23}$$

Intermediate storage equations

For N_{jl} batch stages, there exist at most N_{jl-1} possible positions for storage tanks. Therefore, Eqs. (8.24-8.25) define an upper bound for the storage vessels.

$$VT_{j,i,s} \geq 2ST_{i,j,l}B_{i,j,l,s}su_{j,l} \qquad \forall i,l,s,j = 1,2,\dots,N_{j,l-1} \tag{8.24}$$

$$VT_{j,i,s} \geq 2ST_{i,j,l}B_{i,j+1,l,s}su_{j,l} \qquad \forall i,l,s,j = 1,2,\dots,N_{j,l-1} \tag{8.25}$$

Here, $VT_{j,i,s}$ represents the tank size, $ST_{i,j,l}$ the size factor for each storage tank and $su_{j,l}$ is a binary variable that determines if a tank is allocated after batch stage *j* or not. Using Eq. (8.11) in Eq. (8.13) and Eq. (8.25), the storage constraints are rewritten as follows.

$$Nb_{i,j,l,s} \geq 2\frac{ST_{i,j,l}Q_{i,l,s}}{VT_{j,l,s}} su_{j,l} \qquad \forall i,l,s,j = 1,2,\dots,N_{jl-1} \tag{8.26}$$

$$Nb_{i,j+1,l,s} \geq 2\frac{ST_{i,j,l}Q_{i,l,s}}{VT_{j,l,s}} su_{j,l} \qquad \forall i,l,s,j = 1,2,\dots,N_{jl-1} \tag{8.27}$$

Again, in order to relax the nonlinearities, a set of available discrete sizes for the tank allocated after stage *j*, $STF_{j,l} = \{VTF_{j,l,1}, VTF_{j,l,2}, \dots, VTF_{j,l,w}\}$, is selected. Let $vt_{j,l,w}$ be the binary variable that allows allocating the storage tanks of size *w*. Notice that the first tank, VTF_{jl1}, has a size of zero to represent "no tank allocation". Consequently, Eq. (8.26) and Eq. (8.27) are rewritten as Eq. (8.28-8.30):

$$Nb_{i,j,l,s} \geq 2\sum_{w\neq 1} \frac{ST_{i,j,l}Q_{i,l,s}}{VTF_{j,l,w}} vt_{jlw} \qquad \forall i,l,s,j = 1,2,\dots,N_{jl-1} \tag{8.28}$$

$$Nb_{i,j+1,ls} \geq 2\sum_{w\neq 1} \frac{ST_{i,j,l}Q_{i,l,s}}{VTF_{j,l,w}} vt_{j,l,w} \qquad \forall i,l,s,j = 1,2,\dots,N_{jl-1} \tag{8.29}$$

$$\sum_{w} vt_{j,l,w} = ex_l \qquad \forall l,j = 1,2,\dots,N_{jl-1} \tag{8.30}$$

Eq. (8.30) states that if plant *l* exists, then only one discrete size for a tank after stage *j* has to be selected. Using the continuous variable $ff_{i,j,l,w} = Q_{i,l}\ vt_{j,l,w}$, Eq. (8.28) and Eq. (8.29) become linear and give rise to Eq. (8.31-8.32) using the constraints represented in Eq. (8.33-8.34).

$$Nb_{i,j,l,s} \geq 2\sum_{w\neq 1}\frac{ST_{i,j,l}}{VTF_{j,l,w}}ff_{i,j,l,w} \qquad \forall i,l,s,j=1,2,\dots,N_{j,l-1} \qquad (8.31)$$

$$Nb_{i,j+1,ls} \geq 2\sum_{w\neq 1}\frac{ST_{i,j,l}}{VTF_{j,l,w}}ff_{i,j,l,w} \qquad \forall i,l,s,j=1,2,\dots,N_{j,l-1} \qquad (8.32)$$

$$ff_{i,j,l,w} \leq Q_{i,l}^{UP}vt_{j,l,w} \qquad \forall i,l,j=1,2,\dots,N_{j,l-1},w \qquad (8.33)$$

$$Q_{i,l,s} = \sum_{w} ff_{i,j,l,w} \qquad \forall i,l,s,j=1,2,\dots,N_{j,l-1} \qquad (8.34)$$

If there is an absence of storage tanks between two consecutive stages, then the number of batches must be equal for both of them. In addition, the bounds for the ratio between the numbers of batches of consecutive stages can be calculated as in Eq. (8.35).

$$\begin{aligned} Nb_{i,j,l,s} + \left(\frac{1}{\phi}-1\right)\sum_{w\neq 1} vt_{j,l,w} &\leq \frac{Nb_{i,j+1,l,s}}{Nb_{ijls}} \\ &\leq 1+(\phi-1)\times\sum_{w\neq 1} vt_{j,l,w} \end{aligned} \qquad \forall i,l,s,j=1,2,\dots,N_{j,l-1} \qquad (8.35)$$

Here, ϕ is a constant value corresponding to the maximum ratio allowed between the batches number of consecutive stages.

<u>Objective Function</u>

The investment cost considers both, the batch and storage tanks costs as described in Eq. (8.36).

$$\begin{aligned} EC = &\sum_{l}\sum_{j}\sum_{p}\sum_{n}\sum_{d} \alpha_{j,l}VF_{j,l,p}{}^{(\beta_{j,l})}\, v_{j,l,p}nx_{j,l,n}dxz_{j,l,d} \\ &+\sum_{l}\sum_{j}\sum_{w}\bar{\alpha}_{j,l}VTF_{j,l,w}^{\bar{\beta}_{j,l}}vt_{jlw} \end{aligned} \qquad \forall j,l \qquad (8.36)$$

The first term corresponds to the batch units cost while the second represents the storage tanks cost. Here, in order to avoid nonlinearities, the continuous variable $\rho_{i,j,l,p,n,d}$ is defined given by Eq. (8.37-8.38).

$$\rho_{i,j,l,p,n,d} \geq v_{j,l,p} + x_{j,l,n} + xx_{j,l,d} - 2 \qquad \forall i,j,l,p,n,d \qquad (8.37)$$

$$0 \leq \rho_{i,j,l,p,n,d} \leq 1 \qquad \forall i,j,lp,n,d \qquad (8.38)$$

Thus, the equipment cost can be rewritten as in Eq. (8.39).

$$\begin{aligned} EC = &\sum_{l}\sum_{j}\sum_{p}\sum_{n}\sum_{d} \alpha_{j,l}ndVF_{j,l,p}{}^{(\beta_{j,l})}\, \rho_{i,j,l,p,n,d} \\ &+\sum_{l}\sum_{j}\sum_{w}\bar{\alpha}_{j,l}VTF_{j,l,w}^{\bar{\beta}_{jl}}\, vt_{j,l,w} \end{aligned} \qquad \forall j,l \qquad (8.39)$$

A fixed investment cost is considered (LC) in Eq. (8.40), in which Cpl_l and $Cdep_m$ are the installation cost coefficients, while the total investment cost is described in Eq. (8.41).

$$LC = \sum_l Cpl_l ex_l + \sum_m Cdep_m\, y_m \tag{8.40}$$

$$IC = C_{an}(EC + LC) \tag{8.41}$$

The operating cost, including raw material acquisition, storage, and production cost are considered together in the following expression (Eq. (8.42)).

$$OC_s = \sum_{sp}\sum_r\sum_i\sum_l Craw_{sp,r} Q_{sp,r,i,l,s} + \sum_i\sum_l\sum_m Cd_{i,m} Q_{i,l,m,s} + \sum_i\sum_l Cprod_{i,l} Q_{i,l,s} \qquad \forall s \tag{8.42}$$

Here, $Craw_{sp,r}$, $Cd_{i,m}$, and $Cprod_{i,i}$ are the associated costs for raw material acquisition, storage, and production cost, respectively. The Q amounts are expressed in kg per time horizon, therefore the cost parameters are given in \$/kg. The distribution costs at the entire SC are also considered in this model represented through the Eq. (8.43).

$$TC_s = \sum_{sp}\sum_r\sum_i\sum_l Ctraw_{sp,r,l} Q_{sp,r,i,l,s} + \sum_m\sum_i\sum_l Ctp_{i,l,m} Q_{i,l,m,s} + \sum_i\sum_m\sum_k Ctd_{i,m,k} Q_{i,m,k,s} \qquad \forall s \tag{8.43}$$

In Eq. (8.43), $Ctraw_{sp,r,l}$, $Ctp_{i,l,m}$, and $Ctd_{i,m,k}$ are cost coefficients that depend on the product transported and the covered distance. Eq. (8.44) summarizes the total cost for each scenario.

$$TCost_s = TC_s + OC_s \qquad \forall s \tag{8.44}$$

Eq. (8.45) describes the economic revenue of selling the final product in each scenario, where $Price_i$ is the selling price of product *i* in \$/kg. The profit at each scenario is obtained through the difference among economic revenue and associated costs at each scenario realization as represented in Eq. (8.46).

$$Sales_s = \sum_i\sum_m\sum_k Q_{i,m,k,s} Price_i \qquad \forall s \tag{8.45}$$

$$PROFIT_s = Sales_s - TCost_s \qquad \forall s \tag{8.46}$$

In Eq. (8.47) the total expected profit is described, in which the associated probability of each scenario is taken into account. Additionally, costs which do not depend on the scenario realization are considered in this equation, denoted as *IC*.

$$EProfit = \left(\sum_s PROFIT_s\, Prob_s\right) - IC \tag{8.47}$$

For more details on the model, the reader is invited to check *Corsano et al., (2011)*.

8.3. Methodology

As stated before, this proposed approach aim to evaluate different financial risk metrics along the process performance as a way to promote the identification of an economically efficient solution. Particularly, this approach comprises four essential steps as shown in Fig. 8.2. A stochastic MOO model is formulated in step 1. Step 2 solves the stochastic MOO problem using a customized strategy that provides as output a set of solutions that are later normalized in step 3. Finally, these normalized solutions are filtered in order to obtain a reduced subset of alternatives with better overall performance. A detailed description of each step is provided in the following subsections.

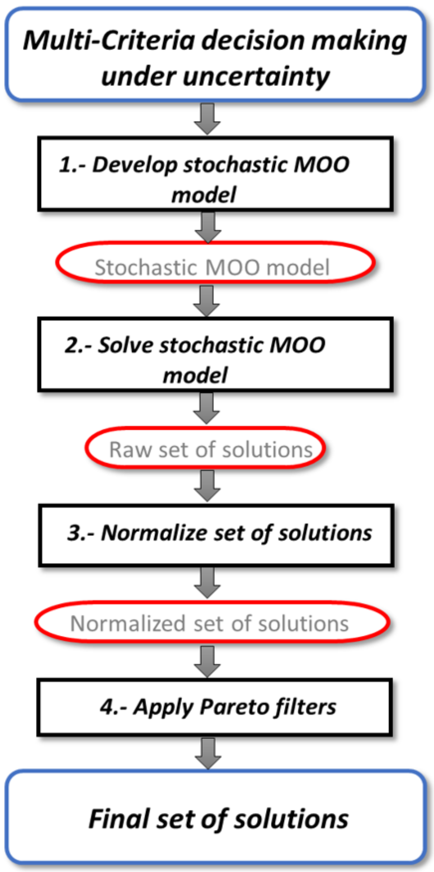

Fig. 8.2. Overview of the proposed methodology.

8.3.1. Multi-scenario two-stage stochastic programming model

Hence, the original deterministic single objective (SO) model was reformulated into a multi-scenario two-stage stochastic problem of the following form (see Eq.(8.48)), henceforth known as model *(P)*:

$$
\begin{aligned}
(P) \quad & \max_{x\,y} \; f(x, y, \theta) \\
s.t. \quad & \\
& h(x, y, \theta) = 0 \\
& g(x, y, \theta) \leq 0 \\
& x \in \mathrm{X}, y \in \mathrm{Y}, \theta \in \Theta
\end{aligned}
\tag{8.48}
$$

Here, x and y are the first and second-stage decision variables, respectively, whereas θ denotes the uncertain parameters values that belong to the corresponding space Θ. First-stage decisions may contain integers due to allocation requirements. $f(x, y, \theta)$ represents the objective function; $h(x, y, \theta)$ and $g(x, y, \theta)$ are vectors of equality and inequality constraints. Commonly, uncertain parameters are described via scenarios, and, model *(P)* can be re-written as follows:

$$
\begin{aligned}
&(P) \qquad \max_{x, y_s} \; f_{ob} = \sum_{s}^{S} prob_s \, f(x, y_s, \theta_s) \\
&s.t. \\
&\qquad h(x, y_s, \theta_s) = 0 \qquad \forall s \in S \\
&\qquad g(x, y_s, \theta_s) \leq 0 \qquad \forall s \in S \\
&\qquad x \in X, y_s \in Y, \theta_s \in \Theta
\end{aligned}
\tag{8.49}
$$

Here, f_{ob} represents the expected value for the objective function of the problem *(P)*. θ_s is the vector of values taken by the uncertain parameters in the scenarios s and $prob_s$ is the probability of occurrence of scenario s belonging to the set S.

Model *(P)* can be interpreted as follows: First stage decision variables (x) must be taken before a realization of the uncertain variables (θ_s) becomes known (here and now decisions). However, such decisions need to satisfy as well the second-stage set of constraints. Therefore, recourse actions need to be taken (second-stage decision variables for each one of the considered scenarios y_s) with an associated impact over the objective function. Hence, given a set of first-stage decisions x, each realization of θ_s leads to recourse costs given by the value of the second-stage decisions (y_s). Note that the characterization of the different scenarios to be considered can be evaluated via sampling on the corresponding probability functions.

To manage the risk associated with the decision-making problem under uncertainty, some risk metrics are included in the model as additional criteria to be optimized. A detailed description of these metrics is presented next.

(i) *Downside Risk (DR): DR* represents the positive deviation from a defined target (generally denoted by Ω). *DR* can be expressed as shown in Eq. (8.50):

$$DR_{\Omega} = E[\delta_{\Omega s}] = \sum_{s} prob_s \, \delta_{\Omega s} \tag{8.50}$$

where

$$\delta_{\Omega s} = \begin{Bmatrix} \Omega - Profit_s & \text{if } Profit_s < \Omega \\ 0 & \text{otherwise} \end{Bmatrix} \qquad \forall s \in S \tag{8.51}$$

Here, $Profit_s$ accounts for the profit in scenario $s \in S$.

(*ii*) *Risk:* This metric also requires the definition of a target, but it measures the probability of not achieving this target rather than the deviation from it. *Risk* is mathematically expressed as follows:

$$Risk_{\Omega} = \sum_{s} prob_s \, Z_{\Omega s} \tag{8.52}$$

Where, $Z_{\Omega s}$ is a binary variable whose value is determined as follows:

$$Z_{\Omega s} = \begin{Bmatrix} 1 & \text{if} & Profit_s \leq \Omega \\ 0 & & \text{otherwise} \end{Bmatrix} \qquad \forall s \in S \tag{8.53}$$

Notice that even if both, *DR* and *Risk*, provide a measure of the deviation of the solution from a given target, the calculation of the latter involves a bigger computational effort since it requires the definition of binary variables for each scenario.

(iii) Value at Risk (VaR) and Opportunity Value (OV): These metrics assess the performance of a solution in a given region of the cumulative probability curve. More precisely, the *VaR* is the difference between the expected profit and the profit for a cumulative probability at a defined confidence level (typically 5%), while the *OV* is conceptually equal to *VaR*, but covers the upper side of the cumulative risk curve (typically a percentile of 95%). Hence, these values are usually used together in order to explore both sides of the cumulative risk plot.

(iv) *Worst Case (WC):* The *WC* has been adopted as an alternative to control the probability of meeting unfavorable scenarios. It leads to a simple formulation that requires a low computational effort (see Eq. (8.54)).

$$WC \leq Profit_s \qquad \forall s \in S \qquad (8.54)$$

For more details about the above risk metrics and their implementation in supply chain models, the reader is referred to the works by *Aseeri et al. (2004), Aseeri and Bagajewicz (2004), Bonfill et al. (2004), Barbaro and Bagajewicz (2004)* and *Applequist et al. (2000)*. Finally, the stochastic model that optimizes a set of risk metrics can be formally expressed as follows:

$$\begin{aligned}
(P) \quad & \max_{x\,y} \ \{f_1(x, y_s, \theta), \dots, f_{ob}(x, y_s, \theta), \dots, f_{|OB|}(x, y_s, \theta)\} \\
s.t. \quad & \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (8.55) \\
& h(x, y_s, \theta) = 0 \qquad \forall s \in S \\
& g(x, y_s, \theta) \leq 0 \qquad \forall s \in S \\
& x \in X, y_s \in Y, \theta \in \Theta
\end{aligned}$$

Where f_{ob} represents the different objective functions of the problem (e.g. $f_1 = EProfit$, $f_2 =$ -*DR*, $f_3 =$ -*Risk*, etc.). A detailed mathematical model description from where the expected profit was calculated is presented in the following subsection. Note that the proposed approach is general enough to accommodate other risk metrics as well.

8.3.2. Solution strategy (Sample Average Approximation algorithm).

Solving *(P)* (step 2 in Fig. 8.2) is challenging due to the number of scenarios and objectives. To expedite its solution, a strategy based on the SAA algorithm is proposed. A general overview of the decomposition strategy used to solve model *(P)* is described as follows *(Shabbir and Shapiro, 2002; Kostin et al., 2012)*.

The model in its deterministic form considering only one scenario at a time and optimizing the profit as the unique objective is first solved. Then, the values obtained for the first-stage variables (i.e., the design of the supply chain) are fixed and the expected profit in the model *(P)* is optimized again, but this time considering all the $|S|$ scenarios. An iterative approach is employed by replacing the parameters at each solution of the deterministic model solved in step one (corresponding to one particular scenario) to obtain the optimal supply chain design for each of the remaining $|S|$-1 scenarios. At the end, $|S|$ different solutions are generated.

