

Chapter 10

Methods and Tools for Hydrogen Supply Chain Design

Jesus Ochoa Robles, Sofía De-León Almaraz
and Catherine Azzaro-Pantel

Laboratoire de Génie Chimique, Université de Toulouse, CNRS, Toulouse, France

ACRONYMS

AHP	analytic hierarchy process
AML	algebraic modelling languages
ANP	analytic network process
AUGMECON	augmented ϵ -constraint method
CCS	carbon capture and storage
DEMATEL	decision making trial and evaluation laboratory
DP	dynamic programming
ELECTRE	elimination and choice translating reality
GA	genetic algorithms
GHG	greenhouse gas
GIS	geographic information systems
HFCV	hydrogen fuel cell vehicle
HSC	hydrogen supply chain
LCA	life cycle assessment
LCC	life cycle costing
LP	linear programming
MCDM	multicriteria decision making
MILP	mixed integer linear programming
MINLP	mixed integer nonlinear programming
M-TOPSIS	modified TOPSIS
NIS	negative ideal solution
NPV	net present value
NSGA-II	nondominated sorting genetic algorithm

PCA	principal component analysis
PEM	proton exchange membrane
RA	risk assessment
RHS	right-hand-side
SAA	sample average approximation
SC	supply chain
SCM	supply chain management
SCND	supply chain network design
SO	solid oxide
TOPSIS	Technique for Order Preference by Similarity to Ideal Solution

10.1 INTRODUCTION

This chapter presents the different approaches that can be used for the solution of hydrogen supply chain design problem. The reader must be aware that this chapter constitutes a companion paper to the following chapters of this book. The objective is to propose guidelines for the methodological choices that emerge as the best options for solution strategies. Some of the formulations are illustrated in the dedicated chapters of this book.

HSC analysis and design can be viewed as a multiscale and multiobjective problem, with several criteria related to cost, environmental impact, and safety, among others. Some of the decisions that must be made in HSC design are as follows: what are the best places to build hydrogen production facilities? How large should the facilities be? Where does each facility get its feedstock from? What kinds of energy sources and production technology constitute the best choices? Which demand centers are served by each production facility? Which mode of hydrogen delivery is used for each demand center? These questions must be answered by considering simultaneously the abovementioned criteria.

This chapter is divided into two sections. [Section 10.2](#) first presents the description of some optimization frameworks according to the type of problem (e.g., linear, nonlinear) and some significant solution strategies that can be used. The HSC problem can be viewed as an optimization problem with both integer (number of production plants, storage facilities, and transport units) and continuous variables (e.g., hydrogen production and flow rates). This section also distinguishes the mono and multiobjective formulations. [Section 10.3](#) focuses on multiobjective optimization methods because they are well suited to the HSC problem. Special attention is paid to the chosen techniques. Some approaches for decision support orientation based on multicriteria decision aid following the multiobjective optimization step are also reviewed. At the end of this section we examine how the HSC design optimization framework can be linked with a spatially detailed infrastructure model. Finally, this chapter ends with some guidelines that can be useful for the practitioner.

10.2 METHODOLOGICAL FRAMEWORKS FOR SUPPLY CHAIN DESIGN

In the design and management of a supply chain, the best global performance should ideally be sought, so as to achieve better performance of a single link of the chain. The decisions that must be made involve different levels of the supply chain and need to be supported by robust tools to evaluate the impact of various decisions prior to implementing them in the real environment. In this context, system modelling is used to predict the behaviors of the supply chain as variations of network configurations. Supply chain modelling aims at minimizing or maximizing an objective function through the identification of decisions and tradeoff solutions that satisfy conflicting objectives at the same time, so that optimization approaches, which are generally based on mathematical models, are largely used to design supply chains (Akbul et al., 2014; Kim et al., 2011; Liu and Papageorgiou, 2013; Pishvaei et al., 2011).

10.2.1 General Decision Levels in a Supply Chain

Several decision levels are classically considered in a supply chain related to different time horizons:

- *Strategic planning*: this level refers to a long-term horizon (several years) and has the objective of identifying strategic decisions for a production network and defining the optimal configuration of a supply chain: capacity sizing, technology selection, sourcing, facility location, production allocation, and others. Future demands resource and management for the entire supply chain must be anticipated.
- *Tactical planning*: this level refers to a mid-term horizon (around 1 year) and has the objective of fulfilling demand and managing material flows, with a strong focus on the tradeoff between the service level and cost reduction: production allocation, supply chain coordination, transportation policies, inventory policies, safety stock sizing.
- *Operational planning*: this level refers to a short-term period (1 day to 1 year) and has the objective of determining material/logistic requirement planning: allocation of customer demands, vehicle routing, and plant scheduling.

10.2.2 Methods for Supply Chain (SC) Management and Design

Different methods and tools have been used and reported in the supply chain management (SCM) and design literature (see Table 10.1 for some examples) and are not specific to the HSC case.

The literature review shows that the most common approach in designing and modelling supply chains is optimization through mathematical models. As opposed to simulation based approaches, these models utilize formal

TABLE 10.1 Different Ways to Optimize SCM

Technique	Reference	Application
Linear programming	Kim et al. (2011)	Optimal design of biomass SC network under uncertainty, in the South-eastern region of the United States.
	Liu and Papageorgiou (2013)	Global process SC optimization problem, considering cost, responsiveness, and customer service level simultaneously.
	Perea-López et al. (2003)	Predictive control strategy to find the optimal decision variables to maximize profit in SC with multiproduct batch plants.
	Pishvaei et al. (2011)	Robust optimization model for handling the inherent uncertainty of input data in a closed-loop SC network design problem in business environment.
	Soylu et al. (2006)	Systematic approach to identify the synergy among different energy systems.
	Tsiakis and Papageorgiou (2008)	Optimal configuration of a production and distribution network subject to operational and financial constraints.
	van Dyken et al. (2010)	Biomass supply chain with different types and the relationship between moisture and energy.
Nonlinear programming	Akgul et al. (2014)	Model of carbon negative energy generation in the UK to examine the potential for existing power generation assets.
	Shabani and Sowlati (2013)	SC configuration of a typical forest biomass power plant.
Dynamic programming (DP)	Buffett and Scott (2004)	Optimization of the inventory level and minimization of the total cost.
	Choi et al. (2006)	A multiproduct supply chain under demand uncertainty.
	Gigler et al. (2002)	DP model for an agricultural chain of willow biomass fuel to an energy plant.
Markov chains	Busse et al. (2012)	Price interdependencies between the German biodiesel and related agricultural and energy markets.
	Kurata and Liu (2007)	Determination of the frequency of the price discount, including or excluding a supplier's inventory decision.

TABLE 10.1 Different Ways to Optimize SCM—cont'd

Technique	Reference	Application
Analytical hierarchy (AH)	Haq and Kannan (2006)	Evaluation of vendor selection in a company in the southern part of India.
Analytical network process (ANP)	Agarwal et al. (2006)	SC encapsulating market sensitiveness, process integration, information driver and flexibility measurement.
	Tseng et al. (2009)	Novel hierarchical evaluation framework to assist the expert group for optimal supplier selection in SC management strategy.
Network equilibrium model	Nagurney and Toyasaki (2005)	Reverse supply chain management of electronic waste, including recycling.
Game theory	Bai et al. (2012)	SC design incorporating farmers' decisions on land use and market choice into the biofuel.
Fuzzy and neuro-fuzzy	Shaw et al. (2012)	Integrated approach for selecting the appropriate supplier in the supply chain, addressing the carbon emission issue.

optimization techniques to allow advanced decisions to be captured and to provide comprehensive integrated solutions ([Hugo et al., 2005](#)). The aim of such methods is to find optimal configurations according to some specific criteria (e.g., economic, safety, environmental aspects). One of the main advantages of this type of modelling is that mathematical models form a bridge to the use of high-powered mathematical techniques and computers to analyze the problems ([Hillier and Lieberman, 2001](#)).

The use of mathematical programming for designing a supply chain consists of three major steps as reported in [Grossmann et al. \(2000\)](#):

- i. The representation of all possibilities from which the optimal solution is extracted by defining the so-called superstructure; a superstructure is defined as the set of all possible connections in a network.
- ii. The formulation of a mathematical model includes generally discrete and continuous variables. The main components of a model are:
 - (a) the optimization criteria, which are expressed as mathematical functions, and
 - (b) the constraints, which can be either of the equality or inequality type.
- iii. The resolution of the mathematical model to determine one or more optimal solutions.

