

THÈSE

En vue de l'obtention du

DOCTORAT DE L'UNIVERSITÉ DE TOULOUSE

Délivré par :

Institut National Polytechnique de Toulouse (INP Toulouse)

Discipline ou spécialité :

Génie des Procédés et de l'Environnement

Présentée et soutenue par :

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le vendredi 14 février 2014

Titre :

MULTI-OBJECTIVE OPTIMISATION OF A HYDROGEN SUPPLY CHAIN

Ecole doctorale :

Mécanique, Energétique, Génie civil, Procédés (MEGeP)

Unité de recherche :

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Remerciements

Je tiens tout d'abord à remercier les différents organismes qui ont mis les moyens financiers pour l'aboutissement de cette thèse : CONACYT et la Secretaría de Educación Pública du gouvernement mexicain.

Mes plus sincères remerciements à Catherine AZZARO-PANTEL pour m'avoir acceptée dans son équipe, je lui suis très reconnaissante pour m'avoir fait partager ses compétences scientifiques et humaines et pour sa confiance en mon travail. Un grand merci également à Ludovic MONTASTRUC qui a été un vrai guide pour moi et qui a toujours eu des idées originales et brillantes.

Je remercie l'ensemble des membres du jury d'avoir accepté d'examiner mon travail, plus particulièrement Bruno GRANO qui m'a fait l'honneur d'être Président du jury, Nathalie MAZET et Patrick SIARRY qui ont rapporté sur cette thèse. Stéphan ASTIER qui est une source d'inspiration pour tout ce qui concerne les énergies renouvelables. A Serge DOMENECH pour ses commentaires, ses conseils pertinents et les pistes scientifiques. Merci aussi à Laurence GRAND-CLEMENT pour ses questions.

Mes plus profonds remerciements vont à Marianne BOIX qui m'a soutenue pendant les trois ans de thèse avec ses conseils et connaissances scientifiques et qui est a été très sympathique et professionnelle.

Un petit mot aussi pour Oscar BAEZ qui m'a présenté le Laboratoire de Génie Chimique et qui m'a encouragé pour faire ma thèse.

J'ai à cœur de remercier Séverine RENGNET et Delphine MATHOU de Midi-Pyrénées Innovation qui ont ouvert la porte à ce travail pour être connu des personnes concernées, ce qui m'a permis de travailler sur un projet concret. Elles se sont investi profondément dans ce projet en permettant des visites sur les sites de production et en me présentant les experts dans le monde de l'hydrogène et les acteurs industriels. Merci Séverine et Delphine pour toujours avoir une attitude très positive et proactive. Merci de votre confiance !

A mes amis et collègues Alexandrine DUPIN-JANSON, Christophe SALINGUE et Alex DE NARDI mille fois merci de leur aide, leur patience, leur efficacité et leur bonne humeur. Je suis contente de compter sur vous même longtemps après avoir fini le projet, notre amitié est un cadeau.

Mes remerciements vont aussi à Claudine SAUVAL, Bertrand CHAUVET, Jocelyn ESPERON, Christophe HEVIN et Christophe TURPIN pour votre aide et vos conseils. Merci aussi aux stagiaires qui ont travaillé avec moi pendant cette thèse : Francisco, Mario, Sophie, Anaïs, Lea, Antonio et Aymeric.

Je voulais aussi dire un mot pour Lydie, Jesus, Fer, Liz, Lalo et Denisse : merci de m'avoir accueillie en France.

J'embrasse également mes amis du bureau : Marie (the rugby girl), Raulito et Toño, ça a été un grand plaisir de travailler à vos côtés. Merci aussi à Marco et René qui sont des mexicains admirables, je remercie également leurs familles.

A mes amis de l'ENSIACET: Ganna, Feri, Koenraad, Shey, Luis Tequila, Verito, Mary HANOUN, Marie BONNIN, Fifi, Imaine, Ali, Guillaume, Adama, Weifeng, Moises, Janaina, Philippe(s), Juliette, Mayra, Manuel, You, Vincent, Pierre, Isaura, Nicolas, Nick, Benoît, Cristina, Marian, Tatiana, Nayiri, Ahmed, Stephan, Tania, Diana, Lorena, Anthony, Ann, Eduin, Amelie et Leandro.