Note that the standard SAA approximates the solution of a single-objective stochastic problem by solving a series of stochastic sub-problems, each of them with fewer scenarios than the original full space stochastic model *(Verweij et al., 2002; Santoso et al., 2005)*. These scenarios, sampled from the original set of scenarios, approximate the expected objective value of the original problem. After solving each sub-problem, the first stage decisions are fixed in the original model, which is solved iteratively for all the solutions generated. The solution that performs best in the full space model is finally used to approximate the global optimum of the original stochastic model. Hence, in this case, the sub-problems contain one single scenario (i.e., they are deterministic), as opposed to what happens in the standard SAA, which solves sub-problems with more than one scenario.

Note that even if the model *(P)* is a multi-criteria model, the only objective function considered during the process is the profit maximization (i.e., risk metrics are calculated in parallel during the process, but they never act as objective functions). The reason for this is two-fold. First, it is not possible to optimize any risk metric during deterministic optimization (i.e., it considers one scenario only). Second, the stochastic model could allocate any risk metric as the objective function, yet this would entail no significant benefit since the risk can be mainly controlled through modifications in the design of the SC, which has already been fixed in the previous step.

8.3.3. Normalization of solutions.

The SAA method provides as outcome a raw set of solutions (*RSS*) to the problem *(P)*. A normalization step is then applied to facilitate the post-optimal analysis of these solutions. Different normalization algorithms can be applied at this point (see *Bolstad et al., (2003)*). Here, we use the basic interpolation method, which is formulated as follows:

$$\hat{f} = \hat{f}_{lo} + (\hat{f}_{up} - \hat{f}_{lo}) \frac{f - f_{lo}}{f_{up} - f_{lo}} \tag{8.56}$$

Here, $\hat{f}$ represents the normalized value (which varies between bounds $\hat{f}_{lo} = 0$ and $\hat{f}_{up} = 1$) associated to the real value f, while f_{lo} and f_{up} represent respectively the minimum and maximum values taken by this objective among the raw set of solutions *RSS*. At the end of this step, a normalized set of solutions *NSS* is obtained.

8.3.4. Application of Pareto filters.

Model *(P)* potentially contains an infinite number of solutions from which decision-makers should identify the ones that better reflect their preferences. To facilitate this task, the already explained Pareto filters (See Chapter 3) are applied to narrow down the number of Pareto solutions and retain for further inspection solutions showing better overall performance (discarding in turn the rest). Fig. 8.3 illustrates the application of the Pareto filter to this problem.

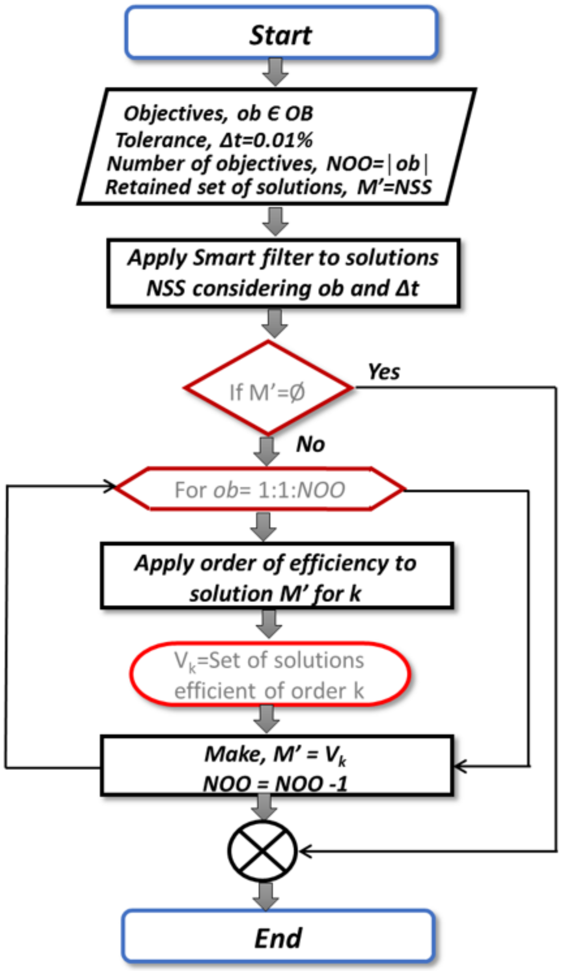

Fig. 8.3. Detailed description of the Pareto filter procedure used to reduce the set of optimal solutions.

A general description of each step in the above algorithm follows is explained in Chapter 3.

8.4.Case study.

The proposed approach is now illustrated through its application to the design and planning problem of a supply chain with embedded batch facilities.

The system considers three raw material sources, which can feed five potential batch plants with up to three phases. Different discrete sizes are considered for each batch unit (0.3 m^3, 0.5 m^3, 0.75 m^3, 1 m^3 and 1.2 m^3) and intermediate storage tank (3m^3, 5 m^3, 10 m^3). Final products can be stored in three warehouses before being sent to three customer zones. The remaining system parameters are provided in Appendix B.5.

The model optimizes the design of the required supply chain network (i.e. allocation decisions, production and capacity levels and flows between the SC nodes) considering the effects of the potential planning decisions. The model also determines the optimal design of the embedded batch plants (i.e. the plants structure) considering parallel unit duplication, allocation of storage tanks, and unit size. Binary variables are used in the mathematical model in order to represent the allocation decisions of a particular site/unit.

Product demand was considered as the only uncertain parameter and modeled through a normal distribution. One hundred scenarios were generated via Monte Carlo sampling in order to discretize the normal distributions, assuming the mean values in Table B.11 (See Appendix B) and a variance of 15%. It is important to highlight that Monte Carlo sampling is used as a crude method to illustrate the generation of scenarios in the proposed methodology as explained in Chapter 3.

The minimum number of scenarios to be considered in order to ensure a representative solution was determined by two methods. First, by solving the SAA for an increasing number of scenarios and then stopping when the difference between the expected profits of the best two consecutive solutions provided by the SAA was less than 5%. Second, the methodology proposed by *Law and Kelton (2000)*, which has been applied to stochastic problems *(Sabio et al., 2014)*was considered (see Appendix B.6). This later approach was solved considering a relative error of 0.1 and a confidence level of 1%, leading to a minimum number of scenarios of 73. Notice that the identification of a reduced is out of the scope of this chapter. In fact, *Law and Kelton (2000)* approach was used without generality since this approach is significantly faster than the one presented in Chapter 6, even though the latest one is more efficient in terms of the size of reduced set of scenarios.

The deterministic model contains 3,222 equations, 2,086 continuous variables and 223 binary variables. Even if 73 were identified as representative enough, 100 scenarios were used so as to evaluate the capabilities of the proposed approach to discard a significant number of non-dominated or repeated solutions. The stochastic model (100 scenarios) has 178,552 equations, 153,061 continuous variables and the same number of binary variables (223). All the runs were implemented in GAMS 23.9 and the problem was solved using CPLEX on a Windows XP computer with Intel®Core™i7 CPU(920) 2.67GHz processor with 4.00 GB of RAM. It takes approximately 27.3 seconds to generate each solution of the deterministic model. It is important to mention that the stochastic model that includes all the scenarios and maximizes the expected profit as unique criterion cannot be solved in 86,400 seconds (24 hours) (i.e., after this CPU time, CPLEX is unable to close the optimality gap below 5% even when optimizing only the expected profit; so much larger CPU times are expected when dealing with several risk metrics simultaneously).

As shown in Table 8.1, two cases differing in the risk metrics are investigated. The targets required in the calculations of the risk metrics were defined as follows. A SAA was applied and the associated result for each deterministic optimization was plotted in (Fig. 8.6). Later, the target values were defined by identifying the lower, middle and upper parts of these cumulative distributions. Each curve in Fig. 8.6 represents a specific SC configuration with associated planning decisions. Expected profit values range from \$530,000 to \$1,334,000. In the figure, we have highlighted the solution with maximum expected profit (*maxEProfit*) as well as two curves that may be appealing for risk-averse and risk-taker decision makers. A Risk-Averse solution corresponds to that in which lower probabilities of small/high profits are found. On the contrary, a solution with larger probabilities of high profits (at the expense of increasing as well the probability of low benefits) is appealing for a *Risk-Averse* behavior.

Solutions behave differently in the uncertain parameters space, as it can be noticed by the performance of the three highlighted solutions. For instance, *maxEProfit* has a probability of 19% of not exceeding a target value of Ω= \$1.00M, while this probability increases gradually to 25% and 55% in the *Risk-Averse* and *Risk-Taker* solutions, respectively. Here, the *maxEProfit* solution represents a very conservative choice that behaves better than the remaining solutions for a wide range of target values (Ω <\$1.15M), however for higher target values this solution shows poor performance. Notice that the better performance attained in the Risk-Averse and Risk-Taker solutions in the upper part of the probability curve is obtained at the expense of a drop in their expected profit. For instance, the Risk-Taker and Risk-Averse solutions show expected profits of \$971,179 and \$1,057,684, respectively, whereas the maximum expected profit is \$1,100,211.

Between the Risk-Taker and Risk-Averse solutions, there are many intermediate solutions behaving in different ways.

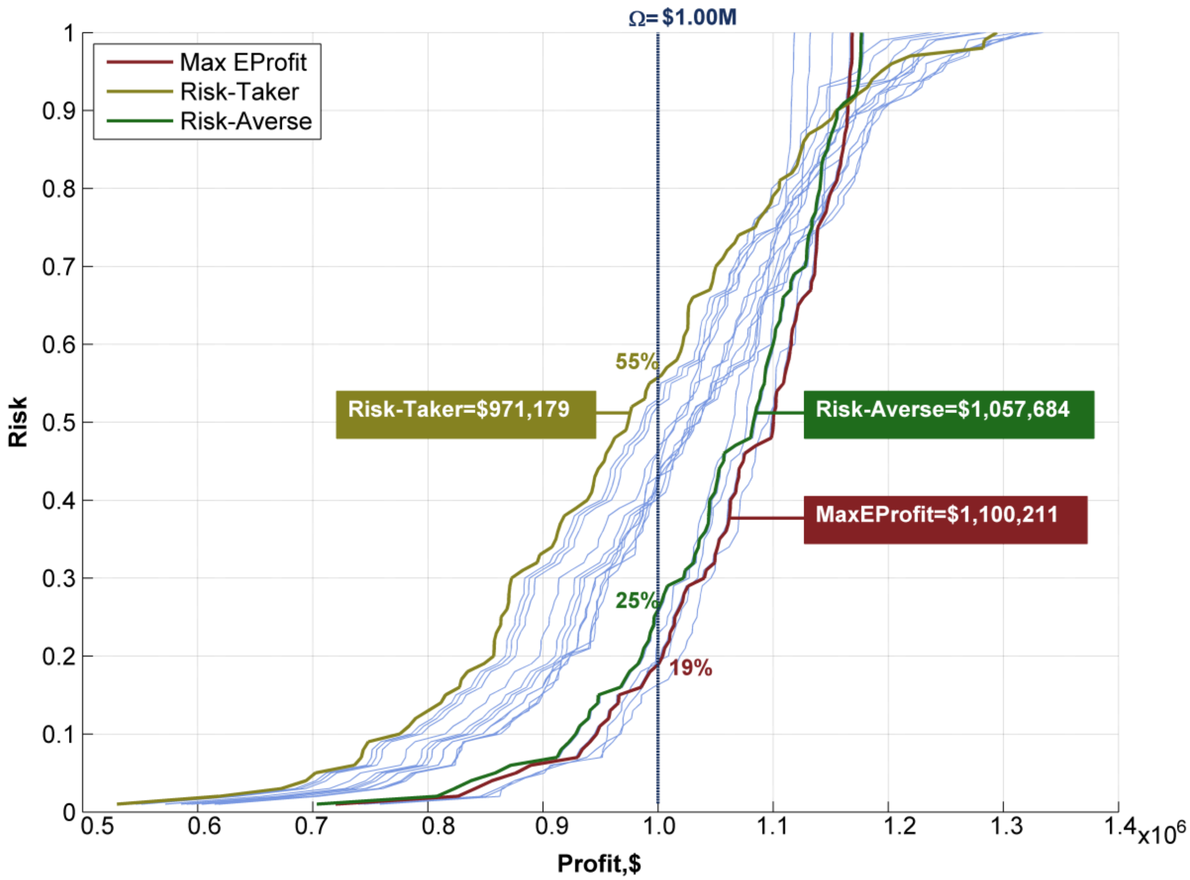

Fig. 8.6. Resulting cumulative risk curves for the 100 scenarios.

All the solutions show essentially the same overall supply chain configuration (see Fig. 8.7), but differ in the detailed design of the plants, as will be explained later. More precisely, they all select plant L4 regardless of the uncertain parameters values, mainly because the required investment and production costs are the lowest. Raw material site S2 supplies all the materials required for producing the four products, because the distribution costs between S2 and L4 are cheaper. The products are delivered to two warehouses, M1 and M3.

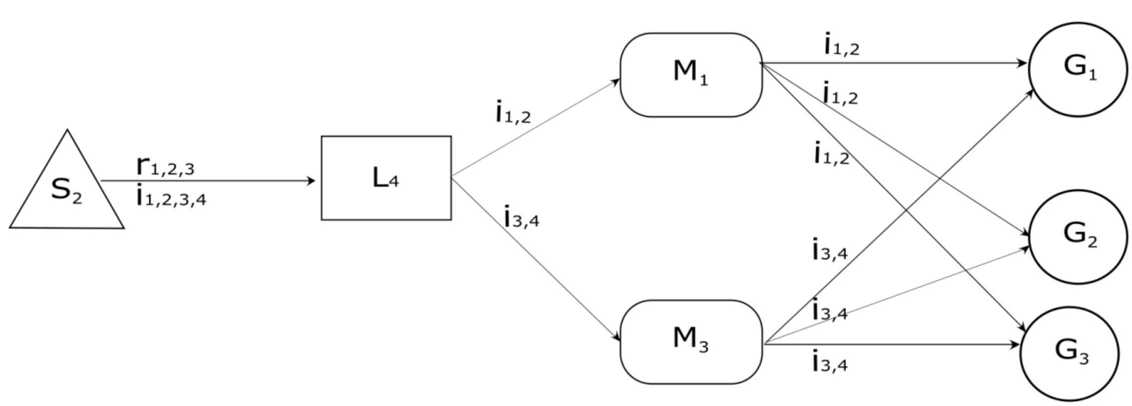

Fig. 8.7 optimal SC design for the 100 demand scenarios.

Table 8.1. List of objectives and target values considered for both cases. Target values Ω are expressed in €·10^3.

First Case		Second Case	
Objective/metric	Target value	Objective/metric	Target value
Eprofit	*N/A*	*Eprofit*	*N/A*
Worst Case (WC)	*N/A*		Ω=530
	Ω=800		Ω=584
Downside Risk (DR)	Ω=950		Ω=637
	Ω=1,050		Ω=691
Value at Risk (VaR)*	*5%*		Ω=745
Opportunity Value (OV)*	*95%*		Ω=798
			Ω=852
			Ω=906
		Risk	Ω=959
			Ω=1,013
			Ω=1,066
			Ω=1,120
			Ω=1,174
			Ω=1,227
			Ω=1,281
			Ω=1,335

*The percentage target value for *VaR* and *OV* are the probability value in the cumulative plot.

8.4.1. First case: Expected profit, worst case, downside risk, value at risk and opportunity value

Here, *WC, DR, VaR* and *OV* were considered as performance criteria (objectives) in addition to *Eprofit*. For the *DR* calculation, three target values were used corresponding to the lower, middle and upper parts of the cumulative distribution curve. For the *VaR* and *OV*, the standard 5% and 95% percentiles were set (See Table 8.1).

After the application of the proposed algorithm, 100 solutions were obtained, each one with specific values of the decision variables, expected cost and financial risk metrics. From here, a 100 x 7 matrix was produced (henceforth known as matrix N) using the values of each performance criteria in each scenario. Matrix N is normalized according to the procedure described in section 8.4.3. Note that some of the deterministic solutions may be suboptimal (in the space of the objectives considered in the analysis), or repeated (i.e. the model yields the same first-stage decision values when solved for two different scenarios). The Pareto filters were applied next using this matrix.

Fig. 8.8 is a parallel coordinates plot that represents in the horizontal axis the normalized objectives and in the vertical one the performance attained by every solution in each such objective. The objectives are normalized as described previously (0 is the best value and 1 is the worst) and the Smart filter (first step of Pareto filters, section 8.4.4) was executed with a tolerance value of Δt=0.01%. As explained in Chapter 3, the dominated solutions are identified and removed by the filter, so finally the number of solutions was reduced from 100 to the 20 which remain in Fig. 8.8 (depicted by polylines, which intersect each other in at least one point).