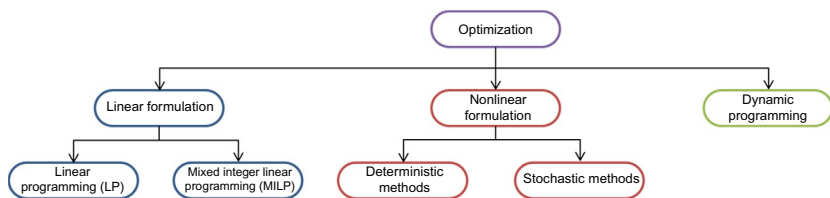


FIG. 10.1 Classification of the main methods of optimization (Adapted from Collette, Y., Siarry, P., 2003. *Multiobjective Optimization: Principles and Case Studies*. Springer.)

Traditionally, the main focus of the research studies dedicated to supply chains has been minimizing the overall cost or maximizing the total revenue as a single-objective optimization problem.

The most common optimization frameworks for capturing SC problems are summarized in Fig. 10.1. These can be classified as either *linear* or *nonlinear programming* or *dynamic programming*. Initially, the majority of these studies were based on a monoobjective formulation.

10.2.2.1 Linear Formulation

A linear formulation is used when the problem (objective functions and constraints) is linear (Hillier and Lieberman, 2001). Two methods can be used, linear programming (LP) and mixed integer linear programming (MILP).

- LP models are used for the efficient allocation of limited resources in known activities in order to meet the desired goals (for instance, maximizing profits or minimizing costs). Linear programming problems can involve decision variables that can take integer values. When integer variables are restricted to the binary variables (0–1), the corresponding problem is called the *binary integer programming problem*. An integer variable can be defined such that it determines whether a processing unit should be invested in or not.
- In the case of both integer and continuous variables, the problem is referred as a mixed-integer linear programming one. Because of its capability to naturally capture logical conditions, applications of MILP have been widespread in areas of investment planning, supply chain, and logistics management, energy industry planning, engineering design, and production scheduling (Hugo et al., 2005). MILP methods consist of maximizing or minimizing an objective function as a function of parameters, variables, and several constraints on these variables (Haeseldonckx and D’haeseleer, 2011).

The use of *integer variables* in general, and binary ones in particular, dramatically broadens the capabilities of linear programming modelling, enabling the

disjunction of constraints, the logical implication and general restrictions to the model incorporating certain nonlinear behaviors of reality. Many practical optimization problems lead to the consideration of an extremely large number of feasible solutions, so that the problem can be viewed as a combinatorial one.

The solution of the system of linear equations that are involved in the problem formulation can be performed by using the Gauss-Jordan method. When problems become larger (more parameters, variables and constraints), the Gauss-Jordan method is generally combined with a branch-and-bound method in order to converge to an optimal solution as quickly as possible (Haeseldonckx and D'haeseleer, 2011).

Mathematically, the MILP problem can be expressed as follows:

$$\text{Min } cx + dy$$

subject to

$$Ax + By \geq b$$

$$L < x < U$$

$$y = \{0, 1, 2, \dots\}$$

where x is a vector of variables that are continuous real numbers, and y is a vector composed of variables that can only take integer values. In this expression, $cx + dy$ is the objective function, and $Ax + By \geq b$ represents the set of constraints. L and U are vectors of lower and upper bounds on the continuous variables, and $y = \{0, 1, 2, \dots\}$ represent the integer variables.

With regard to the solution of the MILP problems, several algebraic modeling languages (AML) were developed with the aim of allowing users to express LP and other optimization problems in a natural, algebraic form similar to the original mathematical expressions, such as AIMMS, AMPL, GAMS, etc. For instance, GAMS includes well-known algorithms for the solution of MILP (Geletu, 2008): Branch & Bound, Benders Decomposition, Cutting Plane (Gomory) algorithm and Branch & Cut. Usually these algorithms are used in combination with the simplex algorithm and/or the interior-point method. For instance, some of the solvers that can solve MILP problems are BARON, BDMLP, LINDO GLOBAL, MOSEK, OSL, XPRESS, and CPLEX (Mansini et al., 2015).

It must be highlighted that linear programming is the most used technique to optimize the SC. Several applications can be found, such as biomass supply chains (Kim et al., 2011; van Dyken et al., 2010), the optimization of the SC under financial constraints (Liu and Papageorgiou, 2013; Tsiakis and Papageorgiou, 2008), in energy systems (Soylu et al., 2006), in business environment (Pishvaei et al., 2011), or in multiproduct batch plants (Perea-López et al., 2003).

10.2.2.2 Nonlinear Formulation

The nonlinear formulation can be tackled by two main methods, either *deterministic* or *stochastic* algorithms procedures. In the nonlinear deterministic models, no randomness is associated. Then, given a particular input, a deterministic algorithm obviously produces the same type of output (Prawda, 2004).

- Mixed integer nonlinear programming (MINLP) refers to mathematical programming with, on the one hand, continuous and discrete variables, and, on the other hand, nonlinearities in the objective function(s) and constraints. The use of MINLP is a *deterministic* approach of formulating problems where it is necessary to simultaneously optimize the system structure (discrete variables) and its parameters (continuous variables). MINLP problems are difficult to solve because they combine all the difficulties of both of their subclasses: the combinatorial nature of mixed integer programs and the difficulty in solving nonconvex (and even convex) nonlinear programs (Bussieac and Pruessner, 2003).

The general form of a MINLP is:

$$\text{Min } f(x, y)$$

subject to

$$g(x, y) \leq 0$$

$$x \in X$$

$$y \in Y$$

The function $f(x, y)$ is a nonlinear objective function and $g(x, y)$ a nonlinear constraint function. The variables x , y are the decision variables, where y is required to be an integer vector. X and Y are bounding-box-type restrictions on the variables. Nonlinear formulations with mathematical MINLP can be found in Akgul et al. (2014) and Shabani and Sowlati (2013).

- *Stochastic programming* is used when random-valued parameters and objective functions subject to statistical perturbations are part of the problem formulation (Coello et al., 2007). The stochastic models can incorporate uncertainty in parameters, such as demand, costs, potential sites, and distances, and then fall into probabilistic approaches and scenarios (Patay, 2008). Metaheuristics cannot guarantee that an optimum can be obtained. The stochastic methods are divided into neighborhood techniques, such as Simulated Annealing, Tabu Search, and evolutionary algorithms, and among others genetic algorithms, evolutionary strategies, and evolutionary programming (Tabkhi, 2007).

10.2.2.3 Dynamic Programming

Dynamic programming (DP) is an optimization approach that changes a complex problem into a less complex one by separation of the problem into simpler and smaller problems (Bellman and Dreyfus, 1962; Momoh, 2008). The method

used by dynamic programming is recursive, which means that the method calls itself, adding information each time, until the conditions of stopping are met.

According to [Chinneck \(2006\)](#), the method steps are the following ones:

1. Dividing the problem into small problems and finding the optimum solution for each small problem.
2. Enlarging the small problem and finding the optimum solution to the next problem using the previously found optimum solution.
3. Continuing with the second step until the enlarged problem encompasses the entire original problem.
4. Tracking back the solution of the entire problem from the optimum solutions to the small problems solved along the way.

The requirements of this technique are ([García and Moreno, 2000](#)):

- The solution to the problem must be reached through a sequence of decisions, each one in each step.
- Such sequence of decisions must satisfy the optimum principle.

Several works using dynamic programming for supply chain problems have been reported in the dedicated literature. [Williams \(1983\)](#) develops a dynamic programming algorithm for simultaneously determining the production level and distribution batch sizes at each node within a supply chain network.

[Buffett and Scott \(2004\)](#) propose a technique for use in supply chain management that assists the decision making process for purchase of direct goods. Based on projections for future prices and demand, request-for-quotes (RFQs) are constructed and quotes are accepted that optimize the level of inventory each day, while minimizing total cost. The problem is modeled as a Markov decision process (MDP) and Dynamic programming is then used to determine the optimal quote requests and accepts at each state in the MDP.

A similar approach has been adopted by [Choi et al. \(2006\)](#) for multiproduct supply chains under uncertainty modelled through Markov chains. They use an approach based on stochastic dynamic programming (DP), which can generate a dynamic operating policy that incorporates information about the uncertainty in the problem at each time step.