Je remercie de plus Philippe DUQUENNE, Ivonne RODRIGUEZ, Pascal FLOQUET et Vincent GERBAUD pour leur gentillesse et leur simplicité.

Je souhaite remercier le personnel technique et administratif du laboratoire et en particulier Alain PHILIPPE (qui m'a toujours poussée à m'intégrer à l'équipe du LGC), Dany, Kinou, Patricia, Maria, Jean-Luc et Claudine. Ce fut un plaisir de traiter avec vous.

Un pensé pour Luc PIBOULEAU et Quentin BERNICAL.

Un grand merci adressé à Elia et André FOURNOU qui en France, ont été mon plus grand soutien.

Merci à Igor pour son amitié et pour avoir été présent à la journée de la soutenance de thèse.

A Laci qui as finit sa thèse quelques mois avant moi et qui a été un exemple de sérénité et de sagesse, merci de m'accompagner dans la dernière ligne droite.

J'ai à cœur de remercier toute ma famille. Merci à mon père et à ma mère pour leur exemple et leur amour, à Carlos et Anita pour votre compréhension, motivation et surtout pour votre bonne humeur!

Résumé

L'hydrogène produit à partir de sources renouvelables et utilisé dans les piles à combustible pour diverses applications, tant mobiles que stationnaires, constitue un vecteur énergétique très prometteur, dans un contexte de développement durable. Les « feuilles de route » stratégiques, élaborées au niveau européen, national ou régional, consacrées aux potentialités énergétiques de l'hydrogène, ainsi que l'analyse des publications scientifiques ont cependant identifié le manque d'infrastructures, comme l'un des principaux obstacles au développement de l'économie « hydrogène ». Cette étude s'inscrit dans le cadre du développement d'une méthodologie de conception d'une chaîne logistique « hydrogène » (production, stockage et transport). La formulation, basée sur une procédure de programmation mathématique linéaire en variables mixtes, implique une approche multicritère concernant la minimisation du prix de revient de l'hydrogène, l'impact sur le réchauffement climatique et un indice de risque, en prenant en compte une échelle tant régionale que nationale. L'optimisation multi-objectif repose sur une stratégie ε-contrainte développée à partir d'une méthode lexicographique menant à la construction de fronts de Pareto offrant un grand nombre de solutions. La procédure d'aide à la décision M-TOPSIS est ensuite utilisée pour choisir le meilleur compromis. Le modèle est appliqué à une étude de cas en Grande-Bretagne, issue de la littérature spécialisée, qui sert de référence pour comparer les approches mono- et multi-objectif. Ensuite, la modélisation et l'optimisation de la chaîne d'approvisionnement d'hydrogène pour la région Midi-Pyrénées ont été étudiées dans le cadre du projet «H_2 vert carburant». Un problème mono/multi-période est traité selon des scénarios d'optimisation basés sur la stratégie ε-contrainte développée à partir d'une méthode lexicographique. Le système d'information ArcGIS® est ensuite utilisé pour valider les solutions obtenues par optimisation multi-objectif. Cette technologie permet d'associer une période de temps aux configurations de la chaîne logistique hydrogène et d'analyser plus finement les résultats de la conception du réseau H_2. L'extension au cas de la France répond à un double objectif : d'une part, tester la robustesse de la méthode à une échelle géographique différente et, d'autre part, examiner si les résultats obtenus au niveau régional sont cohérents avec ceux de l'échelle nationale. Dans cette étude de cas, l'outil spatial ArcGIS® est utilisé avant optimisation pour identifier les contraintes géographiques. Un scénario prenant en compte un cycle économique est également traité. Les optimisations mono et multi-objectif présentent des différences relatives au mode de déploiement de filière, centralisé ou décentralisé, et au type de technologie des unités production, ainsi qu'à leur taille. Les résultats confirment l'importance d'étudier différentes échelles spatiales.

MOTS CLÉS : Optimisation multi-objectif ; chaîne logistique ; hydrogène ; ε-contrainte ; méthode lexicographique ; MILP ; ArcGIS®.