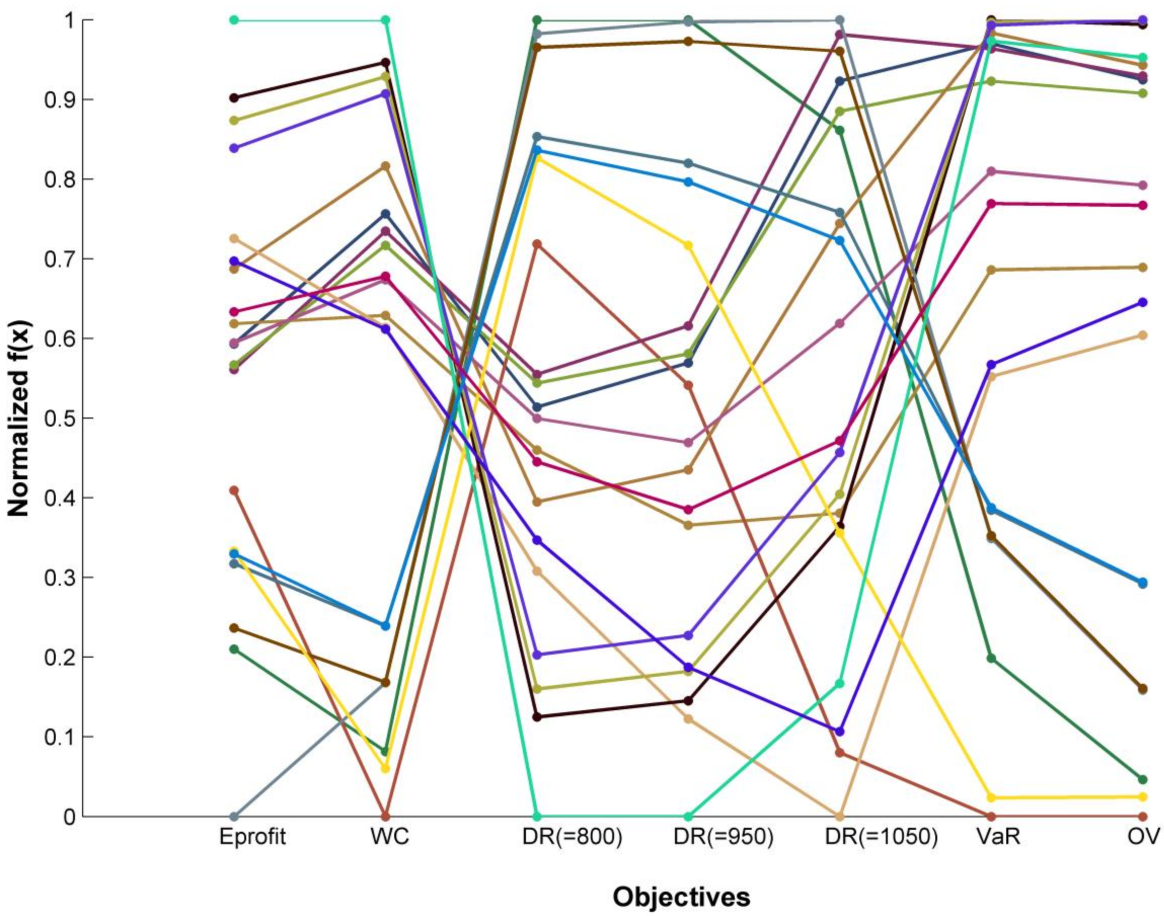

Fig. 8.8. Parallel coordinate plot showing the interactions and relations among solutions for each objective in the first case (matrix N).

Remarkably, some objectives behave similarly, that is, when one increase so do the others and vice versa. This is confirmed by the p-values shown in Table 8.2, which are calculated for the filtered solutions. Two metrics are assumed to be statistically correlated when the p-value is below 0.05 (typical significance value). According to this, metric DR(Ω=1050) is uncorrelated with WC, VaR and OV (see highlighted values in Table 2).

Table 8.2. P-value for each pair of objectives considered for filtered solutions in case 1.

	P-Value						
	Eprofit	WC	DR (Ω=800)	DR (Ω=950)	DR (Ω=1,050)	VaR	OV
Eprofit							
WC	0.00						
DR (Ω=800)	0.00	0.00					
DR (Ω=950)	0.00	0.00	0.00				
DR (Ω=1,050)	0.01	**0.43**	0.01	0.00			
VaR	0.00	0.00	0.00	0.01	**0.76**		
OV	0.00	0.00	0.00	0.00	**0.74**	0.00	

The order of efficiency step was next applied (second step of Pareto Filters, section 8.4.4) in order to identify non-dominated solutions in all the subsets of objectives of cardinality k. Starting from $k = 7$, the value of k was reduced gradually until no solution satisfies the corresponding optimality level (no solution is optimal for all the subsets of k-objectives). For each value of k < 7, a reduced subset of solutions was obtained. Table 8.3 displays the size of the subsets for each order of efficiency, in which a reduction of 80, 90 and 95% (from 20 to 4, 2 and 1, respectively) in the number of solutions were obtained using k=6, k=5 and k=4, respectively.

Table 8.3. Number of solution retained in matrix N for each order of efficiency.

	Matrix N				
Order of efficiency	k=7	k=6	k=5	k=4	k=3
Number of solutions	20	4	2	1	0

To guarantee the quality of the solutions kept in each subset, their performance for each objective was analyzed. Fig. 8.9(a) shows the lower bound for the solutions (best performance) retained in each subset of k-objectives for the group of objectives in matrix N. Note that the lower bound for k=7 is 0 for all of the objectives, since this represents the original solution space (and consequently includes the best solutions identified by the SAA). The efficient solutions of order $k = 6$ show similar bounds as those solutions in the original set ($k = 7$), with just a small deviation in the value of *Eprofit* (the best *Eprofit* in the original set is \$1,100,211, and in the set k=6 is \$1,047,408) Moreover, solutions retained for lower orders of efficiency (k < 6), present worse bounds in multiple objectives. On the other hand, Fig. 8.9(b) shows the upper bound for the solutions retained in each subset of k-objectives. Here, the value of all the objectives in subset k=7 is 1, since it includes the worst performance solution in the original solution space. In this case, a bigger deviation from the original subset k=7 would be preferred, as this would imply that bad solutions would have been discarded. By analyzing simultaneously Fig. 8.9(a) and (b), it can be seen that solutions in the subset k=6 show good performance compared with the original set ($k = 7$). Hence, the filter is stopped at k=6, when 4 solutions are kept. This represents an overall reduction of 96% in the size of the original set of solutions (from 100 to 4).

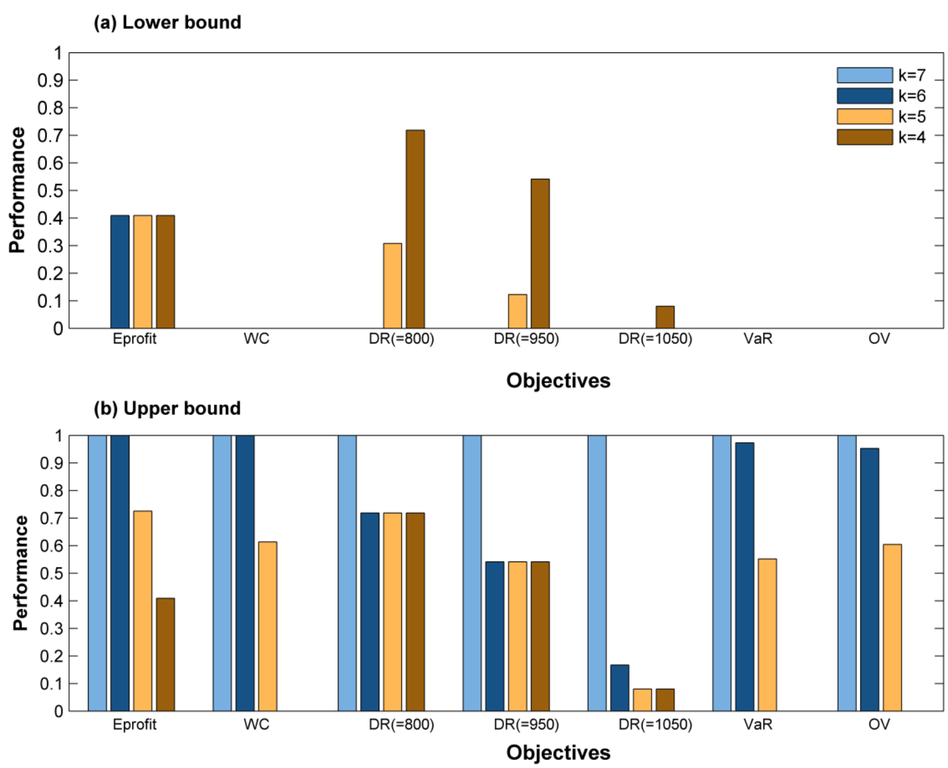

Fig. 8.9. Normalized bounds for solutions with efficiency of order k for the first case. (a) Lower bound. (b) Upper Bound.

Fig. 8.10 shows the risk curves associated with each solution for the reduced set of *k*=6, while Fig. 8.11 and Table 8.4 show their configurations.

Table 8.4. Batch plant design for the reduced set of solutions in case 1.

First case (k=7)									
Configuration	Order of efficiency	*Eprofit* (M$)	**Demand Satisfaction (%)	Batch stage capacities (m^3)			*Storage tanks (m^3)		
				J1	J2	J3	J1	J2	J3
1	k=4	1.047	71	1	0.75	0.5	0	3	10
2	k=5	1.007	82	1.2	0.75	0.5	0	5	10
3	k=6	0.971	100	1.2	1	0.5	0	0	0
4	k=6	1.010	82	1.2	0.75	0.5	0	5	0

*Storage tanks represent the capacity of the tank installed at the exit of each unit J.
** Demand satisfaction level corresponds to the worst-case scenario.

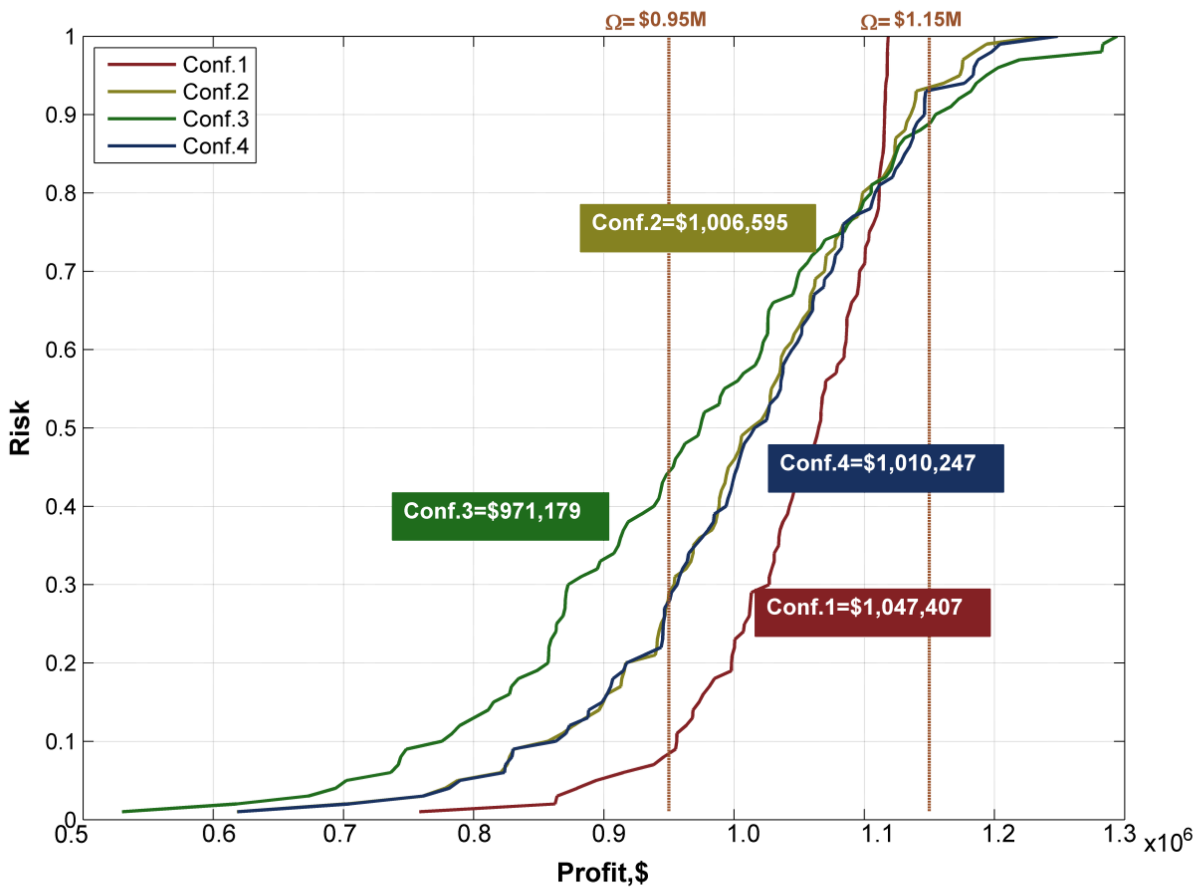

Fig. 8.10. Cumulative risk curves for the solution in the reduced set of case 1.

To get insight into how the model manages the risk associated with the investment, solutions 1 and 4 (configurations 1 and 4, respectively), which are two of the alternatives kept after applying the Pareto filters are studied in detail. Solution 1 reflects a conservative attitude towards risk, with low probabilities of profits below $0.95M (9%), but a probability of large profits (say above $1.15M) of 0%. On the other hand, solution 4 reflects a riskier attitude, with a probability of 28% for profits below $0.95M, but a larger probability of high profits (10% for a target of $1.15M). As seen in Fig. 8.11, the risk-averse solution (configuration 1) implements a design with small capacities for the equipment units and storage tanks. This first case study aims to identify a solution reflecting a conservative attitude towards risk, as most of the objectives focus on improving the performance in the lower part of the profit distribution. Hence, configuration 1 is therefore kept as it represents a conservative arrangement (smaller equipment sizes and consequently lower potential loses that lead to a higher expected profit).

It is worth to mention that in configuration 1 (see Table 8.4) demand satisfaction can be compromised and in fact drops to 71% in the worst-case scenario, because the capacity of the supply chain is reduced with the aim of avoiding risk. On the contrary, the risk-taker solution (configuration 4) installs equipment units with higher capacity (and only one storage tank) that can ensure a demand satisfaction of 82% in the worst case. Finally, Solution 3 is the riskiest design, since no single storage is considered and the highest capacities are installed. This leads to higher operation and installation costs as well as less profit on average, but on the other hand allows fully satisfying the demand in all the scenarios. Hence, this design attains higher maximum profits in scenarios with large demands, but this is accomplished at the expense of worse performance in scenarios with low demand.

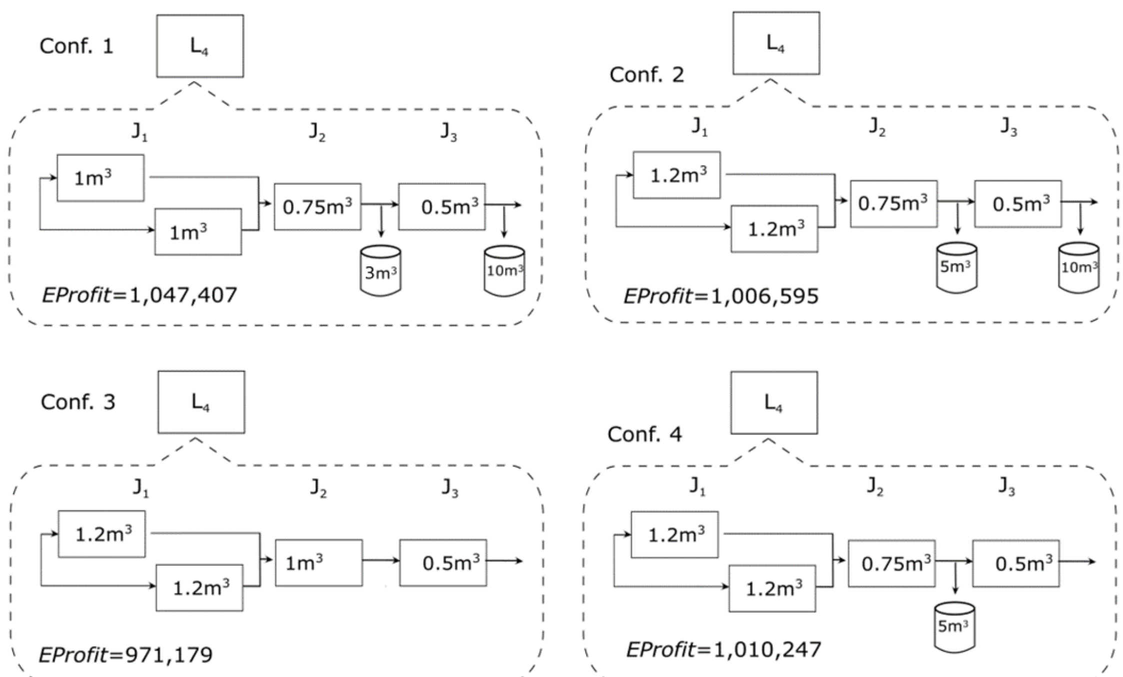

Fig. 8.11. Batch plant configuration scheme for the reduced set of solutions found in the first case study.

8.4.2. Second case: Expected profit and risk at different target values

For this case, Risk was considered as the only additional objective to the expected profit. Sixteen target values were evenly distributed in the complete solution space for this calculation (see Table 8.1).

The first step (Smart filter) was applied considering a tolerance of Δt=0.01%, thereby reducing drastically the number of solutions from 100 to 10 (i.e. a reduction of 90%) by removing dominated and repeated solutions. The relationships between objectives are shown in Fig. 8.12.

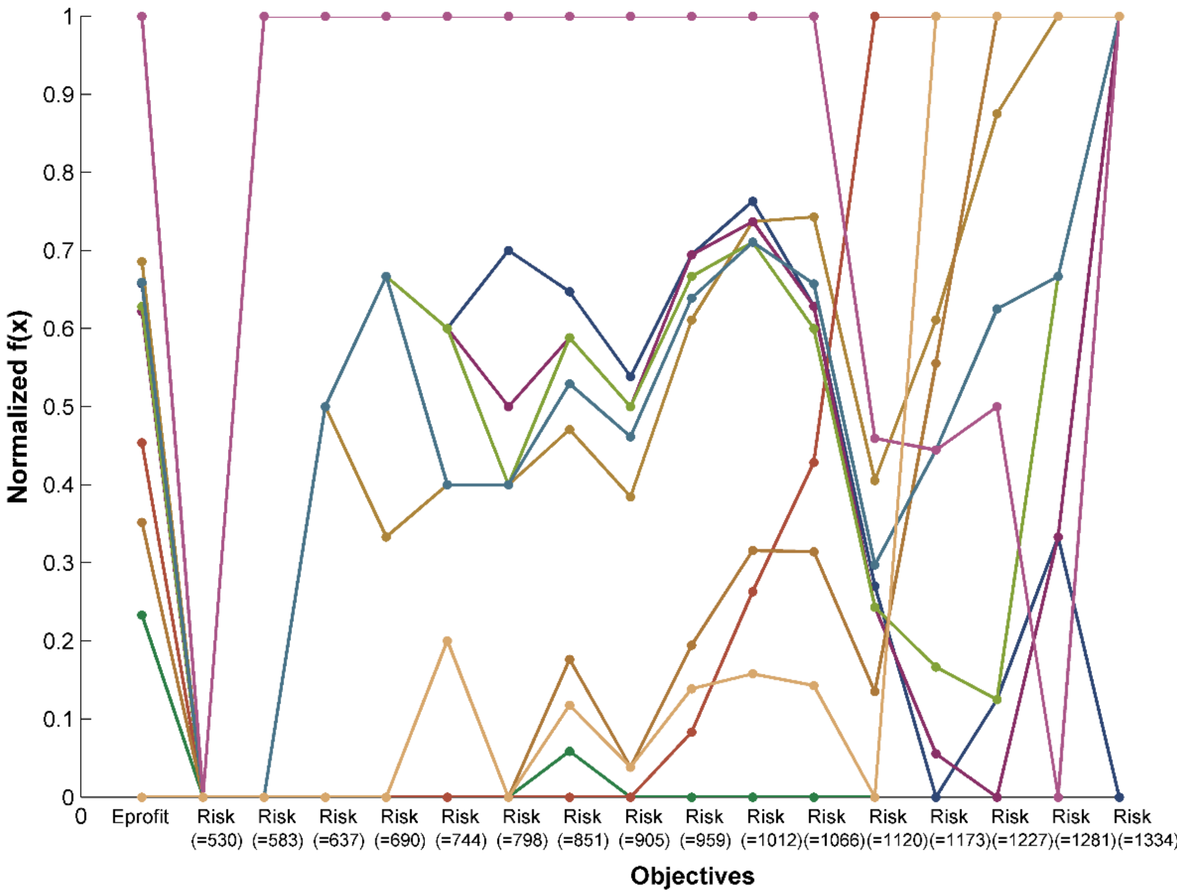

Fig. 8.12. Cumulative probability for the solution in the reduced set of case 1.