[Gigler et al. \(2002\)](#) have also developed a methodology for optimization of agricultural chains using DP, taking into account quality development of a product as a function of the process conditions. The methodology optimizes the route of the chain that returns the minimum integral cost. DP has been firstly applied to a supply chain of bananas (four stages) and then to a chain of willow biomass fuel to an energy plant (7 stages).

Even if dynamic programming is a very elegant framework for analyzing supply chain systems, it is mostly used at a theoretical level to characterize the optimal policy. This approach is yet limited in its applicability; as the number of state variables increases, the state space size grows exponentially, a phenomenon known as the curse of dimensionality, rendering the standard dynamic programming approach impractical.

10.2.2.4 Other Methods for Supply Chain Modelling

In contrast to optimization methods, many researchers have developed an equilibrium model of competitive supply chain networks (Nagurney et al., 2002). The *equilibrium model* captures both the independent behavior of the various decision makers as well as the effect of their interactions. The equilibrium model is drawn from economics and, in particular, from network economics. Nagurney et al. (2002) developed a supply chain network equilibrium model for the case of consumers demand for the product that can be expressed as a deterministic function.

- *Queuing models*, such as *Markov chains*, have also been used to investigate supply chain problems for many years (e.g., Toktaş-Palut and Ülengin, 2010), in the determination of biodiesel prices (Busse et al., 2012) or discounted prices (Kurata and Liu, 2007).

Markov chains can be described as follows. Let us denote S a set of states, $S = \{s_1, s_2, \dots, s_r\}$. The process starts in one of these states and moves successively from one state to another. Each move is called a step. If the chain is currently in state s_1 , then it moves to state s_j at the next step with a probability denoted by p_{ij} , and this probability does not depend upon the states the chain was in before the current state. In some SCs, the probabilities are used to model the times of some tasks.

- *Game theory* can be defined as “the study of mathematical models of conflict and cooperation between intelligent rational decision makers.” It provides general mathematical techniques for analyzing situations in which two or more individuals make decisions that will influence one another’s welfare (Myerson, 2013). In SC, for example, Majumder and Groenevelt (2001) present a two-period model of remanufacturing. An original equipment manufacturer competes with a local remanufacturer under many reverse logistics configurations. Another example is support in the decision between land use and market choice for biofuel (Bai et al., 2012).
- *Neural networks* and *fuzzy systems* combine the advantages of fuzzy systems (e.g., interpretability, use of vague or inexact data) with the learnability of neural networks, so that the parameters of fuzzy systems can be learnt by neural networks according to existing requirements. In Marx-Gomez et al. (2002), fuzzy logic is used to forecast the prognoses for the amount of time of returned product, and in Shaw et al. (2012) to select the correct supplier.

10.2.2.5 Multiobjective Formulation

Multiobjective optimization is now a popular approach to modelling supply chains, especially green supply chains (Srivastava, 2007), and in particular for sustainable design of distributed energy supply systems because it allows for the antagonistic objectives of economic and environmental performance

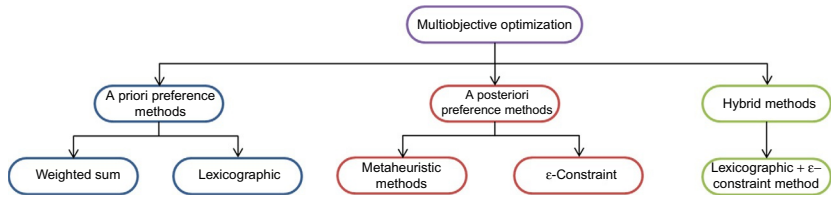


FIG. 10.2 Multiobjective optimization methods.

to be evaluated and optimized simultaneously. Tradeoff solutions are found through this approach giving the decision makers a way to incorporate many objectives and preferences in a single decision framework.

The general formulation of a multiobjective optimization problem is:

$$\text{Min } [f_1(x), f_2(x), \dots, f_k(x)]$$

subject to

$$g(x) \leq 0$$

$$h(x) = 0$$

$$x \in S$$

where f_i (with $i = 1$ to k) is a function of $R^{n1} \times [0, 1]^{n2}$ in R , $g(x) \in R^m$, $h(x) \in R^p$ and x is an element of S . $R^{n1} \times [0, 1]^{n2}$ in R .

Such an optimization scheme is implied when there is a conflict between two or more objectives, even if the most profitable infrastructure may not necessarily be the least environmentally damaging. Because of this tradeoff, there is no single solution to this class of problem, but rather a set of nondominated solutions called *Pareto front*. A solution belonging to the Pareto front is said to be Pareto-optimal if there are no other solutions that can better satisfy all of the objectives simultaneously and any improvement in one objective leads to the worsening of at least one other objective.

Several solution methods have been developed for multiobjective optimization problems and can be classified as the a priori, a posteriori, and *hybrid* methods (Collette and Siarry, 2003), including scalar, interactive, fuzzy, and meta-heuristic methods (see Fig. 10.2).

A Priori Preference Methods

With these methods, the decision maker defines the tradeoff to be applied (preferences) before running the optimization method. The aggregative methods belong to this family (in which the objective functions are gathered into one objective function). More precisely, the weighted sum, goal programming, and lexicographic methods (among others) can be mentioned (Collette and Siarry, 2003). The drawback is that the decision maker never sees the whole

picture (the set of efficient solutions). Hence, the most preferred solution is “most preferred” in relation to what the decision maker has for comparison so far (Mavrotas, 2007, 2009).

- *Weighted sum*

The goal of the weighted sum is to transform the problem so that it turns into a monoobjective optimization problem, for which various methods of solution exist. The simplest way to proceed is to take each objective function, associate a weight with the objective function, and then take a weighted sum of objective functions. Hence, a new, unique objective function is obtained. The weighting factors are assigned a priori, and are modified to obtain the Pareto front, with all nondominated solutions (or satisfactory solutions). The major problem with this method is the variation of the weighting factors, which often leads to Pareto fronts with a low density of solutions (Hernandez-Rodriguez, 2011). It can be used only when the feasible space of values of the objective function is convex. In the weighting method, the weighted sum of the objective functions is optimized. The problem is stated as follows:

$$\text{Min } (w_1 \times f_1(x) + w_2 \times f_2(x) + \dots + w_p \times f_p(x))$$

subject to

$$g(x) \leq 0$$

$$h(x) = 0$$

$$x \in S$$

By varying the weights w_i it is possible to obtain different efficient solutions.

- *Lexicographic method*

Lexicographic problems arise naturally when conflicting objectives exist in a decision problem but for reasons outside the control of the decision maker, the objectives have to be considered in a hierarchical manner (Khorram et al., 2010). This method can be viewed as an “a priori” approach with aggregation using constraints in a decoupled method. In the lexicographic ordering, the objectives are ranked according to the order of importance. The optimization process starts minimizing the most important objective and proceeds according to the assigned order of importance of the criteria. An alternative is to randomly select an objective when there is no more rank available. One disadvantage of this method is that it tends to favor certain objectives, making the Pareto front converge to a particular region. The main advantage is its simplicity and computational efficiency, making it competitive with other ideas, such as weighted sum of objectives

(Collette and Siarry, 2003). In general, the lexicographic problem can be expressed as follows:

$$\text{Lexmin } \{f_1(x), f_2(x), \dots, f_r(x)\}$$

subject to

$$g(x) \leq 0$$

$$h(x) = 0$$

$$x \in S$$

To solve the problem, the following procedure, known as the sequential method, is adopted. First, $f_1(x)$ is minimized, and an optimal solution x^* is determined ($f_1(x^*) = \beta_1$). The problem is then solved minimizing $f_2(x)$ subject to $f_1(x^*) = \beta_1$, and so on at the q iteration:

$$\text{Lexmin } \{f_q(x) : f_i(x) \leq \beta_i, i = 1, \dots, q-1\}$$

subject to

$$g(x) \leq 0$$

$$h(x) = 0$$

$$x \in S$$

If either the last equation has a unique optimum or $q = r$, then its optimal solution is a preemptive optimum. Otherwise, one proceeds to iteration $q+1$ (Khorram et al., 2010).