Abstract

Hydrogen produced from renewable sources and used in fuel cells both for mobile and stationary applications constitutes a very promising energy carrier in a context of sustainable development. Yet the strategic roadmaps that were currently published about the energy potentialities of hydrogen at European, national and regional level as well as the analysis of the scientific publications in this field have identified the lack of infrastructures as a major barrier to the development of a « hydrogen » economy. This study focuses on the development of a methodological framework for the design of a hydrogen supply chain (HSC) (production, storage and transportation). The formulation based on mixed integer linear programming involves a multi-criteria approach where three objectives have to be optimised simultaneously, i.e., cost, global warming potential and safety risk, either at 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 reported in the literature survey and dedicated to Great Britain for validation purpose, comparing the results between mono- and multi-objective approaches. In the regional case**,** the modelling and optimisation of the HSC in the Midi-Pyrénées region was carried out in the framework of the project "*H_2 as a green fuel*". A mono/multi period problem is treated with different optimisation scenarios using ε-constraint and lexicographic methods for the optimisation stage. The geographic information system (GIS) is introduced and allows organising, analysing and mapping spatial data. The optimisation of the HSC is then applied to the national case of France. The objective is twofold: on the one hand, to examine if the methodology is robust enough to tackle a different geographic scale and second to see if the regional approach is consistent with the national scale. In this case study, the ArcGIS® spatial tool is used before optimisation to identify the geographic items that are further used in the optimisation step. A scenario with an economic cycle is also considered. Mono- and multi-objective optimisations exhibit some differences concerning the degree of centralisation of the network and the selection of the production technology type and size. The obtained results confirm that different spatial and temporal scales are required to encompass the complexity of the problem.

KEYWORDS: Multi-objective optimisation; supply chain; hydrogen; ε-constraint; lexicographic method; MILP; ArcGIS®.

Resumen

El hidrógeno obtenido a partir de fuentes renovables puede ser utilizado en las pilas de combustible para diversas aplicaciones tanto móviles como estacionarias y constituye un vector energético muy prometedor en un contexto de desarrollo durable. Las hojas de ruta estratégicas elaboradas a nivel Europeo, nacional o regional se han dedicado a estudiar las potencialidades del hidrógeno. Tanto las hojas de ruta como las publicaciones científicas han identificado la falta de infraestructura como uno de los principales obstáculos en el desarrollo de la economía del hidrógeno. Este estudio se sitúa en el marco de desarrollo de una metodología de diseño de la cadena de suministro del hidrógeno (producción, almacenamiento y transporte). La formulación está basada en un procedimiento de programación matemática lineal en variables mixtas (MILP) que implica un enfoque multi-criterio relacionado a la minimización de costo, el impacto ambiental y el índice de riesgo, tomando en cuenta, una escala tanto regional como nacional. La optimización multi-objetivo se lleva a cabo a través de una estrategia de ε-restricciones para obtener los frentes de Pareto ofreciendo un gran número de soluciones. La metodología de ayuda a la toma de decisiones M-TOPSIS es enseguida utilizada para encontrar el mejor compromiso. El modelo es aplicado primeramente a un caso de estudio en Gran Bretaña tomado de la literatura especializada que sirve de referencia para comparar los enfoques mono- y multi-objetivo. En seguida, la modelización y la optimización de la cadena de suministro del hidrógeno son aplicados a la región Midi-Pyrénées en el marco del proyecto "H_2 carburante verde". Un problema mono/multi-periodo es tratado dependiendo el tipo de escenario. La resolución se basa en las estrategias del método lexicográfico y ε-restricciones. Posteriormente, el sistema de información ArcGIS® es utilizado para validar las soluciones obtenidas por optimización multi-objetivo. Esta herramienta permite asociar un periodo de tiempo a las distintas configuraciones de la cadena de suministro del hidrógeno y analizar más detalladamente los resultados de la red. La extensión del modelo matemático al caso nacional Francés responde a un doble objetivo: de una parte, probar la robustez del método a diferentes escalas geográficas; por otro lado, examinar si los resultados obtenidos a nivel regional son coherentes con los de escala nacional. En este estudio de caso, la herramienta ArcGIS® es utilizada previa optimización para identificar restricciones geográficas. También en este caso se estudia un escenario de optimización siguiendo el ciclo económico. Las optimizaciones mono- y multi-objetivo presentan diferencias relacionadas al tipo de configuración (centralizada o descentralizada), al tipo de producción y al tamaño de las unidades. Los resultados confirman la importancia de estudiar diferentes escalas espaciales.