Notice that most of the 17 objectives behave similarly. By calculating the p-values shown in Table 8.5, it can be seen how for 3 objectives (i.e., Risk(Ω=530), Risk(Ω=1120) and Risk(Ω=1335)) a complete lack of statistical correlation is found (p-values higher than 0.05). The highlighted values in Table 8.5 represent the lack of correlation among metrics. The rest of the objectives correlate each other and prove the correlation among risk metrics.

The second part of Pareto filter was next applied (order of efficiency filter) providing a deeper reduction in the pool of available solutions. Starting with the solutions obtained from the Smart filter ($k = 17$), the non-dominated solutions in all the subsets of objectives of cardinality k were found by reducing gradually the value of k until no solution satisfied the corresponding optimality level.

Table 8.5. P-values for each pair of objectives in matrix P.

	P-Value															
	Eprofit	Ω= 530	Ω= 584	Ω= 637	Ω= 691	Ω= 745	Ω= 798	Ω= 852	Ω= 906	Ω= 959	Ω= 1013	Ω= 1066	Ω= 1120	Ω= 1174	Ω= 1227	Ω= 1281
Eprofit																
Ω=530	**0.51**															
Ω=584	**0.07**	**0.83**														
Ω=637	0.00	**0.52**	0.03													
Ω=691	0.00	**0.37**	**0.09**	0.00												
Ω=745	0.01	**0.45**	0.02	0.00	0.00											
Ω=798	0.00	**0.22**	0.03	0.00	0.00	0.00										
Ω=852	0.00	**0.35**	0.05	0.00	0.00	0.00	0.00									
Ω=906	0.00	**0.43**	0.02	0.00	0.00	0.00	0.00	0.00								
Ω=959	0.00	**0.35**	**0.10**	0.00	0.00	0.00	0.00	0.00	0.00							
Ω=1013	0.00	**0.31**	**0.15**	0.00	0.00	0.00	0.00	0.00	0.00	0.00						
Ω=1066	0.00	**0.45**	**0.08**	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00					
Ω=1120	**0.23**	**0.90**	**0.60**	**0.70**	**0.83**	**0.82**	**0.73**	**0.96**	**0.77**	**0.79**	**0.54**	**0.22**				
Ω=1174	0.05	**0.09**	**0.83**	0.04	0.01	0.02	0.02	0.01	0.03	0.01	0.01	**0.05**	**0.78**			
Ω=1227	**0.08**	**0.16**	**0.77**	0.04	0.00	0.02	0.03	0.02	0.03	0.01	0.02	**0.09**	**0.88**	0.00		
Ω=1281	0.01	**0.25**	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.02	**0.85**	0.02	0.01	
Ω=1335	**0.66**	0.00	**0.76**	**0.67**	**0.49**	**0.55**	**0.30**	**0.48**	**0.56**	**0.52**	**0.50**	**0.71**	**0.91**	**0.16**	**0.22**	**0.32**

Table 8.6 shows the results of this filter in which reductions of 40, 60 and 90% (from 10 to 6, 4 and 1, respectively) were obtained for subsets *k*=16, *k*=15 and *k*=14 (and *k*=13), respectively. For further analysis *k*=13 will be omitted, since subsets for *k*=14 and *k*=13 are equal (i.e., they contain the same solution).

Table 8.6. Number of solution retained in matrix N for each order of efficiency.

	Matrix P					
Order of efficiency	k=17	k=16	k=15	k=14	k=13	k=12
Number of Solutions	10	6	4	1	1	0

Using the same procedure than in the previous subsection, in this case Fig. 8.13(a) shows that the first subset (i.e., *k*=16) provides an important reduction in the number of available solutions, showing similar performance than the original subset (*k*=17). For *k*=16 only the objective Risk(=1227) shows a slight deviation from the best performance. This means that these solutions in subset *k*=16 have 30% less probability of achieving a profit of $1,227,000 than the best solution in the set *k*=17. Solutions with lower orders of efficiency (*k*<16) show a significant deterioration in their performance, specifically in the last four objectives (i.e., Ω ≥ 1174). Analyzing both figures it can be seen how the subset *k*=16 performs similarly to the subset *k*=17, but additionally eliminates solutions with poor performances (see objectives (Ω≤1066) in Fig. 8.13(b)). In view of the above, it can be concluded that the last sets of solutions (i.e., orders *k*=15, *k*=14) perform better on average, but discard points with significantly better performance in some criteria. Therefore, in this case the filter is stopped at *k*=16 with a reduced subset of six solutions, which represents a total reduction of 94% in the original number of solutions (from 100 to 6).

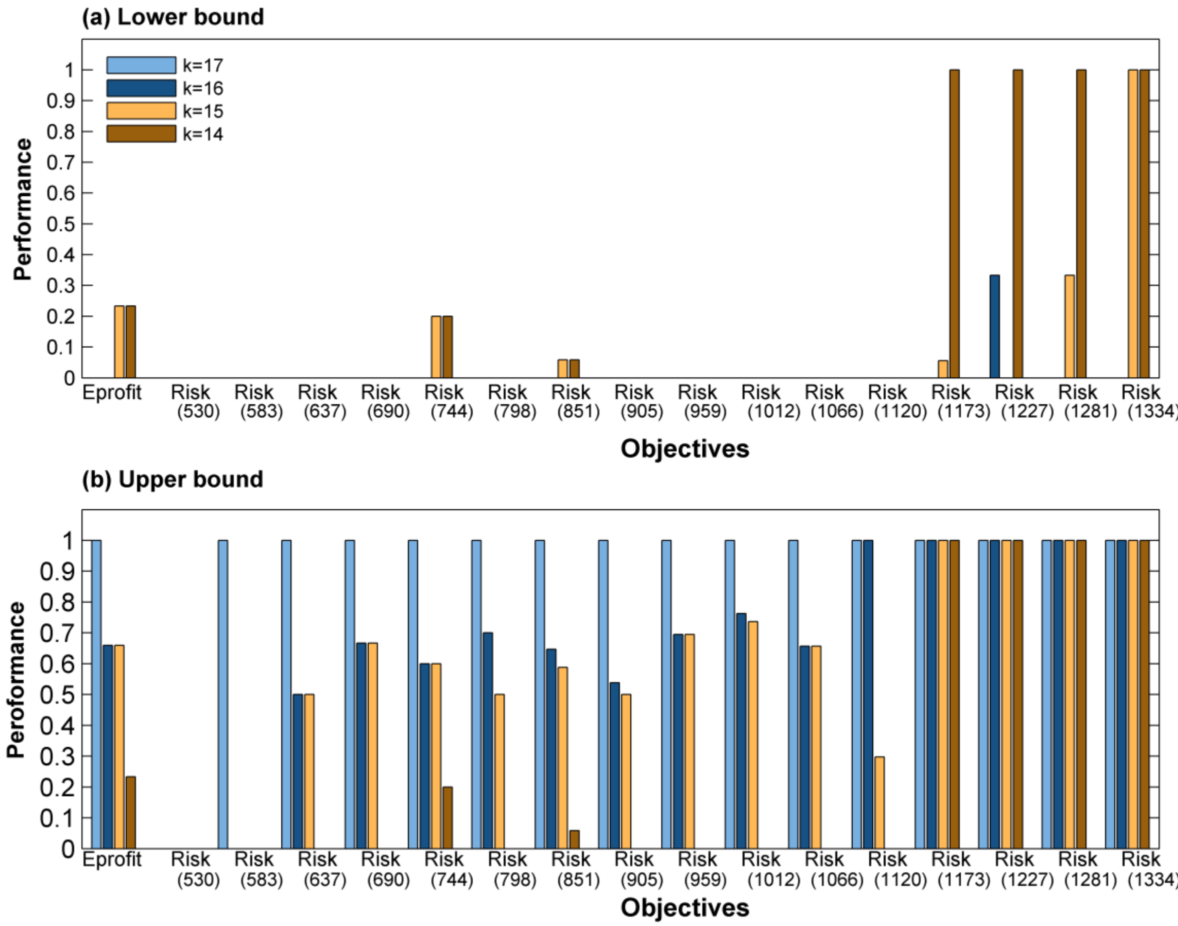

Fig. 8.13. Normalized bounds for solutions with efficiency of order k for the second case-(a) Lower bound. (b) Upper Bound.

Table 8.7. Batch plant design for the reduced set of solutions in case 2.

Second case (k=17)									
Configuration	Order of efficiency	*Eprofit* (M$)	**Demand Satisfaction (%)	Batch stage capacities (m^3)			*Storage tanks (m^3)		
				J1	J2	J3	J1	J2	J3
5	*k*=14	1.073	76	1	0.75	0.5	0	5	10
6	*k*=16	1.024	93	1.2	0.75	0.5	0	0	5
7	*k*=16	1.047	71	1	0.75	0.5	0	3	10
8	*k*=15	1.028	92	1.2	1	0.5	0	5	5
9	*k*=15	1.027	89	1.2	1	0.5	0	5	0
10	*k*=15	1.024	85	1.2	1	0.5	0	5	0

*Storage tanks represent the capacity of the tank installed at the exit of each unit J.
** Demand satisfaction level corresponds to the worst case scenario.

Table 8.7 displays information on the batch plant designs associated with each solution in the reduced subset, while Fig. 8.14 shows the cumulative distribution curves for those solutions.

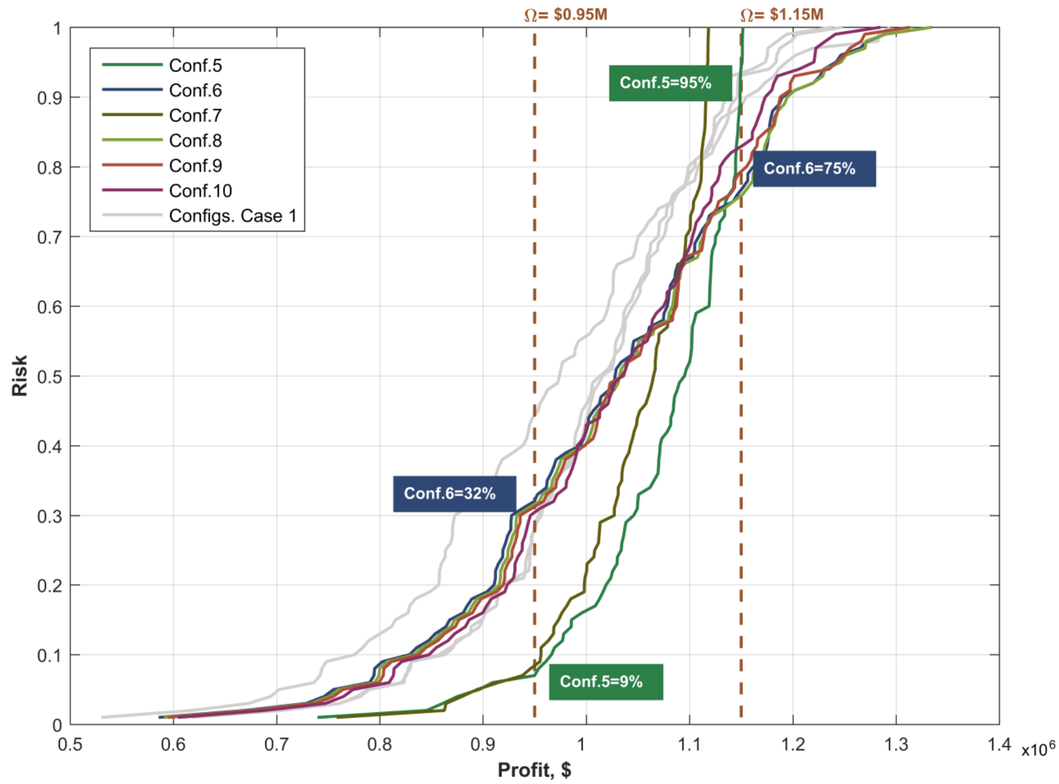

Fig.8.14. Cumulative probability curves for the solution in the reduced set of k=16 for case 2.

This second case study reflects a more balanced attitude towards risk. To get insight into how the model manages risk, let us study solutions 5 and 6. At the lower part of the profit distribution, there is a clear advantage of solution 5 over 6, since their probabilities of profits below \$0.95M are 9% and 32%, respectively. However, for large profits (say above \$1.15M) these solutions behave differently achieving probabilities of 95% and 75% in configurations 5 and 6, respectively. Notice how for lower profits (Ω=\$0.95M) solution 5 is more conservative and vice versa for larger profits (Ω=\$1.15M).

According to Fig. 8.15, where the identified configurations have been displayed, solution 5 represents a very conservative configuration, but the most conservative one is configuration 7, as it provides the smallest equipment capacity at the expense of small profits (compared with solution 5). Analyzing the worst demand satisfaction level attained, configuration 6 is the best choice since its satisfaction rate is the highest one (93% in their worst scenario), while configuration 5 is the least reliable, with a satisfaction of 76% (See Table 8.7).

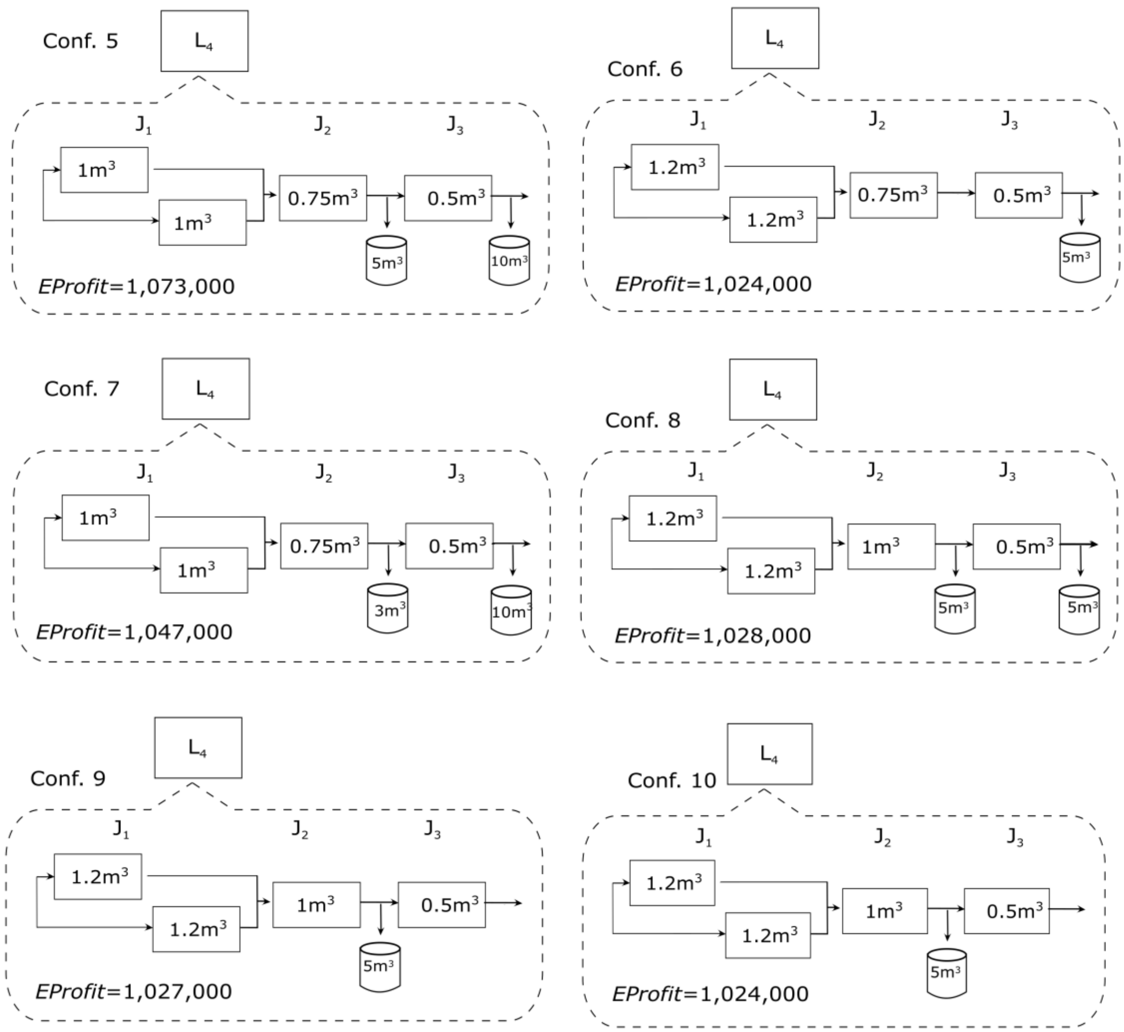

Fig. 8.15. Batch plant configuration scheme for the reduced set of solutions found in the second case study.