A Posteriori Preference Methods

With these methods, the decision maker chooses the solution by examining solutions computed by the optimization model. Methods belonging to this family produce, at the end of the optimization, a tradeoff surface (Collette and Siarry, 2003). This kind of method produces many solutions, whereas only one will be chosen by the decision maker, and a lot of time may be invested to find the Pareto front. The value of using this kind of method within a multi-criteria optimization framework is that it does not require the a priori articulation of preferences by the decision maker. Instead, the aim is to generate the full set of tradeoff solutions and not to present only one single “best” alternative. From the set of alternatives, the decision maker can then further investigate interesting tradeoffs and ultimately select a particular strategy that satisfies his/her willingness to compromise (Hugo et al., 2005). In the a posteriori method, the solutions of the problem are generated and then the decision maker is involved, in order to select among them, the most preferred one.

- *Metaheuristic methods*

Metaheuristic methods can be used as a nonaggregative approach. They are particularly useful to treat problems known as “black box” ones in which no mathematical property of the problem is known (Boix, 2011). This category includes genetic algorithms, tabu search, simulated annealing, ant colonies, neural networks, etc. In the case of the HSC, this method has been rarely used (Nepal et al., 2011) because linear constraints and equality constraints (balance equations must be satisfied with a small tolerance, gap inferior to 0.001%) are involved in a major way in the formulation.

- *The ϵ -constraint method*

In the ϵ -constraint method, introduced by Haimes et al. (1971), all but one of the objectives are converted into constraints by setting an upper or lower bound to each of them, and only one objective is to be optimized (Liu and Papageorgiou, 2013). By varying the numerical values of the upper bounds, a Pareto front can be obtained. The ϵ -constraint technique fits into the family of “a posteriori” approaches with aggregation using constraints in a decoupled method (Collette and Siarry, 2003). This method presents some advantages compared to the a priori methods, for example, for linear problems, the weighting method is applied to the original feasible region and results in a corner solution (extreme solution), thus generating only efficient extreme solutions. Yet, the ϵ -constraint method alters the original feasible region and can produce nonextreme efficient solutions. An additional advantage of the ϵ -constraint method is that the number of the generated efficient solutions can be controlled by properly adjusting the number of grid points in each one of the objective function ranges.

In the ϵ -constraint method, one of the objective functions is optimized using the other objective functions as constraints, incorporating them in the constraint part of the model as shown below:

$$\text{Min } f_1(x)$$

subject to

$$f_2(x) \leq \epsilon_2$$

$$f_3(x) \leq \epsilon_3$$

$$f_p(x) \leq \epsilon_p$$

$$x \in S$$

By parametrical variation in the right-hand-side (RHS) of the constrained objective functions (ϵ_i), the efficient solutions of the problem are obtained. This method is yet easy to implement even if, in some cases, an intensive computation time is required.

However, one of its key disadvantages is that the generated solution largely depends on the selected vector ϵ (Liu and Papageorgiou, 2013).

The main difficulty of this method lies in determining Nadir points (in which the criteria are their worst values). To tackle this problem, a hybrid method can be used as the augmented ϵ -constraint method (AUGMECON) proposed by Mavrotas (2007, 2009).

Hybrid Methods

The works reported in Mavrotas (2007, 2009) shed new light on determining Nadir points combining the ϵ -constraint method with the lexicographic one. According to Liu and Papageorgiou (2013), the decision makers may not have any preference for any objective, that is, all the objectives are equally important. In this case, it is crucial to generate a fair solution in which all normalized objective function values are as close to each other as possible. In order to generate such solutions, the lexicographic can easily be coupled to the ϵ -constraint method.

The AUGMECON method (Mavrotas, 2007, 2009) is an effort to effectively implement the ϵ -constraint method for producing efficient solutions. To determine Utopia and Nadir points in the classical ϵ -constraint method, the most common approach is to take upper and lower bounds from the payoff table (the table with the results from the individual optimization of the p objective functions). In a minimization problem, the Nadir value is usually approximated with the maximum of the corresponding column. However, even in this case, it must be sure that the obtained solutions from the individual optimization of the objective functions are efficient solutions. In order to overcome this limitation, the AUGMECON method proposes the use of lexicographic optimization for every objective function in order to construct the payoff table with only efficient solutions. A simple remedy to bypass the difficulty of estimating the Nadir values of the objective functions is to define reservation values for the objective functions. The reservation value acts like a lower (or upper for minimization objective functions) bound. Values worse than the reservation value are not allowed.

10.2.2.6 Multiple Criteria Decision-Making Approaches

Designing sustainable supply chains requires complex decision support models that must deal with multiple dimensions of sustainability while taking into account specific characteristics of products and their supply chain. When the decision space involves continuous variables, multiobjective optimization techniques, such as mathematical programming problems with multiple objective functions, can be used as abovementioned. Yet multiobjective optimization techniques lead to a set of alternatives, among which the decision maker has to choose a solution for implementation purposes. In that context, multicriteria decision making (MCDM) that deals with discrete decision spaces where the decision alternatives are predetermined is a useful approach to quantify trade-offs between economic, social, and environmental criteria. The analysis of the

dedicated literature shows that the use of MCDM approaches for designing SCs is a rather new, but emerging, research field (Banasik et al., 2016). Many of the MCDM methods share the concepts of alternatives and attributes. A set of finite alternatives represent different choices of action available to the decision maker. Alternatives need to be prioritized with respect to the multiple attributes with which the MCDM problems are associated. Attributes are also referred to as goals or decision criteria, and may be in conflict with each other, may not be easily represented in a quantitative way and may be stochastic or fuzzy. Without being exhaustive, some of the most used MCDM methods are the following ones:

AHP/ANP: Analytic hierarchy process (AHP) is a pairwise comparison-based method proposed by Saaty (1980). An MCDM problem is first formulated as a hierarchy including several levels. The first level represents the goal, the second level shows the main decision criteria, the next levels show the subcriteria, and the last level indicates the alternatives. The elements of each level are compared in a pairwise fashion forming a pairwise comparison matrix.

The *analytic network process* (ANP) developed by Saaty (1996) is a multi-stage decomposition method used to solve decision making problems involving more than one criterion. It is a comprehensive decision making technique that captures the outcome of the dependence and feedback within and between the clusters of elements. Analytical hierarchy process (AHP) (Saaty, 1980) serves as a starting point for ANP. ANP consists of two steps, the first is a control hierarchy or network of criteria controlling the interactions and the second is a network of influences among the elements and clusters. It can be said that ANP uses a network without levels, as it is used in AHP (Ravi et al., 2005). Typically, in AHP the top element of the hierarchy is the overall goal for the decision model. ANP can treat complex problems with strong dependencies among factors (Sarkis, 1999).

ELECTRE: The ELECTRE (elimination and choice translating reality) method was introduced by Roy (1968). The basic concept of the ELECTRE method is to deal with “outranking relations” by using pairwise comparisons among alternatives under each one of the criteria separately. The decision maker is requested to assign weights or importance factors in order to express their relative importance. The ELECTRE method elicits the so-called concordance index, defined as the amount of evidence to support the conclusion that alternative A_j outranks or dominates alternatives A_i , as well as the discordance index, the counterpart of the concordance index. The ELECTRE method is sometimes unable to identify the most preferred alternative. It only produces a core of leading alternatives. This method has a clearer view of alternatives by eliminating less favorable ones. This method is especially convenient when there are decision problems that involve a few criteria with a large number of alternatives as it saves much time.

TOPSIS/M-TOPSIS: TOPSIS (Technique for Order Preference by Similarly to Ideal Solution) was developed by Hwang and Yoon (1981) as an alternative

to the ELECTRE method: the basic concept of this method is that the selected alternative should have the shortest distance from the Positive Ideal Solution (PIS) and the farthest distance from the Negative Ideal Solution (NIS) in a geometrical sense. Yet, one of the problems related to TOPSIS is that it can cause the phenomenon known as rank reversal (García-Cascales and Lamata, 2012), in which the alternative order of preference changes when an alternative is added to or removed from the decision problem.

Ren et al. (2007) presented a novel, modified TOPSIS (M-TOPSIS) method to evaluate the quality of the alternative and to deal the rank reversal problem. In M-TOPSIS, the positive ideal solution (D_i^+) and negative ideal solution (D_i^-) in finite planes are found (as in the TOPSIS Method) first and then the $D^+ D^-$ plane is constructed. D^+ is the x -axis and D^- is the y -axis. The point (D_i^+, D_i^-) represents each alternative ($i = 1, 2, \dots, n$). The point A ($\min(D_i^+), \max(D_i^-)$) is the “optimized ideal reference point.” Finally, the relative distance from each evaluated alternative to the ideal reference point (A) is calculated to determine the ranking order of all alternatives.