PALABRAS CLAVE: Optimización multi-objetivo; cadena de suministro; hidrógeno; ε-restricciones; método lexicográfico; MILP; ArcGIS®.

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INTRODUCTION GÉNERALE

L'hydrogène produit à partir de sources renouvelables et utilisé dans les piles à combustible pour diverses applications, tant mobiles que stationnaires, mais également pour des usages de niche (engins de manutention, groupes électriques de secours, fourniture de courant pour des sites isolés, applications nomades…), constitue un vecteur énergétique très prometteur, dans un contexte de développement durable. Certes, à l'heure actuelle, le coût de production d'hydrogène reste encore prohibitif par rapport au prix des combustibles fossiles utilisés dans les transports, mais les dernières avancées de la technologie, conjuguées au prix élevé du pétrole, ont amélioré sa compétitivité. Un point clé du développement de la filière hydrogène repose sur la démonstration de faisabilité de l'infrastructure pour produire, stocker et distribuer l'hydrogène, en surmontant de nombreux obstacles à la fois techniques, économiques, et sociaux.

Un certain nombre de « feuilles de route » stratégiques, élaborées au niveau européen, national ou régional ont été consacrées aux potentialités énergétiques de l'hydrogène et seront mentionnées dans le cadre de ce travail. Elles ont pour objectif majeur d'éclairer les enjeux industriels, technologiques, environnementaux et sociétaux et de mettre en avant les verrous associés concernant l'hydrogène. Leur analyse, ainsi que la synthèse des publications scientifiques récentes du domaine, s'accordent sur la nécessité de développer des études systémiques de démonstration de faisabilité de la filière, pour valider l'intérêt technico-économique de la production et de la valorisation de l'hydrogène produit à partir de sources renouvelables : ces travaux impliquent le développement de modèles basés sur des scénarios économiques de déploiement de la filière.

Ce travail de doctorat, qui s'inscrit dans ce contexte, est exclusivement consacré à des applications de l'hydrogène à des fins d'électromobilité. Mais au-delà de son intérêt comme carburant propre et viable, l'hydrogène pourrait également devenir une des pierres angulaires du système énergétique dans le cadre de l'accroissement des énergies renouvelables et intermittentes : l'hydrogène est identifié comme un moyen flexible de stocker l'énergie électrique pour les applications transport et stationnaire, sur le réseau et hors réseau. Le stockage d'énergie par le vecteur hydrogène a non seulement du potentiel pour le marché du stockage, mais également pour la valorisation de ces énergies stockées dans d'autres marchés, notamment celui du transport de masse. L'hydrogène a donc de sérieux atouts à faire valoir, qui dépassent les aspects qui seront spécifiquement abordés dans ce manuscrit et qui renforcent la portée de ce travail.

L'étude proposée dans ce mémoire est dédiée au développement d'un modèle de chaîne logistique de l'hydrogène, basé sur une procédure de programmation mathématique linéaire en variables mixtes, prenant en compte une approche multicritère impliquant le prix de revient de l'hydrogène, l'impact sur le réchauffement climatique et un indice de risque. Elle analyse l'impact de différentes sources d'énergies et de divers procédés de production d'hydrogène, de différents modes de stockage et de distribution. Plusieurs scénarios de demande basés sur des études prospectives récentes seront étudiés sur l'horizon 2020-2050, selon des approches mono- et multi-périodes. L'analyse s'inscrit dans l'objectif global de division par quatre des émissions de gaz à effet de serre à l'horizon 2050 par rapport à leur niveau de 1990 (facteur 4[1]). Les stratégies étudiées seront précisées et justifiées au fur et à mesure de la présentation des études. Le modèle développé a été conçu de façon générique et évolutive pour s'adapter, par exemple à l'extension à d'autres sources d'énergies ou à la modification du découpage des territoires. Si les études ont impliqué nécessairement un aspect temporel, des caractéristiques d'ordre territorial se sont avérées déterminantes (disponibilité de ressources renouvelables, contraintes géographiques…). Différentes analyses ont ainsi été menées à deux niveaux d'échelle spatiale, régionale (cas de la région Midi-Pyrénées) et nationale (cas de la France).