8.5.Conclusions

A systematic methodology to support risk management in optimization under uncertainty problems has been proposed. Such a solution framework incorporates several stochastic metrics that assess the performance of a solution considering the whole space of uncertain parameters. The proposed strategy combines optimization under uncertainty considering multiple risk metrics with a systematic approach for the selection of the most promising alternatives. The capabilities of this approach have been successfully proved using as test-bed a multi-scenario multi-objective design and planning supply chain model of a batch process production process. Numerical results show that the proposed approach accelerates the search for supply chain design alternatives behaving in different manners in the uncertain parameters space. Furthermore, Pareto filters narrow down the number of each such alternative, ensuring that the final design selected performs well for a wide range of economic targets. In addition, by combining different risk measurements, the final solution identified by the decision-maker is more robust and bypass significant losses.

The proposed tool assists decision-making by incorporating several risk metrics in the modeling framework and by avoiding subjectivity when selecting the final solution. This approach can be used in a wide variety of engineering problems in which multiple conflicting objectives and/or different performance criteria must be simultaneously considered.

Despite the significant advantages of the proposed approach, all the criteria have considered equally important. However, if a more accurate representation of the decision-maker preference for each objective might lead to subjectivity problem since the approach is not suitable for systematically represents these preferences. Therefore, the following chapter uses ELECTRE-IV method to overcome such a limitation.

8.6.Nomenclature

Abbreviations

MOO	Multi-objective optimization
SC	Supply chain
SCM	Supply Chain Management
MILP	Mixed integer linear programming
PSE	Process system engineering
SAA	Sample average approximation
RAR	Risk Area Ratio
SO	Simple Objective
VPI	*Value of Perfect Information*

Indexes

sp	Suppliers
r	Raw material
l	Plants
j	Batch stages
i	Products
m	Warehouses
g	Customer zones
s	Scenarios
sol	Solutions
d	Parallel unit in phase
w	Tanks sizes
p	Batch unit discrete sizes

Parameters

Ω	Target value for risk metrics
D_{ig}	Demand product i for each customer zone *g*
$prob_s$	Probability of occurrence for scenario s
$\hat{f}_{lo}$	Lower bound in normalized scale
$\hat{f}_{up}$	Upper bound in normalized scale
f_{lo}	Lower bound in objective value
f_{up}	Upper bound in objective value
Δt	Tolerance value for Smart Pareto filter
$fl_{r,i,j}$	Conversion factor of raw material *r* to produce product *i* in batch stage *j*
Φ	Maximum ratio allowed between batches of consecutive stages.
$Price_i$	Selling price of product *i*
$Q_{i,l}^{UP}$	Upper bound for production of product *i* in plant *l*.

$Q_{i,l}^{LO}$	Lower bound for production of product *i* in plant *l*.
Q_m^{max}	Upper bound of storage capacity of warehouse *m*.
$Cd_{i,m}$	Storage cost of product *i* at storage *m*.
$Cprod_{i,l}$	Production cost of product *i* at plant *l*.
$Craw_{sp,r}$	Raw material acquisition cost from supplier *sp* and raw material *r*.
$Ctp_{i,l,m}$	Distribution cost of product *i* among production plant *l* and storage site *m*.
$Ctd_{i,m,g}$	Distribution cost of product *i* among storage site *m* and customer zone *g*.
$ST_{i,j,l}$	Size factor for each storage tank for contain product *i* at batch stage *j* in plant *l*.
$VTF_{j,l,w}$	Discrete size *w* for storage tanks in stage *j* of plant *l*.

Sets/subsets

N_s	Set of supplier sites.
N_r	Set of raw materials.
N_l	Set of batch plants.
N_j	Set of batch stages.
N_i	Set of products.
N_m	Set of warehouses.
N_g	Set of customer zones.
S	Set of different scenarios.
SS	Set of different solutions belonging to NSS.
Sol	Set of different solutions form model P.
RSS	Raw set of solutions.
$\bar{x}_s^*$	Optimal set of solutions for scenario *s*.
$\bar{y}_s^*$	Second stage variables in the full optimal solution.
xx^*	Optimal solution for order of efficiency algorithm.
s_s^*	Optimal set of solutions for the entire set of scenarios *s*.
NSS	Normalized set of solutions.
Ob	Objectives under analysis.
NOO	Number of objectives under analysis.
V_k	Set of solution efficient of order *k*.
RS	Set of rejected solutions.
P	Solution retained after Smart Pareto filter.
M'	Set of candidate solutions.
c'	Counter set.
cc'	Counter set.
K	Order of efficiency.
Θ	Space of uncertain parameters.

Variables

x	Vector of first-stage decision variables.
λ	Random vector associated to an uncertainty behaviour.
y	Vector of second-stage decision variables.
$\delta_{\Omega s}$	Positive deviation of the profit value from the target Ω in scenario *s*.
$Profit_s$	Profit obtained for scenario *s*.
$\hat{f}$	Normalized value.
f	Real objective value.
Eprofit	Objective (Expected profit).
$Q_{sp,r,i,l,s}$	Material amount of raw material *r* send from supplier site *sp* to plant *l* in order to produce product *i* at scenario *s*.
$B_{i,j,l,s}$	Batch size of product *i* at stage *j* in plant *l* for scenario *s*.
$NP_{j,l}$	Number of in phase units for stage *j* in plant *l*.
$Nb_{i,j,l,s}$	Number of batches of product i in stage j of plant l.

$VF_{j,l,p}$	Discrete size p for batch units in stage j of plant l
$ee_{i,j,l,p,d,s}$	Non-negative continuous variable
$VT_{i,j,s}$	Tank size installed for contain product i from batch stage j at scenario s
SS_c	Normalized solution c
$Size_{ijl}$	Size required for batch stage j to produce 1kg of final product i in plant l
DR	Downside risk
WC	Worst case
VaR	Value at risk
OV	Opportunity value
$Risk$	Financial risk
$VZ_{j,i,s}$	Batch unit size of stage j of plant l at scenario s
$ff_{i,j,l,w}$	Continuous variable that is equal to Q_{il} if batch stage j is installed with tank size w
$\rho_{i,j,l,p,n,d}$	Auxiliary variable to skip nonlinearities
Cpl_l	Installation cost of plant l
$Cdep_m$	Installation cost of storage m
LC	Total allocation cost
IC	Total investment cost
EC	Equipment acquisition cost
C_{an}	Capital charge factor
OC_s	Total operating cost at scenario s
TC_s	Total distribution cost of scenario s
$Ctraw_{sp,r,i,l}$	Distribution cost of raw material r among supplier site sp to production plant l in order to produce product i
$TCost_s$	Total cost including operating and investment cost
$Sales_s$	Total revenue obtained by selling product i.

Binary Variables

$Z_{\Omega s}$	1 if Profit for scenario *s* is lower than the target Profit Ω.
ex_l	Takes value 1 if plant *l* is allocated.
$zz_{i,l}$	Is equal to 1 if product *i* is produced in plant *l*.
$yy_{m,s}$	Takes value 1 if warehouse *m* is allocated for scenario *s*.
$xz_{j,l,d}$	Takes value 1 if stage *j* of plant *l* has *d* parallel units in phase.
$su_{j,l}$	Determines if a tank is allocated after batch stage *j*.
$vt_{j,l,w}$	Takes value 1 if a tank of size *w* is allocated in batch stage *j* and plant *l*.
$v_{j,i,p}$	Takes value 1 if a batch stage *j* is allocated to produce product *i* and with size *p*.

Chapter 9

A multi-item negotiation approach for the management of resource SCs.

Previous chapters stress the importance of a detailed and accurate knowledge of the process conditions for a decision-making (Chapter 6 and Chapter 7), while Chapter 4 and 5 present strategies evaluating the effect of multiple decision criteria over the final solution. The capabilities of these strategies have been tested independently and for a centralized decision-making scheme (i.e. only one decision maker for the entire system); nevertheless, such a scheme may not represent a realistic problem, especially when dealing with largescale networks with independent enterprises, since these SC echelons can operate in standalone conditions. Therefore, in this chapter, the study of non-cooperative environments introduced in Chapter 5 is extended to consider the uncertainty in the reaction of the different players and the role of third parties, leading to an integrated negotiation framework for the design and operation of a decentralized supply chains under competitive market environments. Thus, departing from the mathematical formulation representing the competitive leader-follower situation presented in Chapter 5, the uncertainty management strategies introduced in Chapters 6, 7 and 8 are now applied in order to assess the consequences of the uncertain follower behavior on the leader decisions and the overall system. The impact of the follower design decisions over the leader objective is controlled in the optimization by the use of a pre-defined set of follower designs. The framework uses a Scenario-Based Dynamic Negotiation (SBDN) formulation capable to assess the system uncertainties to produce a set of potential solutions/options, which are later, evaluated for several decision criteria (including economic and environmental) using the ELECTRE-IV method. Ultimately, the proposed integrated approach promotes the identification of single agreements that improve the process robustness, feasibility and sustainability altogether. Remarkably, such solutions must represent the leader and follower interests under a win-win negotiation partnership despite the uncontrollable/unpredicted behaviors resulting from the follower decisions as well as the presence of third-parties also affecting the resulting negotiation (fixing base-prices).

9.1.Background on negotiation frameworks.

The market globalization as well as the constant changes in the market dynamics leads to a need of strategies that provide stability to the resulting current complex industrial scenario. Therefore, the Process System Engineering (PSE) research, which focuses on the development of fast, robust and reliable tools for designing and managing industries, faces nowadays the main challenge associated to the increasing presence of suppliers/producers competition in this worldwide volatile market environment, leading to non-cooperative situations and, very often, conflicts of interest (i.e. objective functions) *(Zamarripa et al., 2014)*.

Few works have been carried out to analyze the SCs coordination in competitive environments. For instance, *Hjaila et al. (2016a)* propose a framework capable of model the third parties' role/interaction in a polystyrene production/distribution SC. The work was later expanded to evaluate/coordinate the relations between two independent SC's and their associated competitors (third parties) in order to ensure a win-win situation *(Hjaila et al., 2016b)* using an Scenario-Based Dynamic Negotiation (SBDN) framework. The competitor's behaviors were described through a defined set of scenarios, nonetheless, the reliability of the final solution is not guaranteed due to an inaccurate uncertainty management. Therefore, an appropriate uncertainty formulation, like the two-stage stochastic programming framework, has to be included in the SBDN strategy.

Similarly, in the line of integrated design and operation of a decentralized SCs under a competitive environment, *Yue and You (2015)* evaluated the role of follower's discrete decisions in a negotiation leader-follower optimization problem using a novel mixed integer bi-level programming framework. However, the main shortcoming of their formulation is the fact that the follower's discrete decisions highly depend on the leader decisions, which compromise the actual applicability of the final design solution since it enforces the collaboration between the leader and the follower. Consequently, a more sophisticated strategy that explicitly considers the follower's design decisions is needed (regardless of the leader's behavior).

Additionally, the dynamism in the current competitive business environment and the growing interests on designing sustainable processes has created an opportunity area. Actually, negotiation strategies and "Green" engineering must be combined to improve the traditional independent economic and environmental assessments and, until now, the simultaneous representation of multiple leader/follower objectives in the final solution remains as an open issue in the current literature. In order to overcome such an issue, a robust multi-criteria decision-making tool should be used within a negotiation strategy. Many methods can be used as decision-support tools, nevertheless, due to its previously identified advantages, ELECTRE-IV have gain attention as the most complete decision-making approach (Chapter 3).

In order to address these issues, a negotiation framework is proposed for the design and management of MO (e.g.: sustainable) SC under non-cooperative environments. Such a framework allows evaluating a set of negotiation contracts, identifying the best one for multiple criteria. Ultimately, this solution strategy identifies a negotiation contract that holds feasible disregarding the uncontrollable/unpredicted behaviors associated to a follower as well as the set of third parties compromising the competitive system.

9.2.Problem Statement

Consider two independent SC's working in a non-cooperative environment, being one a net resource consumer (e.g wastewater generator) and the other one a resource regenerator (e.g treatment plant) . Particularly, the resource consumer and regenerator are considered as leader and follower, respectively. Both are functional SC's with their own independent suppliers/markets, but the leader is the participant that takes the initiative to improve its benefits by searching for a suitable resource disposal price as well as buying recovered water (being one of the options to and from the follower SC respectively). Hence, in order to push the agreement towards a win-win policy, the systematic search of a profitable collaboration is required. Remarkably, the identified agreement must consider the uncertain behavior of the external conditions, the follower design decisions (which remains unknown for the leader) as well as additional efficiency indicators from both leader's and follower's perspectives. Therefore, the negotiation may be complex and under some circumstances, a feasible agreement may not be found.

A water network within a shale gas (the same one presented in Chapter 5) was used as motivating example. The general decentralized schemes of the water and shale gas networks are displayed in Fig. 9.1, defining the two entities, the shale gas producer (as the wastewater generator or leader) and the wastewater treatment tasks (as the wastewater regenerator or follower), as well as the third parties (competitors). The detailed description of the case study can be found in Chapter 5; however, for completeness of this section the main elements that describe the problem are commented.

- A set of freshwater sources $s \in S$ from which supplier s can satisfy the freshwater requirements.
- Shale sites $i \in I$ in which a set of wells can be chosen $j \in J$.
- Treatment facilities including centralized facilities (CWT;$c \in C$), disposal wells ($d \in D$) or onsite treatment plants ($o \in O$).

In addition to these network elements, in order to represent the negotiation approach, a set of supply chains ($sc \in SC$) has to be defined in the mathematical model formulation linking each one to its corresponding negotiation partner (being the leader ($l \in SC$) and the follower ($f \in SC$). Moreover, a set of third parties are included (leader external providers *xv*, follower external clients *xc*, and external customers *m*).

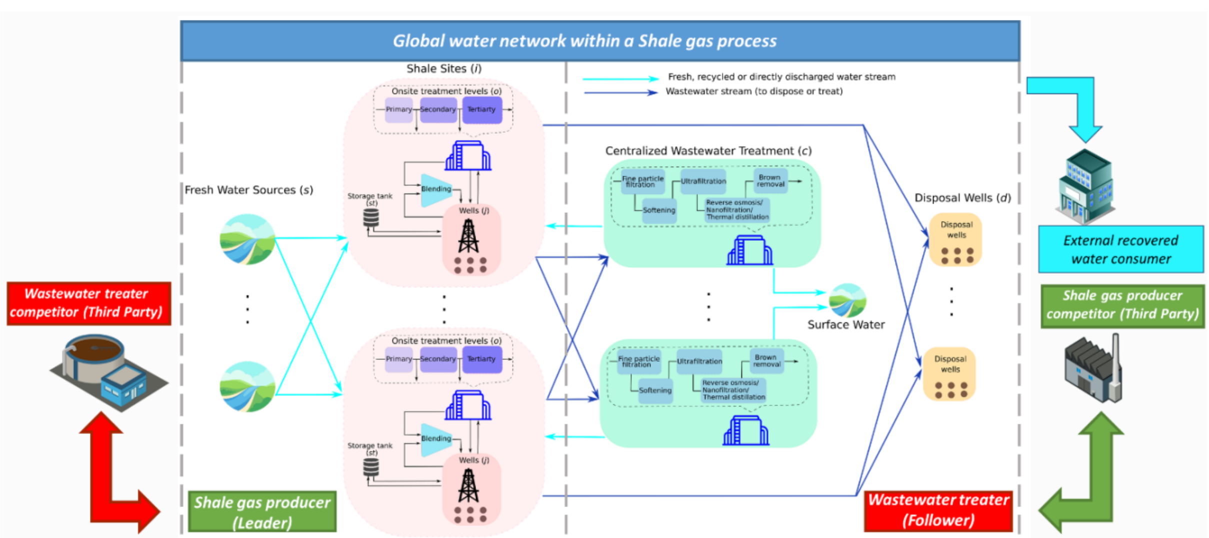

Fig. 9.1 Decentralized SC network.

Furthermore, the goal is to maximize the economic vector for each participant SC by modifying the traditional strategic and tactical management decisions. Note that by activating the follower operations, the global sustainability is promoted; thus, freshwater savings will be considered here as an environmental indicator. Further details regarding process data, equipment description and nominal capacities, as well as the mathematical equations that describe this problem can be found in Chapter 5. However, the following section presents the main equations modified to adapt the negotiation approach to the original mathematical formulation.