10.2.2.7 Supply Chain Network Design Under Uncertainty

Uncertainty in the supply chain is an issue that is difficult to deal with, and that increases the complexity of a supply network. Supply chain uncertainty can be defined by the lack of information about the environment of the supply chain, about the processing capacities or the lack of prediction of the impact of some control actions (van der Vorst and Beulens, 2002).

Three sources of uncertainty can be identified as upstream (supply) uncertainty, internal (process) uncertainty, and downstream (demand) uncertainty (Davis, 1993). Among these three sources, the demand is seen as the most severe parameter due to its volatile nature and the consequences of an inaccurate forecast. In addition, because some of the relevant technologies are still in the process of maturing, many important parameters, such as processing costs and yields, are highly uncertain. There are also uncertainties regarding the future course of energy policies, such as carbon taxes.

Grossmann and Guillén-Gosálbez (2010) reviewed major contributions in process synthesis and supply chain management, including the handling of uncertainty and the multiobjective optimization of economic and environmental objectives, and highlighted the need to develop sophisticated optimization and decision support tools to help in exploring diverse system alternatives under uncertainty.

The majority of the approaches to managing these sources of uncertainty seek to reduce uncertainty at its source, and to cope with it, thereby minimizing its impact on performance (Simangunsong et al., 2012).

Table 10.2 shows the different techniques to treat the uncertainty of the demand. Three distinct methods are frequently mentioned for representing uncertainty (Chen and Lee, 2004). First, the distribution-based approach, in

TABLE 10.2 Different Ways to Model Demand Uncertainty	
Technique	Reference
Scenario based approach	Tsiakis et al. (2001), Chen and Lee (2004), Almansoori and Shah (2012), Kim et al. (2008), Nunes et al. (2015)
Distribution based approach	Gupta and Maranas (2003), You and Grossmann (2008)
Demand generator	Jung et al. (2004)
Fuzzy based approach	Chen and Lee (2004), Peidro et al. (2009)
Spatially aggregated demand model	Dayhim et al. (2014)

which the normal distribution with specified mean and standard deviation is widely used for modelling uncertain demands and/or parameters. For example, You and Grossmann (2008) used normal distributions and triangular distributions to model the demand, transforming the disjunction of the triangular distribution into MINLP constraints. Second, in the fuzzy-based approach, the forecast parameters are considered as fuzzy numbers with accompanied membership functions. Third and finally, the scenario-based approach is a classical approach, in which several discrete scenarios with associated probability levels are used to describe the expected occurrence of particular outcomes. Yet, the creation of scenarios with their associated probabilities could be a problematic and cumbersome task, especially in real-life SC problems. Also, the use of an adequate number of scenarios could lead to a large-scale optimization problem that may be computationally time consuming.

The objective of any SCND under uncertainty is to achieve a configuration with a good performance even if uncertain parameters are involved. In general, the uncertainty sources include the existing uncertainty in parameters, such as supply, demand, and cost, that are inherently uncertain, and the uncertainty caused by natural or manmade disruptions (Govindan et al., 2017).

10.3 DESIGN OF HYDROGEN SUPPLY CHAINS

This section highlights the current trends for HSC design regarding the general context of supply chain modelling and the typical features of HSC.

Hydrogen-based energy systems have been widely studied and modelled (see Table 10.3). The dominant models used to describe them are supply chain models as opposed to equilibrium models and are quasi exclusively based on the MILP formulation.

TABLE 10.3 Taxonomy of HSC Studies

	Territorial Scale		Time Scale		Objective		Energy Source	Approach	Uncertain Parameters	Observations
	Region	Country	Monoperiod	Multiperiod	Monoobjective	Multiobjective				
Agnolucci et al. (2013)		Great Britain		9 (2020–2060)	Financial		Coal, Natural gas, Biomass (CCS), renewable	MILP		Development of a spatially-explicit MILP model, called SHIPMod (Spatial Hydrogen Infrastructure Mode)
Almansoori and Betancourt-Torcat (2016)		Germany	x		Financial		Natural gas, Coal (CCS), Biomass	MILP		
Almansoori and Shah (2006)		Great Britain	x		Financial		Natural gas, coal, biomass, other renewable sources	MILP		
Almansoori and Shah (2009)		Great Britain		5 (2005–2034)	Financial		Natural gas, coal, biomass, renewable	MILP		

Continued

TABLE 10.3 Taxonomy of HSC Studies—cont'd

	Territorial Scale		Time Scale		Objective		Energy Source	Approach	Uncertain Parameters	Observations
	<i>Region</i>	<i>Country</i>	<i>Monoperiod</i>	<i>Multiperiod</i>	<i>Monoobjective</i>	<i>Multiobjective</i>				
Almansoori and Shah (2012)		Great Britain		3 (2005–2022)	Financial		Natural gas, coal, biomass, other renewable sources	MILP	Demand	Demand uncertainty is modelled using scenario-based-approach
De-León Almaraz et al. (2013)		Great Britain	x			Cost, Ecological, Safety risk	Natural gas, coal, biomass	MILP		ε -constraint method for the multiperiod problem
De-León Almaraz et al. (2014)	Midi-Pyrénées	France		4 (2010–2050)		Cost, Ecological, Safety risk	Natural gas, photovoltaic, wind, hydro, nuclear	MILP		ε -constraint method for the multiperiod problem
Gondal and Sahir (2013)		Pakistan	x		Financial		Biomass	MINLP-GIS		
Guillén Gosálbez et al. (2010)		Great Britain		5 (5 years)		Cost, Ecological	Natural gas, coal, biomass	MILP		The Pareto front is obtained by the ε -constraint method

Han et al. (2013)		Korea	x			Financial, Ecological, Risk	Natural gas (CCS), renewable sources	Fuzzy multiple objective programming		
Hugo et al. (2005)	x			5 (2004–2038)		Financial, Ecological	Natural gas, coal, biomass, other renewable sources	MILP		The territorial scale is not specified, only defined as a “geographical region”
Kamarudin et al. (2009)		Malaysia	x		Cost		Natural gas, coal, biomass, water electrolysis	MILP		Two methods for demand determination: one based on the prediction of vehicle numbers and the other based on the supply of gasoline and diesel
Kim and Moon (2008)		Korea	x			Financial, Safety	Natural gas, renewable sources	MILP		The relative risk index proposed is based on the relative risks of individual components of hydrogen infrastructure

Continued

TABLE 10.3 Taxonomy of HSC Studies—cont'd

	Territorial Scale		Time Scale		Objective		Energy Source	Approach	Uncertain Parameters	Observations
	<i>Region</i>	<i>Country</i>	<i>Monoperiod</i>	<i>Multiperiod</i>	<i>Monoobjective</i>	<i>Multiobjective</i>				
Kim et al. (2008)		Korea	x		Financial		Natural gas, renewable sources	MILP	Demand	Demand uncertainty is modelled using scenario-based-approach
Li et al. (2008)		China		5 (2010–2034)		Financial, Ecological	Natural gas, coal, biomass, and other renewable sources	MILP		
Ochoa Robles et al. (2016)	Midi-Pyrénées	France		4 (2010–2050)		Cost, Ecological, Safety risk	Natural gas, renewable sources	Genetic Algorithms		
Samsatli et al. (2016)		Great Britain		4 (seasons)	Financial		Wind, renewable sources	MILP		
Sabio et al. (2010)		Spain		8		Financial Risk	Natural gas, coal (CCS), Biomass, other renewable sources	MILP	Fuel price	The uncertainty is associated to the operating costs

Woo et al. (2016)	Jeju Island	Korea		12 (months)	Financial		Biomass	MILP		A sensitivity analysis is conducted to provide insights into the efficient management of the B2H2 supply chain
Zhou et al. (2013)						Financial, Ecological		MINLP		The Pareto front is obtained by an adaptive weighted-sum method

A variety of potential hydrogen supply chain pathways can be found that make the problem original compared to more classical supply chain problems:

- the variety of feedstock and/or the major energy source from which the hydrogen is produced. These include fossil resources, such as natural gas and coal, as well as renewable resources, such as biomass with input from renewable energy sources (e.g., sunlight, wind, wave, or hydropower). The studied cases do not yet include all combinations of the factors. Intermittent technologies (wind, photovoltaics) can be used independently or in combination;
- the variety of technologies to produce (including chemical, biological, electrolytic, photolytic, and thermo-chemical) store and distribute hydrogen.
- the size of the facility at which the hydrogen is produced and the transportation requirements to deliver it to the customer;
- the state of the technology used, whether current or to be improved by future developments; most hydrogen and fuel cell technologies are still in the early stages of commercialization. The generation of hydrogen from fossil resources (such as natural gas), its transmission, distribution, and use within industry and the refining sector are based on mature technologies and applied on a large scale, and are not the main focus of this work, but meanwhile, they can help to build early markets and infrastructure. Major differences in the degree of maturity of some technologies must be highlighted; although alkaline electrolyzers are a mature and affordable technology, PEM and SO electrolyzers show a greater potential to reduce capital costs and to increase efficiency;
- differences also exist, for example, whether or not the carbon dioxide (CO₂) byproduct is sequestered when hydrogen is produced from fossil fuel;
- various markets with multiple uses (mobility, power, industry, buildings, and others);
- multiple stakeholders: policy and government decision makers, strategic investors, stakeholders of hydrogen technologies for production, distribution, and storage.
- integration of different geographical scales: regional and national levels to develop hydrogen solutions.

10.3.1 Problem Formulation for HSC Design

As presented in [Table 10.3](#), several methods can be chosen to present the taxonomy of HSC problems. Following the guidelines of the general presentation on SC modelling, some typical features of HSC are highlighted in what follows.

10.3.1.1 Deterministic Optimization Approaches for HSC Design

Not surprisingly, following the general trends that have been previously observed for SC problems, the optimization formulation is the classical way

to tackle HSC design with a specific focus on MILP, as can be observed in [Table 10.3](#). The inputs of such models are constituted by a set of options for the production, storage, and transportation, while the outputs are relative to the type, numbers, location, and capacity of the production, storage, and transportation.

The network design problem can be characterized according to different levels of interest:

- type of problem: location, allocation, routing, location-allocation, location routing,
- planning level considering the strategic, tactical, or operational aspects,
- temporal dimension, for example, either static or dynamic,
- type of data (deterministic, stochastic),
- type of approach (optimization, simulation),
- time horizon (short, medium, or long term),
- geographic dimension according to the problem definition.

It must be emphasized that the application of hydrogen to vehicle use serves as an incentive to deploy HSC. Several energy sources are generally considered, whether based on fossil fuels or renewable origins.

The model developed in [Almansoori and Shah \(2006\)](#) can be considered as a precursor model to the optimal design of a network (production, transportation, and storage) for vehicle use in which the network is demand driven. The model was applied to a case study in Great Britain. The model was then extended in 2009 by the same authors ([Almansoori and Shah, 2009](#)) to consider the availability of energy sources and their logistics, as well as the variation of hydrogen demand over a long-term planning horizon, leading to phased infrastructure development as well as the possibility of selecting different scales of production and storage technologies. Other works ([Almansoori and Shah, 2012](#)) take into account demand uncertainty arising from long-term variation in hydrogen demand using a scenario-based approach. The model adds another echelon, including refueling stations and local distribution of hydrogen, minimizing the total daily cost.

[Guillén Gosálbez et al. \(2010\)](#) design an HSC for vehicle use. The design task is formulated as a bi-criterion MILP problem. A case study in Great Britain is introduced to illustrate the capabilities of the proposed approach. The model optimizes an economic and environmental objective. The economic objective is given by the total discounted cost, and the environmental impact is measured by its contribution to climate change. The problem is decomposed into two levels. The first level is represented by the original MILP model, while the second level refers to the original problem without the variables of production and storage facilities, adding some binary variables to represent the selection of the different technologies. The advantage of this methodology is the reduction of combinatorial complexity of the problem, and thus, its computational effort.

Sabio et al. (2010) also design an HSC for vehicle use. The objective is to determine the optimal design of the production-distribution network. The model is formulated as an MILP problem, controlling the variation of the economic performance of the hydrogen network. A case study in Spain is applied. The uncertainty in the fuel price is introduced into the operating costs of the network.

Recent models have been focusing on the integration of carbon capture and storage technologies, as well as on the utilization of pipelines, resulting in several scenarios of centralized HSCs using fossil fuels instead of renewable energies, if CCS technology is available. One example is the SHIPMod developed by Agnolucci et al. (2013), that is an optimization-based framework involving a multiperiod spatially-explicit MILP formulation, for the design of HSC and CCS pipeline networks over a long planning horizon. These authors have highlighted that varying the level and the spatial pattern of demand has significant impacts on both the optimal supply system and on the overall costs of delivered hydrogen. In the work of Moreno-Benito et al. (2016), the SHIPMod model has included additional options, such as hydrogen imports in the United Kingdom for a multiperiod problem until 2070 in order to minimize the present value of the total infrastructure cost using a discounted cash flow analysis. These works have also developed a hierarchical procedure to reduce the computational time by initializing the solutions in a two-stage approach.

Almansoori and Betancourt-Torcat (2016) propose an approach for the design of the HSC under emission constraints, taking into account the use of carbon capture storage. The problem is formulated as an MILP model. The objective to be optimized is the total network cost, and it was applied to the future supply chain in Germany in the year 2030, showing that the carbon emission target and CO₂ tax are effective strategies for reducing emissions.

Samsatli et al. (2016) present a model that integrates wind-hydrogen electricity networks using an MILP formulation, comprising wind turbines, electrolyzers, fuel cells, and compressors. Some constraints linked to the installation of wind turbines were added. The objective is the total cost of the network, and it was applied in Great Britain, showing the optimal path to install the pipeline network throughout the country.

Some reported works for the optimal design of an HSC involve a mixed integer nonlinear programming (MINLP) formulation. Most of the problems of optimization of the HSC are MINLP because of the nonlinear nature of the objectives, more particularly, the cost objective. For example, Zhou et al. (2013) study the environmental impact of hydrogen consumption, especially the greenhouse gas (GHG) emissions, and propose a hydrogen network integration (HNI) for refinery hydrogen management. They present a systematic mathematical modelling methodology for the optimal synthesis of sustainable refinery hydrogen networks. The proposed mixed integer nonlinear programming (MINLP) model accounts for both the economic and the environmental aspect of the hydrogen network. The total annual cost is employed to evaluate

the economic efficiency of the network, while the environmental performance is assessed by the total CO₂ emission of the network. A multiobjective optimization is carried out via the Pareto front generation, which is obtained by an adaptive weighted-sum method. Then a superstructure-based mixed integer optimization methodology is proposed for the integration of the hydrogen network integration aimed at balancing the economic and environmental objectives for sustainable development.

10.3.1.2 Multiobjective Optimization and MCDM

Initially, HSC modelling was mainly tackled by monoobjective optimization (see Table 10.3). In these studies, the objective to be considered has been based on cost considerations. Considering a multiobjective formulation, the problem decision support for HSC design will have to encompass cost consideration, environmental impact, and risk, for which several models exist, such as life cycle costing (LCC), life cycle assessment (LCA), and risk assessment (RA). The literature analysis shows that only significant criteria belonging to each category are considered in the methodological frameworks developed.

Environmental impact in terms of life cycle assessment (LCA) has been considered by Guillén Gosálbez et al. (2010). The risk of combustion or explosion of leaked H₂ in hydrogen infrastructure has been investigated in several studies (Kim and Moon, 2008; Landucci et al., 2010; Rosyid et al., 2007). Kim et al. (2008) have integrated the safety hazard risks with the economic cost of hydrogen supply chains.

The literature survey also reveals that the multiobjective optimization problem is often solved with an ϵ -constraint method, or less frequently with the weighted-sum method (Zhou et al., 2013), and produces Pareto-optimal curves that reveal the tradeoffs among the three objectives.

Guillén Gosálbez et al. (2010) proposed a bi-criterion formulation that considers simultaneously the total cost and life cycle impact of the hydrogen infrastructure and developed an efficient solution method that overcomes the numerical difficulties associated with the resulting large-scale MILP. More precisely, the cost criterion is represented by the total discounted cost, calculated as the summation of the discounted costs associated with each time period, whereas the environmental impact is measured through its contribution to climate change.