9.2.1. Mathematical formulation

The equations affected are mainly the financial ones. For example, Eq. (9.1) represents the total sales for each participant SC considering the prices associated with internal and external consumers ($p_{r',sc',t}$ and $pr_{r,m,t}$, respectively).

$$Sales_{sc,s} \leq \sum_{t\in T}\sum_{r\in R}\sum_{m\in M} pr_{r,m,t}\cdot xdem_{r,sc,m,t,s} + \sum_{t\in T}\sum_{r^i\in R} p_{r',f,t}\cdot Q_{r'sc',s} \qquad \forall sc \in SC;\ f \in SC; s\in S \tag{9.1}$$

Similarly, the cost for each participant is calculated considering the raw material purchase, transport, storage, production, and the negotiation resource, as shown in Eq. (9.2). Finally, the maximization of the individual SC profits $Prof_{sc,s}$ is displayed in Eq. (9.3), which consist in the difference between the individual economic sales and costs.

$$Cost_{sc,s} = \sum_{t\in T}\left(CRM_{sc,t,s} + CTR_{sc,t,s} + CST_{sc,t,s} + CPRD_{sc,t,s}\right) + \sum_{t\in T}\sum_{r^i\in R} p_{r',l,t}\cdot Q_{r'l\ \ ,t,s} \qquad l \in SC; s\in S \tag{9.2}$$

$$Prof_{sc,s} = Sales_{sc,s} - Cost_{sc,s} \qquad \forall sc \in SC \tag{9.3}$$

It is important to highlight that the negotiation item ($p_{r'sc\ t}\cdot Q_{r'sc\ t\ s}$) appears in both, sales and cost functions. Remarkably, the leader partner seeks being robust against the unpredictable follower behaviour (uncertain decisions and parameters). Mathematically, such an uncontrollable behaviour is faced through a two-stage stochastic programming formulation. Therefore, the economic objective adopts the following form.

$$EProf_{sc} = \sum_{s\in S}\left(Sales_{sc,s} - Cost_{sc,s}\right)\cdot prob_s \qquad \forall sc \in SC \tag{9.4}$$

Here, $prob_s$ represents the probability of occurrence of scenario s, each of which represents a possible realization of the uncertaint behaviors of the follower and the 3rd parties (suppliers, customers, external clients) being for this particular case equiprobable ($prob_s = \frac{1}{No.of\ scenarios}$) but easily extendible to uneven distributions. Parallely, the reaction of the follower in front of each pricing agreement is modelled using the probability of acceptance over a set of scenarios. Such a probability ($prob\_acceptance_f$) is computed by taking into account the number of scenarios that improve the individual results for the follower SC (see Eq.(9.5)).

$$prob\_acceptance_f = \frac{No.of\ scenarios\ improving\ EProf_f}{Total\ No.of\ scenarios} \qquad \forall f \in SC \tag{9.5}$$

Due to the used formulation, the maximization of the economic revenues for all the participants promotes the operations of the resource regenerators, and consequently, increases the use of recovered wastewater while reducing the freshwater consumption (For any freshwater price higher than 0). Thus, Eq. (9.6) quantifies the net freshwater consumption, where $fw_{s,i,m,t}$ represents the total freshwater withdrawals and $wtcd_{c,t,s}$ accounts for the wastewater recovered.

$$Enfw = \sum_{s\epsilon S}\left(\sum_{i\epsilon I}\sum_{m\epsilon M}\sum_{t\epsilon T} fw_{s,i,m,t} - \sum_{c\epsilon C}\sum_{t\epsilon T} wtcd_{c,t,s}\right)\cdot prob_s \tag{9.6}$$

Remarkably, $prob\_acceptance_f$ and $Enfw$ represent additional decision criteria to $EProf_{sc}$. Finally, the effect of the follower's design decisions over the projections of the leader's decisions are evaluated by solving the leader's model iterativeley for a defined set of follower's designs. Details on the solution strategy are presented in the following section.

9.3. Solution strategy

The competitive environment has been addressed before in this Thesis (Chapter 5), where the balance between the objectives of the two participant SCs was obtained using a traditional bilevel formulation (each level representing the individual economic performance of the leader and the follower). The methodology proposed in this chapter integrates the SAA and the ELECTRE-IV methods presented in previous chapters under the framework of SBDN approach. This strategy allows the explicit consideration of uncertain/unpredicted conditions over the non-cooperative systems associated to the follower and 3rd parties. The proposed strategy consists of four parts as illustrated in Fig. 9.2.

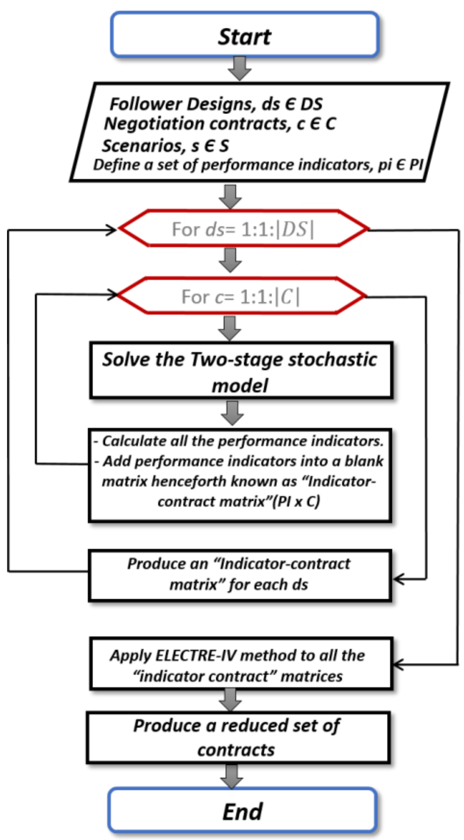

Fig. 9.2 Decentralized SC network.

First, during an initialization step a set of follower designs, potential pricing agreements and performance indicators are defined. The second and third parts consist of an iterative optimization procedure and the collection of the resulting performance indicators respectively. Finally, a post-optimization procedure is required to identify the best overall solution in terms of the decision-maker preferences. The main parts of the algorithm are presented in the following section while the whole algorithm is illustrated in Fig. 9.2.

9.3.1. Iterative optimization procedure.

The most important part of the proposed strategy consists in a reiterative procedure, in which a two-stage stochastic optimization problem was solved for each design and agreement (Fig.9.2). The used single objective (SO) stochastic problem follows the general form of Eq. (9.7).

$$
\begin{aligned}
&\max_{x\ y_s}\ \{EProf_l, EProf_f\} \\
s.t.\quad & \\
&h(x, y_s) = 0 \qquad \forall s \in S \\
&g(x, y_s) < 0 \qquad \forall s \in S \\
&x \in X, y_s \in Y
\end{aligned}
\tag{9.7}
$$

Notice that even if additional performance indicators are considered/calculated (such as expected freshwater consumption and follower reaction "prediction") they do not act as objective functions, and in fact, only the economic objective for both participant SCs were considered.

Additionally, a solution identification strategy was also included during the iterative procedure to overcome the decision making challenge. In this particular case, and without loss of generality, the ELECTRE-IV method was used, even if different solution identification algorithms may be considered. The complete iterative procedure is described next.

1. For each design;
   1.1. For each contract;
      1.1.1. Solve the problem and collect the decision variables.
      1.1.2. Add the results of each scenario into a blank matrix, henceforth known as "scenario matrix"
      1.1.3. Using the information of "scenario matrix" calculate all the post-optimal performance indicators (such as the probability of acceptance, financial risk for each actor, etc.).
      1.1.4. Collect all the performance indicators (from either, optimization and post-optimization calculation) into a blank matrix and generate a new matrix including all these performance indicators for each contract, henceforth known as "Criteria-Contract matrix".
   1.2. Select the solution (or reduced set of solutions) with the best overall performance for all the criteria in "Criteria-Contract matrix" by applying the ELECTRE-IV method.
2. Compare the solution selected at each design to provide the best overall performance for all the follower designs.

9.4. Case study

The capabilities of the proposed strategy are illustrated using a case study seeking for the management of a water network within a shale gas SC originally presented in *Gao and You (2015)* (see Fig. 9.1). This case study was previously used in Chapter 5, thus, problem description and details can be found there and in Appendix B.3. Remarkably, the point 1.1.1 of the solution algorithm has been simplified into a SO function substituting the objective function as in Eq. (9.8) so as to facilitate the solution of the problem and promote the results comparison/discussion.

$$\max \; EProf_{global} := \sum_{sc} EProf_l + EProf_f \qquad \forall l, f \qquad \in SC \quad (9.8)$$

As a way to explore variation in the unpredictable follower decisions two extreme follower designs were considered modifying the complexity of the treatment sites as shown in Fig. 9.3. The most conservative one account for the installation of a single treatment plant and disposal well, while risky designs may install all the possible treatment/disposal units.

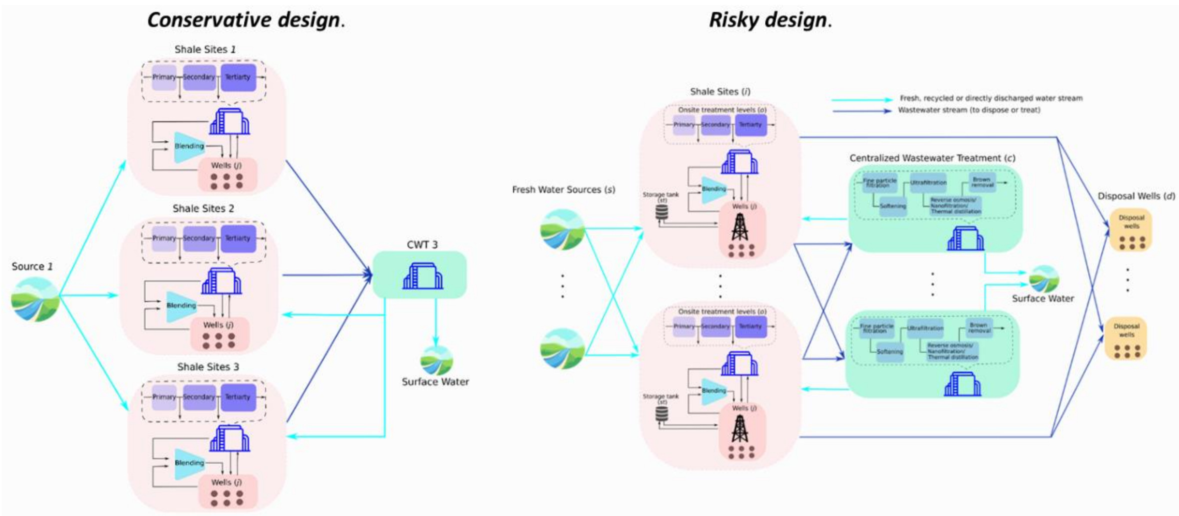

Fig. 9.3 Follower designs.

These designs were analyzed for a set of negotiation contracts. In particular, 50 pricing agreements were considered and generated by combining the 10 wastewater disposal prices and five recovered water prices. These prices were defined based on their average historical values (see Table 9.1).

Table 9.1 Negotiation agreements.

		Wastewater treatment price ($/bbl)				
		0.025	***0.0412***	***0.057***	***0.073***	***0.09***
Recovery treatment Price ($/bbl)	***1.00***	1	11	21	31	41
	1.44	2	12	22	32	42
	1.88	3	13	23	33	43
	2.32	4	14	24	34	44
	2.76	5	15	25	35	45
	3.20	6	16	26	36	46
	3.64	7	17	27	37	47
	4.08	8	18	28	38	48
	4.52	9	19	29	39	49
	4.96	10	20	30	40	50

Finally, 100 scenarios were used as a way to model the unpredictable role of the third parties in the system. Similarly than for the negotiation agreements, each scenario consists of a pair of values for wastewater treatment and recovery wastewater prices that are randomly selected using the average value of $0.075/bbl and $4.0/bbl respectively and an overall standard deviation of 30%. Without loss of generality, the well-known Monte Carlo sampling was used in order to discretize the normal distributions leading to an equiprobable distribution.

For clarity in the comparison analysis, the following discussion will be focused on the conservative follower design. Thus, using such a set of scenarios, the two-stage stochastic model was solved for each one of the negotiation contracts resulting in 50 different solutions for each follower design. Each solution (individual point in Fig. 9.4) accounts for a specific freshwater consumption, a follower's probability of acceptance and, more importantly an associated financial behavior for both, the leader and the follower. These financial behaviors prove that even a small variation in the pricing policies/agreements has a significant effect on the actor's performances. Notice that the $EProf$ ranges differently between the leader and the follower (being \$230,000 and \$338,000, respectively) proving the conflict of interest between actors and confirming that the system in represented by a non-zero-sum game. Fig. 9.4 also includes the player's standalone situation, thus, any contract showing higher economic performances than \$77.05x10^6 and \$1.11 x10^6 for leader and follower respectively represents a feasible option, since they actually improve their best individual performance.

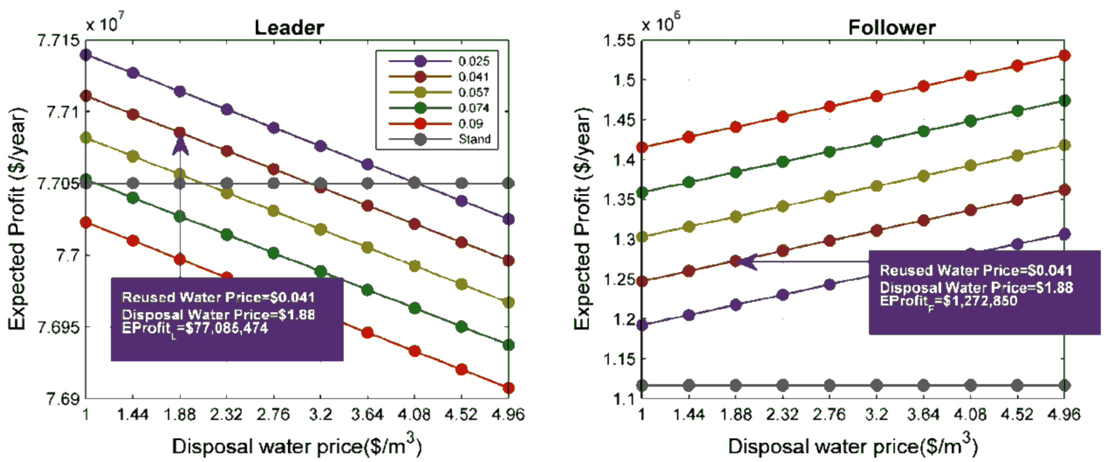

Fig. 9.4. Negotiation behavior for the conservative follower designs.

Within all the negotiation contracts, the follower's expected profit is improved. However, only a small fraction of these contracts produce a win-win situation from the leader's perspective. Therefore, in order to suggest the best agreement, the leader has to measure the positive impact on its economic performance and the probability that the follower accepts a specific contract. Consequently, a set of decision criteria with their decision maker's preferences was defined (Table 9.2) and used within the ELECTRE-IV method framework. It is important to comment that until now only the results associated to the conservative design have been showed; however, the results related to the risky design have been considered for the preference values definition.

Table 9.2. Thresholds values for the considered decision criteria.

Thresholds	Selection Criteria			
	$EProfit_L$	$EProfit_L$	*Water Savings***	*Prob. acceptance*
Indifference	7.70x10^7	1.20x10^6	6.0x10^5	0.55
Preference	7.71x10^7	1.45x10^6	6.80x10^5	0.75
Veto	10.0x10^7	10.0x10^7	7.00x10^5	1

* Values expressed in \$ ** Values expressed in bbl

In general, the ELECTRE-IV method compares all the solutions identifying a single negotiation agreement that leads to the highest positive impact on all the four decision criteria disregarding the follower designs. After applying the ELECTRE-IV method, a single negotiation contract was found as the overall optimum contract (highlighted in Fig.9.4). Such a negotiation contract consists of a reused water price of \$0.041 and a disposal cost of \$1.88 per bbl of water and wastewater respectively. Such a negotiation contract has an associated specific design and coordination plan for the decentralized SC. By analyzing the optimal SC conditions presented in Table 9.3, it can be concluded that, disregarding the follower decisions, the leader is able to propose an agreement leading to an improvement in the entire set of performance indicators for both, leader and follower. In addition, such a negotiation is acceptable for the follower (more than 60% of favorable results) increasing the confidence in the obtained solution.

Table 9.3. Optimal criteria values for each player within the selected negotiation contract.

	$EProfit_L{}^{*}$	$EProfit_F{}^{*}$	$FreshWater^{**}$	$Prob.\ Acceptance$
Conservative	77.085 x10^6	1.272 x10^6	0.820 x10^6	0.73
Risky	77.085 x10^6	1.192 x10^6	0.820 x10^6	0.63
Standalone	77.005 x10^6	1.117 x10^6	1.253 x10^6	N/A
Improvement	0.080 x10^6	0.155 x10^6 0.075 x10^6	0.433 x10^6	

* Values expressed in \$ **Values expressed in bbl

A detailed analysis of the resulting network configuration is discussed in detail in the following section.

9.4.1. Network description and analysis

In this section, the network configuration obtained using the proposed strategy was compared with the one resulting from the traditional centralized scheme in order to illustrate the benefits of considering a decentralized approach.

Both networks are displayed in Fig. 9.5; in the centralized scheme, despite the dependency on the follower decisions (wastewater treatment part), this configuration totally relies on an onsite treatment to reduce the freshwater demands (contributing in around 1,000,000 bbl/year). Even if the centralized treatment plants are employed, they are only considered for disposal purposes and there is not regenerated water coming back to the system after its treatment in the follower sites. Such a behavior is logical from a centralized perspective, since it is assumed that a return transportation task is redundant and even unnecessary.

The decentralized network configuration (i.e. the one obtained with the proposed strategy) produces a well-balanced design that promotes the use of regenerated water from both treatment options onsite and centralized facilities, reusing at least 3,400,000 bbl/year. Such a massive water saving was achieved at the expense of significantly increasing the distribution cost (an increase of about 52% if compared with the centralized approach). Certainty, the resulting configuration provides a robust system that ensures a good process performance for different scenarios.

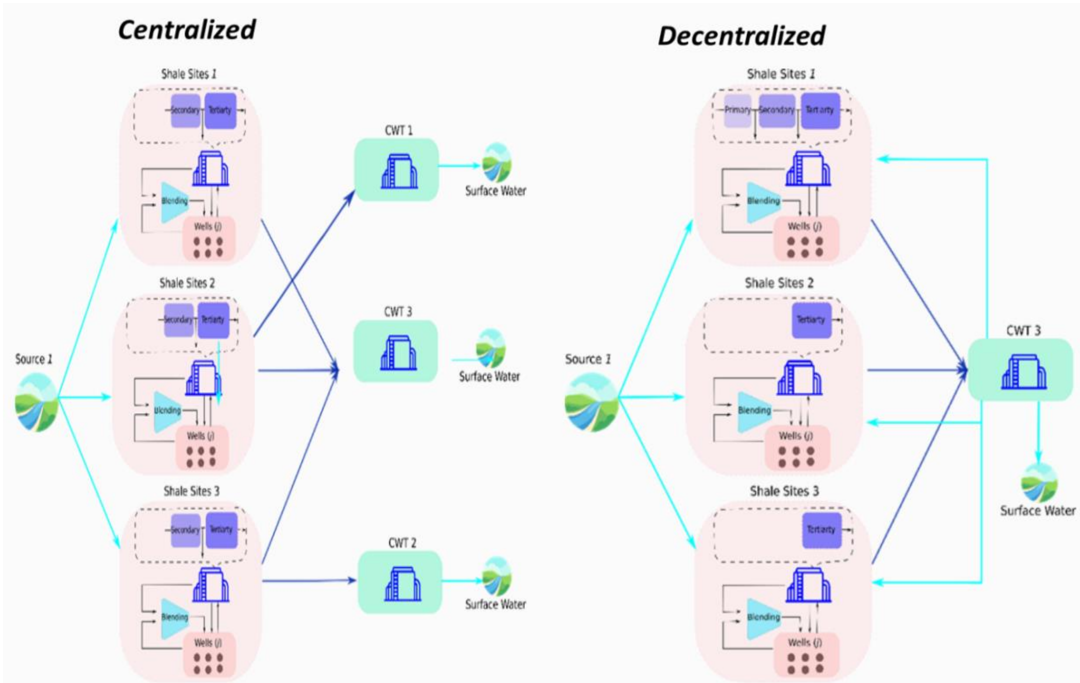

Fig. 9.5. Complete network configuration for: a) centralized and b) decentralized schemes.

The total water management benefit in the centralized scheme is $79,024,590/year, which is 10% greater than the one obtained with the decentralized scheme ($77,085,000/year). Besides the significant difference in the final benefit, both strategies distribute their costs in very different manners: the overall cost distribution of different water management sections is given in Figure 9.6. These results prove that in the decentralized scheme the use of resource regenerator (treatment plants) have been promoted treating the 86% of the total waste, while in the centralized one only 11% of the wastewater is treated. Similarly, it can be noticed that the transportation cost is significantly higher in the decentralized configuration (57% more than in centralized network).

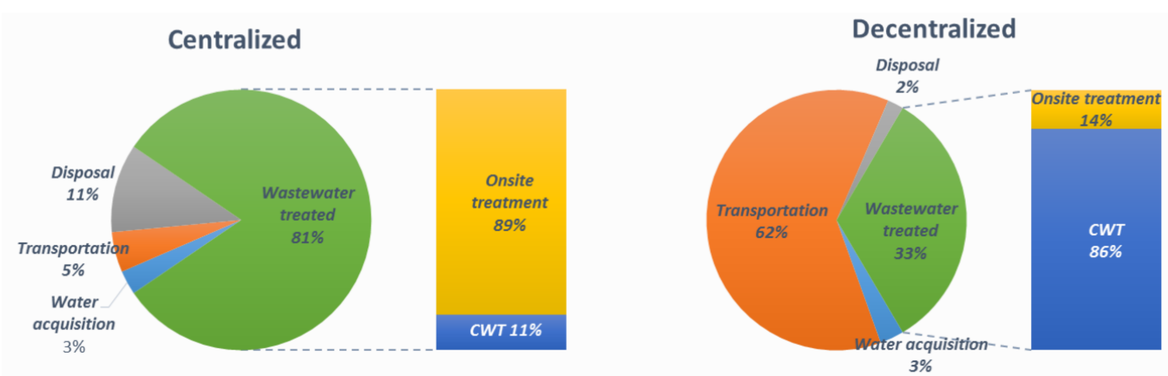

Fig. 9.6. Cost breakdown for: a) centralized/cooperative and b) decentralized/competitive schemes.

Despite their different cost distribution, the one corresponding to water acquisition is the same for both configurations. Even if the above suggests that the resulting water management is the same, Table 9.4 proves otherwise. In fact, the configuration resulting from the competitive approach achieves more than three times more water savings than the cooperative configuration due to the large investment in the use of recovered water.

Table 9.4. Detailed water management costs.

	Cooperative	Competitive
Freshwater *($/year)*	254,470	82,136
Recovered water *($/year)*	2,116	180,700
Total consumed water *(bbl/year)*	6,000,000	5,000,000
Freshwater *(bbl/year)*	5,000,000	1,500,000
Water savings *(bbl/year)*	1,000,000	3,500,000

All the above results illustrate the advantages of the competitive configuration in terms of individual economic benefit as well as global environmental ones.

9.5. Conclusions

This chapter proposes an integrated holistic approach for the effective SC design and management under multiple types of uncertainties and competitive environment supporting the decision-making processes. Particularly, a systematic strategy that allows designing and coordinating a decentralized supply chain through the production of an attractive negotiation contract between two independent SCs is presented. Numerical results prove that the solution strategy is capable of identifying an attractive agreement that has a positive impact on the economic and environmental performances of both partners.

The proposed strategy uses a proper formulation to manage the uncertainty associated to the different actors participating in the system, increasing the reliability of the resulting design and planning decisions associated with each negotiation contract. The above contributes to guarantee the robustness in the design and planning network obtained considering a non-collaborative SC. Additionally, the use of the ELECTRE-IV method as a decision-making tool not only expedites the selection of a unique and reliable negotiation contract but also increases the flexibility of the strategy, being able to consider multiple negotiation items and multiple decision criteria.

As a future work, the proposed strategy needs to be combined with other systematic approaches capable of identifying the proper amount of follower designs and uncertainty scenarios to be considered, in terms of their effect over the quality of the final solution. Such a framework could be based on the scenario reduction methods used in previous chapters of this Thesis.

9.6. Nomenclature

Abbreviations

MO	Multi-objective
SC	Supply chain
SBDN	Scenario-Based Dynamic Negotiation
MILP	Mixed integer linear programming
PSE	Process system engineering
CWT	Centralized wastewater treatment plant
ELECTRE	Life Cycle Assessment
IS	Industrial Symbiosis
G-ICE	Gasifier internal combustion engine
LHV	Lower heating value
MC	Moisture content
MILP	Mixed integer linear programming
ANN	Artificial Neuronal Network

Indices/Subsets

s	Freshwater source
j	Wells
i	Shale sites
xv	Leader external provider
xc	Follower external client
m	External customers
r	Exchangeable item
t	Time period
c	Treatment plant
d	Disposal well
o	Treatment plants
sc	Supply chain
L	Leader
F	Follower

Parameters

$dem_{r,sc,m,t,s}$	Freshwater demand of item *r* for each player *sc*
$p_{r',sc',t}$	Prices associated to internal customer
$pr_{r,m,t}$	Prices associated to external customer
v	Veto thresholds
$Prob_s$	Probability of occurrence of scenario *a*
$Prob\_acceptance_{sc\prime}$	Probability of acceptance of agreement

Variables

$Q_{r'sc't\ s}$	Amount of exchangeable/negotiation item
$CRM_{sc,t,s}$	Cost of freshwater
$CTR_{sc,t,s}$	Transportation cost of water management
$CST_{sc,t,s}$	Storage cost
$CPRD_{sc,t,s}$	Disposal cost
$Prof_{sc,s}$	Profit for each player.
$Sales_{sc,s}$	Total sales for each player and scenario *s*
$Cost_{sc,s}$	Total cost for each player and scenario *s*
$EProf_{sc}$	Expected profit for each player
$EProf_{global}$	Expected global profit
$Enfw$	Expected net freshwater consumption
$fw_{s,i,m,t}$	Freshwater extracted from freshwater suppliers
$wtcd_{c,t,s}$	Wastewater disposed to surface

Part V:

Conclusions and Outlook

Chapter 10

Conclusions and Future Work

10.1. Conclusions

The methodical combination of Multi-Objective strategies with uncertainty management approaches has been attained in this Thesis. The numerical results have proved the positive effect of this combination on the solutions flexibility and robustness compared with the ones obtained through traditional approaches. These methods have resulted in contributions on the following issues.

- Computational effort reduction for both, solutions identification and uncertainty management.
    - The scenario reduction strategies used here allow reducing the computational effort necessary to obtain a robust solution through two-stage stochastic programming methods.
    - The Meta-Multiparametric programming approach expedites the reaction of the decision maker once the uncertainty has been unveiled.
    - The use of Pareto Filters and ELECTRE-IV methods simplify the decision maker tasks, expediting the solution identification ensuring the quality of the decisions through a systematic approach.
- Effective exploitation of modelling and optimization strategies in order to drive to sustainable processes/solutions.
    - Fuzzy based formulations allow reducing the difficulties associated with the decision making, introducing a selection directly at the optimization step skipping the traditional need of post-optimization algorithms.

The integrated discussion of the conclusions obtained from each chapter is next exposed.

Part II. - Efficient Multi-Objective strategies

Along this section, two different strategies were proposed supporting the decision-making process associated with multi-objective and/or multi-criteria problems. These proposed solution strategies can be classified as in-optimization and post-optimization methods. Both methods aim to solve the issues associated to the selection of an optimal solution within the Pareto set. In particular, these methods provide a framework for the systematic generation/evaluation of a single optimal solution disregarding the amount of objectives/criteria at the time that reduce the effect of the decision maker bias. For the in-optimization strategy, a fuzzy-based formulation was implemented considering complex non-linear objective behaviors that accurately represent some cause-effect relationships between raw material consumption/conservation. This fuzzy-formulation was used as a way to bypass the decision making process and directly generate a well-balanced optimal solution for the multi-objective optimization problem. On the other hand, the post-optimization method used consists of a combination of the ELECTRE-IV method and the ε-constraint method (as multi-objective approach) to systematically generate the Pareto frontier and evaluate all the options identifying the single solution that better satisfies the decision maker preferences simultaneously for different criteria.

The capabilities of these approaches have been tasted through the design and planning of a real water management system. For the fuzzy approach, an urban water network was considered. In particular, the case study accounts for rainwater harvesting and regenerated wastewater as alternative water sources for satisfying water demands (in the industrial, domestic, and agriculture sectors) for the city of Morelia in Mexico. The ELECTRE-IV method was proved in a water network system within a shale gas production SC problem.

Numerical results show that in both cases a freshwater consumption savings of at least 13% is achieved, reinforcing the idea that a proper water management, including reclamation and harvested rainwater, are promising and feasible options to reduce the use of freshwater even during drought seasons. Even more, it has been proved that both, Fuzzy and ELECTRE-IV method are useful and reliable to identify an overall better solution satisfying partially or completely the decision maker preferences. Furthermore, these strategies represent alternative ways to assess different challenges in the field of process systems engineering (such as sustainability in either centralized or decentralized schemes).

Part III. - Uncertainty management strategies

In this section, two strategies have been proposed to extend the current approaches to address problems associated to the sustainable management of supply chains under uncertainty (i.e. proactive and reactive approaches). These strategies were aimed to address two main challenges: first, the reduction of the computational effort typically associated to the solution of problems under uncertainty addressed by the traditional approaches and second, the efficient control of the effect of uncertain/unpredictable conditions over the resulting solution.

In order to address the computational effort issue, a scenario-reduction strategy has been proposed as a way to expedite the solution of multi-stage stochastic problems. The basic idea behind this reduction strategy is to find the lowest number of sampling points that accurately represent the uncertainty space. In addition, the reduction strategy has been efficiently combined with a solution identification algorithm and hence, their coordinated application to address the design of a sustainable supply chain under raw material availability and quality uncertainties was justified. Thus, ultimately, a potentially flexible and robust formulation is obtained while reducing the computational effort required for solving the problem.

Conversely, in order to better control the effect of the uncertainty, a meta-multiparametric approach (M-MP) was proposed in which traditional optimization and surrogate-modeling techniques were combined. In particular, a Kriging meta-model was used in order to emulate/predict the expected state of the system in front of parameter variations. The system behavior associated with the uncertain conditions was obtained using an M-MP approach and this information was later used to build and validate the meta-model. As a result, M-MP demonstrated its ability to emulate successfully large complex real-world problems subject to multiple uncertainty sources. The above is of great relevance for the management of sustainability problems since a single meta-model is able to cover the entire uncertainty space enhancing the capabilities of the traditional multiparametric programming.

The capabilities of both approaches have been successfully demonstrated using, as a common case study, the multi-scenario and multi-objective design and management problem of an energy distribution network using biomass as raw material. It is important to emphasize that both methods address the management of different material flows with independent uncertain sources, ensuring a sustainable energy demand satisfaction. Numerical results show that from one side, the scenario reduction strategy systematically reduces the number of scenarios maintaining the accurate representation of the uncertainty solution space, while the surrogate model predicts the system performance with high accuracy and computational efficiency. If compared with traditional optimization approaches (such as two-stage stochastic programming), M-MP may be considered as a more “difficult to apply” strategy, but the detailed information on system behavior provides additional advantages and justifies its potential combination with other sophisticated decision-making strategies.

Notice that even if both strategies achieve computational savings, their focus is devoted to different steps. For the scenario reduction strategy, its improvements are in the optimization step. On the contrary, M-MP addresses the “re-optimization” step (i.e. once the uncertain information changes or is unveiled). Thus, these results prove that both, the systematic reduction of scenarios and the accurate and detailed descriptions of the system behavior are equally relevant for the development of strategies that reduce the computational challenges on uncertainty approaches ensuring a feasible solution.

Part IV. - Functional integrations

In this part, two different frameworks were developed to address MO and uncertainty management strategies. Essentially, solution identification techniques (particularly, Pareto filter and the ELECTRE-IV methods) were combined with an uncertainty management strategy (sample average approximation) in order to address the optimization of a problem under uncertainty. The resulting solution frameworks address the major challenge of considering a large number of decision criteria simultaneously with a large (representative enough) amount of uncertainty parameters.

For the first framework, (let’s say Pareto filters one), a set of uncertainty-aware solutions are generated using the sample average approximation. Later, the Pareto filters are applied to systematically evaluate the solution based on their performances and optimality through a set risk metrics. Remarkably, by employing the risk metrics, this strategy selects the solution with the minimum worst performance.

The capability of this approach has been successfully proved using as test-bed a multi-scenario multi-objective design and planning supply chain model. Numerical results show that both proposed approaches accelerate the search for solution alternatives behaving in different manners within the uncertain parameter space.

The second framework presented also employs SAA approach as uncertainty management strategy and ELECTRE-IV method is used as solution identification approach: However, these approaches are integrated in a scenario-based dynamic negotiation framework (SBDN) that allows formulating a water management problem under non-cooperative environment. Particularly, this framework was exploited for the systematic design and coordination of a decentralized supply chain through the production of an attractive negotiation contract between two independent SC's was presented.

The consideration of negotiation contracts were successfully applied leading to a positive impact on the performance of each one of the objectives considered for all the participants. The proposed strategy uses a proper uncertainty formulation that promotes the generation of robust solutions, increasing the reliability of the resulting design and planning decisions associated with each negotiation contract. Remarkably, the use of ELECTRE-IV method not only expedited the selection of a unique and reliable negotiation contract but also increased the flexibility of the strategy, being able to consider multiple negotiation items and multiple decision criteria.

Besides their differences, both approaches allow to narrow down the number of alternatives, ensuring that the final solution performs well for a wide range of criterion targets. These approaches can be used in different engineering problems ensuring the quality of final solution even for those in which the effect of process uncertainties has to be explicitly considered over the solution performance.

10.2. Future works

The main future research direction may be classified in:

- Evaluate the quality/representativeness of the defined decision criteria.

There is a need for a novel integrated strategy that allows evaluating the quality/representativeness of the selected decision criteria. For instance, in the ELECTRE-IV method, the impact and significance of the defined threshold over the final solution has to be evaluated. Such an issue represents an important gap in the literature and it can be considered as one of the more significant future research topics.

Besides, this can lead to potential contribution in the proper quantification of objectives, since the solution selection strategy is highly sensitive to the quality in the performance of the objectives measurements.

- Include robustness calculation/valorization within a solution identification framework.

The proposed Pareto filters framework uses a very simplified version of the strict robust optimization (Minimax), thus, the combination of minimax concepts on Pareto filters are a promising research area. The above is particularly interesting for its further application on large and complex problems, such as pharmaceutical and petrochemical processes.

- Evaluation of the uncertainty parameters in terms of its effect over the system behavior or solution performances.

As a future work, the proposed strategy needs to be combined with other systematic approaches capable of identifying the proper amount of follower design and uncertainty scenarios to be considered, in terms of their effect over the quality of the final solution. Such a framework could be based on the scenario reduction method used in previous chapters of this Thesis.

Appendices

Appendix A

Publications

This is a list of the publications resulted from the works carried out so far within the scope of this Thesis.

A.1. Indexed journals

i. Published

Medina-González, S.; Pozo, C.; Corsano, G.; Guillén-Gosálbez, G.; Espuña, A. Using Pareto filters to support risk management in optimization under uncertainty: Application to the strategic planning of chemical supply chains. *Computers & Chemical Engineering*, 98: 236-255 **(2017)**. doi.org/10.1016/j.compchemeng.2016.10.008.

Medina-González, S.; Graells, M.; Guillén-Gosálbez, G.; Espuña, A.; Puigjaner, L. Systematic approach for the design of sustainable supply chains under quality uncertainty. *Energy Conversion and Management*, 149: 722-737 **(2017)**. doi.org/10.1016/j.enconman.2017.02.060.

Medina-González, S.; Espuña, A.; Puigjaner, L. An efficient uncertainty representation for the design of sustainable energy generation systems. *Chemical Engineering Research and Design*, 131: 144-159 **(2018)**. doi.org/10.1016/j.cherd.2017.11.044.

Medina-González, S.; Rojas-Torres, M.; Ponce-Ortega, J.M.; Espuña, A.: Guillén-Gosálbez, G. Use of Nonlinear Membership Functions and the Water Stress Index for the Environmentally Conscious Management of Urban Water Systems; Application to the City of Morelia. ACS Sustainable Chemistry and Engineering, 6(6): 7752-7760 **(2018).** doi: 10.1021/acssuschemeng.8b00660.

Medina-González, S.; Shokry, A.; Silvente, J.; Lupera, G.; Espuña, A. Optimal management of bio-based energy supply chains under parametric uncertainty through a data-driven decision-support framework. *Computers & Industrial Engineering*. doi.org/10.1016/j.cie.2018.12.008

ii. Submitted

Medina-González, S.; Gao, J.; You, F.; Espuña, A. Comparing and Extending Multi-Criteria decision-making strategies to address non-cooperative situations: An application to address sustainable supply chain design problems. *AIChE Journal*. (Ready for submission)

A.2. Conference proceeding articles

Medina-González, S.; Shokry, A.; Silvente, J.; Espuña, A. A meta-multiparametric framework: Application to the operation of bio-based energy supply chains. *Computer Aided Chemical Engineering*, (37), 1955-1960 **(2015)**. doi.org/10.1016/B978-0-444-63576-1.50020-0.

Dombayci, C.; Medina-González, S.; Graells, M.; Espuña, A. Integrated management of hierarchical levels: towards a CAPE tool. *Computer Aided Chemical Engineering*, (38), 7-12 **(2016)**. doi.org/10.1016/B978-0-444-63428-3.50006-0.