Hugo et al. (2005) represents the financial objectives as the Net Present Value (NPV) and the environmental objective as the greenhouse gas (GHG) emissions. These authors have developed an optimization-based formulation that investigates different hydrogen pathways in Germany. The model identifies the optimal infrastructure in terms of both investment and environmental criteria for many alternatives of H₂ configurations. This model has been extended and considered as a basis for other works (Li et al., 2008) for a case study in China. At the same time, in Iran, Qadrdan et al. (2008) examined a model

for the investigation of an optimal hydrogen pathway and the evaluation of the environmental impacts of the hydrogen supply system. Another study also considered hydrogen from water, using electricity from hydro and geothermal power in Iceland for exportation (Ingason et al., 2008).

Sabio et al. (2011) take into account eight environmental indicators in a two-step method based on a combination of MILP multiobjective optimization with a postoptimal analysis by principal component analysis (PCA) to detect and omit redundant environmental indicators.

The work of Dagdougui (2011) describes the risk hazards (delimitation and explanation of potential risks in some parts of the hydrogen infrastructure: pipeline and storage tank) to demonstrate the consequences of a hydrogen accident in the case of future infrastructure operation. The risk is integrated into the HSC to minimize the global risk to population and the environment. The model is applied to regional case studies in the region of Liguria (North of Italy) and Morocco. A GIS based methodology was coupled based on the clean feedstock for hydrogen production. Then, the minimization of the cost of installation of new onsite hydrogen refueling stations, the cost of conversion of existing gasoline to hydrogen stations, and the cost of transporting hydrogen fuel to offsite stations is taken into account. The objective of this work was to develop a decision support system for the localization of hydrogen refueling stations, considering the potential of production within a specific boundary region.

The work of De-León Almaraz et al. (2013) involves a formulation-based on mixed integer linear programming with a multicriteria approach in which three objectives have to be optimized simultaneously, i.e., cost, global warming potential, and safety risk, either at the national or regional scale. This problem is solved by implementing lexicographic and ϵ -constraint methods. The solution consists of a Pareto front, corresponding to different design strategies in the associated variable space. Multiple choice decision making based on M-TOPSIS (Modified Technique for Order Preference by Similarity to Ideal Solution) analysis is then selected to find the best compromise. The mathematical model is applied to a case study in Great Britain reported in Almansoori and Shah (2006) for validation purposes, comparing the results between the mono and multiobjective approaches. In the regional case, the modelling and optimization of the HSC in the Midi-Pyrénées region was carried out in the framework of the project “*H₂ as a green fuel*” (see Fig. 10.3). The sensitivity of geographical scale was analyzed in De-León Almaraz et al. (2014) to solve a real problem of the HSC in the former “Midi-Pyrénées” region in France. In order to analyze the economies of scale and the real geographical implications, a comparison between a regional and a national case for France is discussed in De-León Almaraz et al. (2015).

The decision making trial and evaluation laboratory (DEMATEL) method, used to study and solve the complicated and intertwined problem group, has been used by Ren et al. (2013) to analyze the cause-effect relationships among the factors that influence the sustainability of hydrogen supply. The interest of

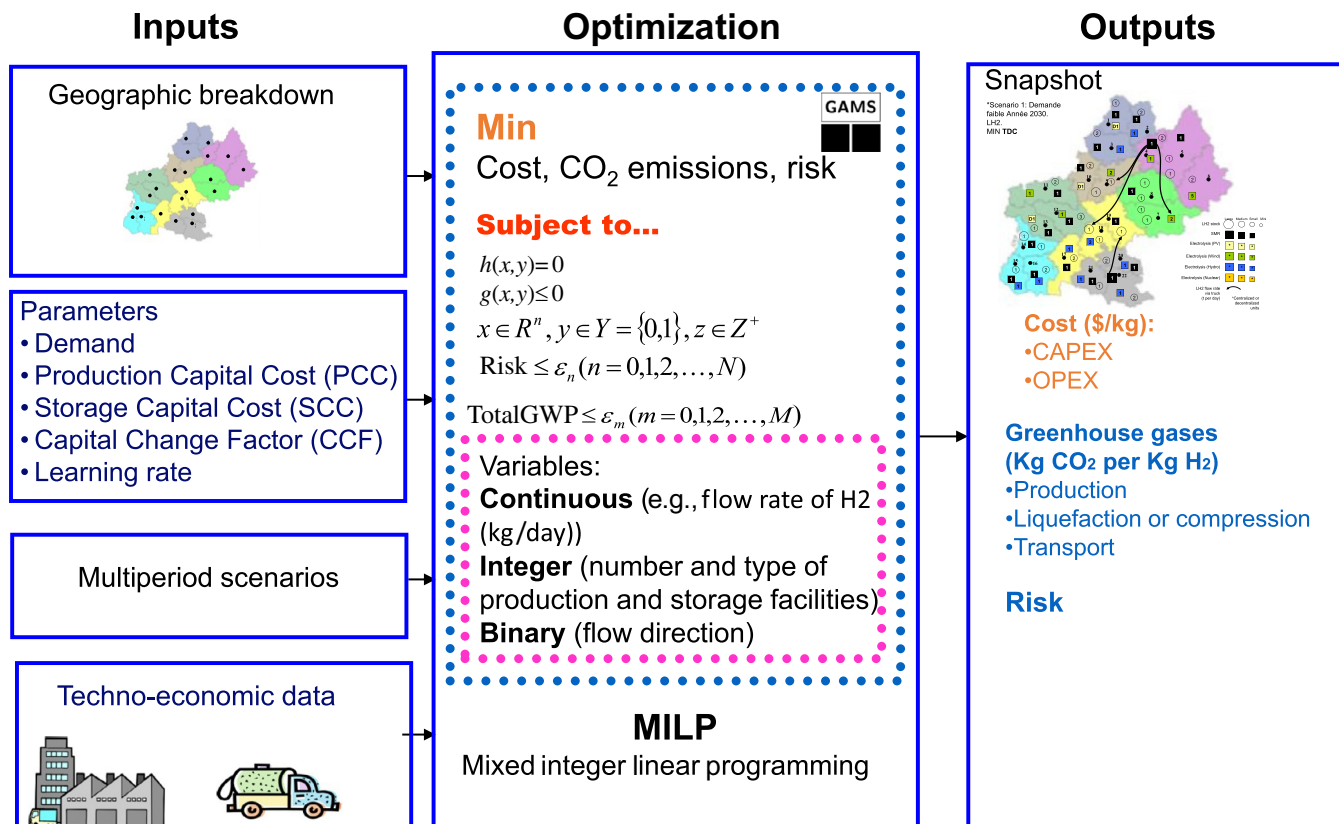


FIG. 10.3 Methodology framework for the “Green H₂ fuel” project (Midi-Pyrénées).

this method, based on graph theory, is to divide multiple criteria into a cause-and-effect group, and the causal relationships in a network relationship map. Four aspects were evaluated: economic, technological, environmental, and societal. A study case was developed in China, and the results are consistent with the current conditions.

Although the weighted-sum method and the ϵ -constraint method are the most used when solving multiobjective problems, it must be emphasized that assigning a set of compatible objectives, as cost efficiency and safety level, is difficult without knowledge of their possible values (Han et al., 2013), leading to a vague final objective and thus an invalid solution. To overcome this difficulty, fuzzy linear programming with multiple objectives constitutes an interesting alternative. In general, in a fuzzy set methodology, it is assumed that there may be a fuzzy goal for each of the objective functions (Sakawa, 2012). The fuzzy set concept can be adopted to provide a clearer theoretical analysis than the others methods (Han et al., 2013). The fuzzy set method consists of minimizing the distance between the ideal and the desired solutions. Following this approach, Han et al. (2013) designed the HI (H₂ infrastructure) considering economic cost efficiency, safety, and low CO₂ emissions simultaneously. An optimization modelling approach is thus proposed to address such multiple objectives in the HI design. The proposed model employs fuzzy multiple objective programming to compute a compromising solution among multiple objectives. Three objective functions are considered: (1) minimization of the total supply cost of the H₂ of the HSC, (2) minimization of the total relative risk of the HSC, (3) minimization the total mitigation cost of CO₂ for the HSC.

The potential of genetic algorithms (GA) via a variant of NSGA-II has also been explored to cope with the multiobjective formulation, in order to produce compromise solutions automatically (Ochoa Robles et al., 2016). In this work, cost and global warming potential have been simultaneously optimized so that the Pareto Front has been directly obtained. The interest of such an approach is that nonlinearities that may be involved in the formulation of the HSC problem can also be taken into account with a generic framework.

10.3.1.3 *Multiperiod Nature*

Initially, static models for HSC were developed (Agnolucci et al., 2013; Almansoori and Betancourt-Torcat, 2016; Almansoori and Shah, 2006, 2009, 2012; Gondal and Sahir, 2013; Kamarudin et al., 2009; Kim et al., 2008; Samsatli et al., 2016). Beyond these static models, planning models over multiple periods have been developed. HSC design has to be considered under dynamic conditions with demand exhibiting different realization at each period from deployment to maturity. This is generally modelled through a multiperiod approach in which the demand profiles vary from one period to another, capturing market dynamics.

In energy supply planning and design, coupling between investment/design decisions and operating decisions constitutes an interesting challenge due to the multiscale nature of the problem. Capacity investment and design decisions are typically made on a much longer time scale than operation decisions, while the operation of existing capacities requires decisions on a much faster time scale. The coupling between these decisions makes the overall decision problem a multiscale one (Lee, 2014).

10.3.1.4 HSC Supply Chain Uncertainty

Stochastic modelling tools are classical approaches to the incorporation of different sources of uncertainty into the decision making process. The demand has been the most studied source of uncertainty (Almansoori and Shah, 2012; Chen and Lee, 2004; Dayhim et al., 2014; Gupta and Maranas, 2003; Jung et al., 2004; Kim et al., 2008; Nunes et al., 2015; Peidro et al., 2009; Tsiakis et al., 2001; You and Grossmann, 2008), whereas other uncertainties, especially those appearing in the coefficients of the objective function (product prices, operating cost, etc.) have received much less attention (Sabio et al., 2010).

Traditionally, stochastic models that consider the variability of the uncertain parameters typically optimize the expected economic performance of the system. These approaches can lead to solutions that perform well on average but have a high probability of unfavorable solutions.

The modelling of the uncertainty represents a major issue in the HSC because it deals with the lack of information or forecasts due to the novel nature of the network.

For example, to solve the stochastic mathematical model, the scenario-based approach is employed in Kim et al. (2008). The scenarios emerge from the assumption that the hydrogen demands are “above average,” “average,” or “below average.” Numerically, “above average” and “below average” scenarios are assumed as +20% and −20% of the average values, respectively. First-stage decisions are generally hydrogen production quantities. All the other decision variables are considered as second-stage decisions, which are defined for each scenario.

Nunes et al. (2015) propose the sample average approximation (SAA) technique to manage the large number of scenarios, which enables the calculation of estimates for the objective function value using Monte Carlo simulations while providing statistically certified quality. This technique consists of repeatedly optimizing a set of random sample scenarios, generating different possible solutions for the problem. Then, these solutions are evaluated using new scenarios to allow the calculation of the statistical properties, evaluating their quality regarding the optimality of the problem.

The previous studies of Almansoori and Shah (2012) and Dayhim et al. (2014) proposed to represent the logistic infrastructure, considering the uncertainty in the demand forecast and sought to evaluate different investment

alternatives. Comparing the new model with that presented by [Almansoori and Shah \(2012\)](#), there is a reduction in the number of variables, which illustrates the effect of the proposed reformulation of the mathematical model and the data analysis performed.

10.3.1.5 Sensitivity Analysis

The parameter values and assumptions of any model are subject to change and error. Sensitivity analysis is the investigation of these potential changes and errors and their impacts on conclusions to be drawn from the model ([Pannell, 1997](#)).

A detailed sensitivity analysis using design of experiments methodology is presented in [Ochoa Robles et al. \(2015\)](#). The importance of hydrogen demand is significantly highlighted, because this factor strongly conditions the optimization criterion of the HSC model. Because the demand for the future HSC is not yet known, its uncertainty is an important issue to be taken into account. The Production Capital Cost is, at a lower level, another significant factor on hydrogen production cost.

[Woo et al. \(2016\)](#) present a new optimization-based approach for design and operation of a renewable hydrogen system from diverse types of biomass, mostly because some works only evaluate technologies that use renewable energy sources in their models, for example, renewable electricity [Kim and Kim \(2016\)](#). The model is tested on an upcoming biomass-to-hydrogen (B_2H_2) supply chain for HFCVs at Jeju Island, South Korea by estimating the expected hydrogen demand in 2040. A sensitivity analysis is conducted to provide insights into the efficient management of the B_2H_2 supply chain.

10.3.1.6 Geographical Information System (GIS)

Literature review reveals that few researchers have used the spatial dimension to construct the infrastructure for hydrogen. In that context, Geographic information systems (GIS), massive software packages providing a range of functions for creating, acquiring, integrating, transforming, visualizing, analyzing, modelling, and archiving information about the surface and near-surface of the earth ([Goodchild, 2009](#)), constitute a powerful tool to develop energy supply chain models. Some examples of geographic approaches include the study of [Ball et al. \(2006\)](#) who developed the MOREHyS (Model for Optimization of Regional Hydrogen Supply) approach to the energy system with the integration of geographic aspects in the analysis by the GIS-based method for Germany. This model identifies the cost-optimal way for constructing and implementing an (initial) hydrogen supply infrastructure, as well as possible tradeoffs between hydrogen production and electricity generation within a country-specific context (high degree of regionalization) ([Ball et al., 2006](#)).

[Johnson et al. \(2008\)](#) also used GIS for modelling regional hydrogen infrastructure deployment using detailed spatial data and applied the methodology to

the case study of a potential coal-based hydrogen transportation system in Ohio with CCS. The objective of this work was to optimize hydrogen infrastructure design for the entire state. The MARKAL model has been applied to the UK and used to develop a GIS-based spatial model to represent the layout of hydrogen infrastructure (Yang and Ogden, 2013).

In the model proposed by Gondal and Sahir (2013), the pipeline network of the natural gas distribution companies has been interfaced with a GIS system. The objective function used is based on profit maximization. An integrated renewable hydrogen model based on a MINLP formulation has been developed based on biomass feedstocks as the input material for hydrogen production in Pakistan because of the strong agrarian economy there. The model involves a statistical database and an up-to-date geographical information system to present accurate and logical results for effective energy planning.

There are very few contributions that have reported to date on hydrogen infrastructure modelling across spatial scales, even if the resulting hydrogen network would depend heavily on the country/region-specific conditions. The framework proposed in De-León Almaraz et al. (2015) has addressed the national and regional scales by linking geographic constraints found by the GIS model to the MILP model.

10.4 CONCLUSIONS

A key point in the development of the hydrogen supply chain is the demonstration of the feasibility of its infrastructure, while many technical, economic, and social obstacles must be overcome. Some strategic roadmaps are currently published about the energy potentialities of hydrogen at the European, national, and regional levels. Their main objective is to evaluate some industrial, technological, environmental, and social issues and to identify the main obstacles associated with the hydrogen economy. A literature review of recent dedicated scientific publications revealed that authors agree on the need to develop systemic studies in order to demonstrate the feasibility of the sector and to validate the technical and economic interest in the production and recovery of hydrogen produced from renewable sources. Such works involve the development of models based on economic scenarios for hydrogen deployment.

Following these guidelines, this chapter has presented the various existing approaches to modelling and optimization of the hydrogen supply chain. Designing the hydrogen supply chain is not a trivial task because different alternatives to produce, store, and distribute H_2 exist.

Most works devoted to hydrogen supply chain modelling are based on mathematical programming approaches and are generally limited to monoobjective (cost minimization) or bi-criteria assessment, generally based on either cost-environment or cost-safety. This is not enough when sustainable development must be taken into account in the strategic stage of any new project, when social, economic, and environmental impacts are interconnected. The spatial- or

GIS-based approach cannot be considered as a general methodology for finding the optimal HSC configuration but can be coupled to mathematical programming to design the HSC. Very few contributions have reported to date on hydrogen infrastructure modelling across spatial scales.

Stochastic methods and genetic algorithms, in particular, have been used more recently for HSC optimization and are well suited to handle multiobjective optimization problems because they are able to search for Pareto solutions simultaneously. More efforts toward robust and sophisticated methods are necessary to deal with demand uncertainty, which is a significant parameter in HSC design.

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