Medina-González, S.; You, F.; Espuña, A. Optimal design and operation of water supply chain networks using scenario-based dynamic negotiation and multiple negotiation terms. *Computer Aided Chemical Engineering*, (40), 1921-1926 **(2017)**. doi.org/10.1016/B978-0-444-63965-3.50322-6.

Audino, F.; Medina-González, S.; Graells, M.; Pérez-Moya, M.; Espuña, A.; Méndez, C. Optimization of a Distributed Wastewater Treatment Network Considering Lumped Parameters Interrelations. *Computer Aided Chemical Engineering*, (40), 2701-2706 **(2017)**. doi.org/10.1016/B978-0-444-63965-3.50322-6.

Shokry, A.; Medina-González, S.; Espuña, A. Mixed-Integer MultiParametric Approach based on Machine Learning Techniques. *Computer Aided Chemical Engineering*, (40), 451-456 **(2017)**. doi.org/10.1016/B978-0-444-63965-3.50322-6.

Lupera, G.; Shokry, A.; Medina-González, S.; Vyhmeister, E.; Espuña, A. Ordinary Kriging: A Machine Learning Tool Applied to Mixed-Integer Multiparametric approach. *Computer Aided Chemical Engineering*, (43), 531-536 **(2018)**.

A.3. Other congresses and workshops

Dombayci, C.; Medina-González, S.; Graells, M.; Espuña, A. Integrated management of batch production systems using domain ontology. *10th European congress of chemical engineering, 3rd European congress of applied biotechnology and 5th European process intensification conference.* **(27-30 September 2015)** *Oral presentation*.

Medina-González, S.; Morakabatchiankar, S.; Graells, M.; Guillén-Gosálbez, G.; Espuña, A.; Puigjaner, L. Sustainable Design of a Bio-Based Energy Network Under Multiple Objectives and Availability/quality Uncertainty. *11th Conference on sustainable development of energy, water and environment systems*, **(04-09 September 2016)**. *Oral presentation*.

Medina-González, S.; Graells, M.; You, F.; Espuña, A. Aplicación del enfoque de negociación dinámica basada en escenarios para el diseño y manejo de redes de suministro de agua. *IV Simposio CEA de Modelado, Simulación y Optimización. MSO optimización 4.0*, **(25-26 January 2018)**. *Oral presentation*.

Appendix B

Case studies data and validations

B.1. Piecewise validation for the case study of Chapter 4.

The relationship between *WSI* and *WC* is displayed in Fig. B1, which shows how the unitary impact of water first goes up, then reaches a maximum, and then declines. Hence, after a given point, further water consumptions do not result in a significant increase of the impact. The inclusion of the sigmoidal behavior associated to the *WSI* thus enables a more realistic assessment of the effect of freshwater usage. In addition, Fig. B1 shows the five intervals considered for the piecewise strategy, which produce an accurate representation of the original sigmoidal behavior.

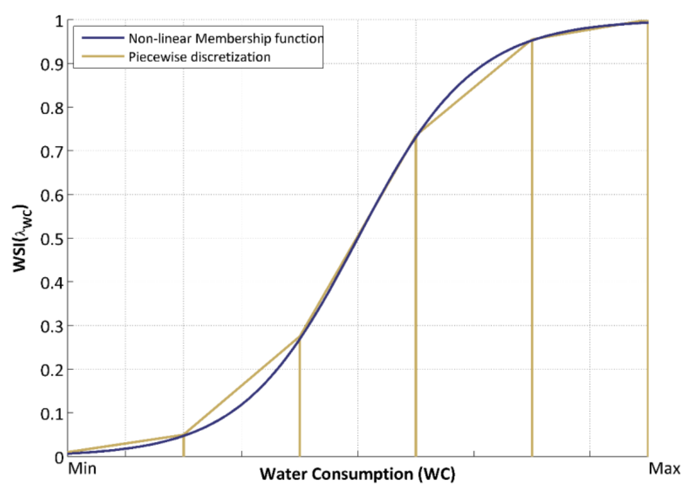

Fig. B1. Graphical membership function representation using our cause-effect approach (blue line) and the fixed piecewise discretization used (gold line).

It is evident that a higher discretization will lead to a better representation of the sigmoidal function. However, it would also lead to more binary variables and therefore larger CPU times. In our case, five intervals produce an accurate enough approximation for the purposes of our study.

B.2. Complementary information for the case study of Chapter 4.

Table B1. Expected monthly precipitation amount (mmH2O).

Month	Year										
	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025
Jan	15.60	15.51	15.41	15.32	15.23	15.14	15.05	14.96	14.87	14.78	14.69
Feb	7.70	7.65	7.61	7.56	7.52	7.47	7.43	7.38	7.34	7.29	7.25
Mar	8.60	8.55	8.50	8.45	8.40	8.35	8.30	8.25	8.20	8.145	8.10
Apr	10.10	10.04	9.98	9.919	9.86	9.80	9.74	9.68	9.63	9.57	9.51
May	41.70	41.45	41.20	40.95	40.71	40.46	40.22	39.98	39.74	39.50	39.26
June	150.70	149.80	148.90	148.00	147.12	146.23	145.36	144.48	143.62	142.76	141.90
July	167.50	166.50	165.50	164.50	163.52	162.54	161.56	160.59	159.63	158.67	157.72
Aug	170.40	169.38	168.36	167.35	166.35	165.35	164.36	163.37	162.39	161.42	160.45
Sept	129.90	129.12	128.35	127.58	126.81	126.05	125.29	124.54	123.79	123.05	122.31
Oct	52.80	52.48	52.17	51.86	51.54	51.24	50.93	50.62	50.32	50.02	49.72
Nov	10.00	9.94	9.88	9.821	9.76	9.70	9.65	9.59	9.53	9.47	9.42
Dec	3.90	3.88	3.85	3.83	3.81	3.78	3.76	3.74	3.72	3.69	3.67
Total	769	764	760	755	751	746	742	737	733	728	724

Table B2. Deviation from the mean value used to calculate the monthly demand.

Month	*%*
January	-8,5
February	4
March	4
April	17,9
May	14,1
June	6,9
July	0
August	0
September	-2,2
October	-2,2
November	-2,3
December	-7,9

Table B3. Constant parameters for the storage devices.

Device	***Coefficient***			
	A($)	B($)	C($/m^3)	D($/m^3)
Tank	28,08		151,968	
Artificial pond		4,9134		4,9895

Table B4. Available freshwater at natural sources.

Source	***Capacity (m^3)***
Deep well	$8x10^6$
Spring	$49x10^6$
Dam	$84.3x10^6$

Table B5. Freshwater demand.

Site/Use	***Demand (m^3/month)***
Domestic	$2.2x10^6$
Agricultural	$0.46x10^6$
Industrial	$0.54x10^6$

Table B6. Storage devises capacities.

Device	***Capacity (m^3)***
Storage tank	50,000
Artificial pond	600,000

B.3. Parameters for the case study of Chapter 5.

Table B7. Parameters for the shale gas case study.

Parameter	Unit	Index	Value
$CC_{i,j,t}$	Mcf/bbl	-	100-200
CS_i	$/bbl	-	0.20-0.50
CI_i	$/bbl	-	100-140
DR	per week	-	0.0018
$FC_{i,c,m,r}$	$	r1	15,800
	$	r2	20,000
	$	r3	23,800
$FD_{i,d,m,r}$	$	r1	238,000
	$	r2	300,000
	$	r3	357,000
$FO_{i,o,q}$	$	q1	15,800
	$	q2	20,000
	$	q3	23,800
$FR_{s,t}$	bbl/week	-	22,000-115,000
$FS_{s,i,m,r}$	$	m1,r1	158,000
	$	m1,r2	200,000
	$	m1,r3	238,000
	$	m2,r1	986,000
	$	m2,r2	1,500,000
	$	m2,r3	1,910,000
LC_i	-	-	0.6-0.7
LO_o	-	o1	1.00
	-	o2	0.98
	-	o3	0.70
$MC_{i,c,m,r}$	bbl	r1	30,000
	bbl	r2	45,000
	bbl	r3	60,000
$MD_{i,d,m,r}$	bbl	r1	30,000
	bbl	r2	45,000
	bbl	r3	60,000
$MS_{s,i,m,r}$	bbl	m1,r1	30,000
	bbl	m1,r2	45,000
	bbl	m1,r3	60,000
	bbl	m2,r1	200
	bbl	m2,r2	400
	bbl	m2,r3	600
RF_o	-	o1	5.67
	-	o2	1.86
	-	o3	0.25
$RW_{i,j,t}$	bbl/week	-	300-500
SC_i	bbl	-	15,000-25,000
SM_i	bbl	-	50,000-80,000
$SP_{i,t}$	$/Mcf	-	0.10-1.00
$TC_{i,c,m}$	$/bbl	-	0.60-3.00
$TD_{i,d,m}$	$/bbl	-	9-18
$TS_{s,i,m}$	$/bbl	m1	0.20-1.00
	$/bbl	m2	10-30
$VC_{i,c,t}$	$/bbl	-	1.00-5.00
$VD_{i,d,t}$	$/bbl	-	0.80-1.20

$VO_{i,o,t}$	\$/bbl	o1	1.60
	\$/bbl	o2	2.00
	\$/bbl	o3	4.50
WA_s	\$/bbl	-	0.04-0.06
$WC_{c,t}$	bbl/week	-	6,000-20,000
$WD_{d,t}$	bbl/week	-	1,000-5,000
$WO_{i,o,q}$	bbl/week	o1,q1	5.000
	bbl/week	o1,q2	10.000
	bbl/week	o1,q3	15.000
	bbl/week	o2,q1	1.000
	bbl/week	o2,q2	2.000
	bbl/week	o2,q3	4.000
	bbl/week	o3,q1	5.000
	bbl/week	o3,q2	10.000
	bbl/week	o3,q3	20.000
$WP_{i,j,t}$	bbl/week	-	90-100

B.4. Technologies characteristic and parameters for the case study of Chapter 6.

Technologies characteristics

The gasifier requires that the inlet material strictly satisfy a physical homogeneity (chipping) and a MC lower than 20% (dried). It is assumed that chipper and dryer work an average of 8 h/d while the gasifier works in average 16 h/d. Onsite storage represents an economic and simple option providing assurance of biomass availability against seasonality as well as aims to reducing pre-treatment/treatment capacities. It is important to notice that this kind of storages is only applicable for primary waste and if secondary waste is considered other type of storage is required.

The chipper and dryer capacities are assumed to have the same capacities employed in micronized food products (MFP) during one day. The required parameters and physical limitations used to model the activities in the mathematical formulation are described below.

1. Biomass generation. The cassava is harvested and subjected to different treatments in Food Industries, which produce a cassava waste with unpredicted properties.
2. Drying. A rotatory drum is used to produce raw material with a MC lower than 20%w/w. This unit has an energy efficiency of 99% and use diesel as utility (with price of $1133.31/t). Rotatory drums capacity is assumed in the range of 0.1 to 5 t/h as states in *(Hamelinck et al., 2005)*.
3. Chipping. Chipping task is mandatory placed after drying one. This unit has an energy efficiency of 96% and similarly to dryer units its available capacities range from 0.1 to 5 t/h *(Velázquez-Martí and Fernández-González, 2009)*.
4. G-ICE system. The system capacity ranges are between 5 and 100 kWe. The main parameters and outputs associated to this equipment are shown in Table A.1. Here, the equipment efficiency represents the main parameter and will affect for Biomass required *(Hamelinck et al., 2002).*
5. Transportation. Solid biomass should be distributed from its origin point to a storage place or to a pre-treatment/treatment sites by tractors. The capacity of that equipment's (Tractors) was set at 10t, which represents the upper level of tractor capacity. The price of transport task depends on the amount of material transported and the distance among sites. Lineal distances among nodes expressed in km are corrected through a tortuosity factor of 1.8 *(Hamelinck et al., 2005).*
6. Distribution grids. This task represents another type of transportation, dealing with energy transportation and not material. LV and MV are considered as "equipment". The LV distribution line has 6% losses in energy terms while MV distribution line losses are proportional to the power demand as stated by Medina-González et al., (2017a).

It is considered that the electricity demand should be partially or totally satisfied. The demand has been estimated for each community considering a direct relation with its population density. Particularly, the highest gross demand is 448.65 kWh/d, while the lowest is 21.17 kWh/d as shown in Table A.2.

Table B.8. Principal output values and specification for the G-ICE system.

Parameters	Values
Tgasif(°C)	702
Flowrate (kg/h)	35.33
LHV(MJ/kg)	6.32
CGE(%)	68
Power(kW_e)	15.8
η(%)	17

Table B.9. Energy demand and population distribution in Atebubu-Amantin district.

Community	Population (2010)	Net demand (kWh/d)	Gross demand LV (kWh/d)	Gross demand MV (kWh/d)
Senso	296	42.43	45	61.63
Old Konkrompe	566	88.6	93.96	119.48
Fakwasi	1881	333.2	353.35	393.67
Kunfia	2834	423.05	448.64	501.92
Trohye	376	58.65	62.2	78.84
Bompa	512	69.88	74.11	114.43
Nwunwom	122	19.97	21.17	31.57
Boniafo	489	84.86	89.99	115.51
Abamba	653	91.1	96.61	122.13

B.5. Parameters for the case study of Chapter 8.

Table B.10. Raw material costs.

	Distribution Cost ($ kg^{-1})					Procurement cost ($ kg^{-1})		
	l_1	l_2	l_3	l_4	l_5	r_1	r_2	r_3
s_1	0.02	0.1	0.08	0.06	0.08	0.02	0.02	0.01
s_2	0.14	0.12	0.14	0.02	0.06	0.02	0.01	0.02

Table B.11.Product demand (Ton).

	i_1	i_2	i_3	i_4
g_1	150	130	150	100
g_2	100	120	150	100
g_3	115	130	150	120

Table B.12. Product distribution cost form plant to warehouse.

	Distribution Cost ($ kg^{-1})											
	m_1				m_2				m_3			
	i_1	i_2	i_3	i_4	i_1	i_2	i_3	i_4	i_1	i_2	i_3	i_4
l_1	0.1	0.17	0.05	0.05	0.2	0.1	0.15	0.15	0.23	0.16	0.11	0.11
l_2	0.2	0.19	0.25	0.25	0.19	0.18	0.35	0.35	0.18	0.19	0.15	0.15
l_3	0.2	0.18	0.25	0.25	0.18	0.15	0.25	0.25	0.15	0.08	0.15	0.18
l_4	0.05	0.1	0.2	0.15	0.15	0.11	0.2	0.2	0.1	0.15	0.15	0.05
l_5	0.2	0.18	0.25	0.25	0.2	0.15	0.25	0.25	0.15	0.15	0.08	0.08

Table B.13. Product distribution cost ($ kg-1) from warehouse to customer.

	m_1	m_2	m_3
g_1	0.08	0.09	0.09
g_2	0.07	0.09	0.08
g_3	0.06	0.07	0.05

Table B.14. Batch parameters.

	Batch parameters													
	Size factors			Operating time (h)			Raw material factor conversion			Production Cost ($ kg^{-1})				
	j_1	j_2	j_3	j_1	j_2	j_3	r_1	r_2	r_3	l_1	l_2	l_3	l_4	l_5
i_1	0.9	0.6	0.4	14	5	7	0.8	0.5	0.7	0.12	0.18	0.12	0.06	0.12
i_2	0.6	0.5	0.4	12	6	4	0.6	0.8	0.8	0.08	0.16	0.06	0.12	0.10
i_3	0.7	0.5	0.4	16	8	5	0.4	0.5	0.5	0.12	0.14	0.14	0.08	0.14
i_4	0.8	0.6	0.4	10	4	5	0.5	0.5	0.5	0.14	0.08	0.14	0.04	0.12

Table B.15. Batch costs.

	Batch investment cost												
	Unit cost coefficient α_{ji} (annualized)					Raw material factor conversion			Production Cost ($ kg^{-1})				
	l_1	l_2	l_3	l_4	l_5	r_1	r_2	r_3	l_1	l_2	l_3	l_4	l_5
j_1	1620	2430	1350	1350	1890	0.8	0.5	0.7	0.12	0.18	0.12	0.06	0.12
j_2	2160	1620	2160	1620	1890	0.6	0.8	0.8	0.08	0.16	0.06	0.12	0.1
j_3	1890	2700	1890	1890	2430	0.4	0.5	0.5	0.12	0.14	0.14	0.08	0.14
Tanks	500	500	500	500	500	0.5	0.5	0.5	0.14	0.08	0.14	0.04	0.12

B.6. Validation of the representativeness of the selected number of scenarios (Chapter 8).

The number of scenarios (i.e., sample size) required to ensure a good estimation of the "real" values in the domain of uncertain parameters is a critical issue in any multi-scenario problem. In this regard, the method proposed by *Law and Kelton (2000)*, represents a promising alternative and it is completely applicable to any stochastic programming model. This approach relies on solving the stochastic model iteratively for an increasing number of scenarios until a given relative error γ is satisfied for a confidence level of 100(1- αα)%. In the context of our problem, this method comprises the following steps:

1. Define an initial number of scenarios ns_0, (as $|S|=s=ns_0$) where s will be updated dynamically during the execution of the algorithm.

2. Solve the specific stochastic model with |S|=s scenarios

3. Compute the confidence interval half-length $\vartheta(s, aa)$ for the mean value of the values in each scenario using the following expression.

$$\vartheta(s, a\alpha) = t_{n-1,\frac{1-a\alpha}{2}}\sqrt{\frac{Var^2(s)}{s}}$$

   Where $Var^2(s)$ is the sample variance, and $t_{n-1,\frac{1-a\alpha}{2}}$ is the critical point of the t-distribution.

4. If $\frac{\delta(s,\alpha)}{|Evalue|} \leq \frac{\gamma}{1-\gamma}$, then stop (i.e., the expected value of the discrete distribution is a valid estimator of the mean of the universe for the relative error and confidence interval defined beforehand). Otherwise, make $s = s + 1$ and go to Step 2.

The work of *Law and Kelton (2000)* provide more details about this procedure.

Author Index

Subject Index

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