Les travaux de doctorat présentés dans ce mémoire ont été menés de janvier 2011 à janvier 2014 au Laboratoire de Génie Chimique, LGC UMR CNRS INPT UPS 5503 au sein de l'équipe COOP (Conception, Optimisation et Ordonnancement des Procédés) du département PSI (Procédés et Systèmes Industriels. Le thème général de recherche de l'équipe COOP concerne l'optimisation et la conception de procédés. La bourse de thèse associée a été octroyée par CONACYT (Consejo Nacional de Ciencia y Tecnología, México). Ce travail a d'ores et déjà donné lieu à un certain nombre de publications (De-Léon Almaraz et al., 2012, 2013a, 2013b, 2014). Elles seront référencées dans les chapitres auxquels elles se rapportent.

Nous avons eu l'opportunité de participer au cours de ce travail au projet *hydrogène vert* au sein de la région Midi-Pyrénées. Il a impliqué différents professionnels issus de secteurs distincts (entreprises, collectivités, universitaires) pour analyser le potentiel de déploiement de la filière hydrogène à des fins d'électromobilité en Midi-Pyrénées (PHyRENEES[2], Midi-Pyrénées Innovation (MPI)[3], WH_2[4] et

[1] Cet objectif est mentionné dans l'article 2 de la loi de programme fixant les orientations de la politique énergétique française (13 juillet 2005).

[2] L'Association PHyRENEES a été créée en octobre 2007 autour de plusieurs partenaires (Ecole des Mines d'Albi, Trifyl, N-GHY, Airbus, GDF, INPT, ARAMIP, Conseil Général du Tarn...).

[3] MPI est une association loi 1901, financée par la Région Midi-Pyrénées, l'état et l'Europe. Elle a été créée en 2006 à l'initiative du Conseil régional avec le concours de l'Etat et d'Oséo, pour améliorer la visibilité du paysage institutionnel et guider les entreprises dans leur démarche d'innovation.

[4] WH_2est une société créée en 2011, qui se positionne comme société de courtage en énergie « H_2 vert » en France.

Trifyl[5]). Nous avons également présenté les résultats du projet *hydrogène vert* dans deux réunions de restitution avec les membres de PHyRENEES et MPI (12 juillet et 25 septembre 2012).

Par ailleurs, le travail proposé dans le cadre de ce doctorat sur ce projet a été sélectionné pour participer au Débat National sur la Transition Energétique[6] le 3 Juin 2013 à Toulouse, organisé en région par MPI.

Nous avons également participé de façon active à des manifestations scientifiques et des événements de vulgarisation scientifique qu'il convient de mentionner dans le cadre de ce sujet sur l'hydrogène dont les actions de promotion sont importantes en phase de transition énergétique : « Fête de la science : les énergies pour tous » (présentation de la voiture à pile à combustible le 14 octobre 2012 à Toulouse); « Journées H_2 dans les territoires » du 16-17 mai 2013 organisée par Trifyl ; « HyVolution 2013, consacré à la filière hydrogène et piles à combustible (http://hyvolution.fr/fr) », organisé par Seiya Consulting du 5 au 8 septembre 2013 (Albi).

Le mémoire de thèse, qui synthétise l'ensemble des travaux menés pendant ces trois années, est organisé en sept chapitres. La présentation de leur contenu est donnée à la fin du premier chapitre qui permet de poser les éléments motivant cette étude et d'introduire de façon plus détaillée les chapitres de ce document :

Chapitre 1 *Motivation de l'étude: l'hydrogène comme carburant alternatif pour le transport*. Ce chapitre introductif a pour but de présenter le contexte énergétique.

Chapitre 2 *Conception de la chaîne logistique « hydrogène »*. L'objectif de ce chapitre est de présenter le concept de la chaîne logistique de l'hydrogène et les principales activités qui y sont impliquées, i.e., production, stockage, transport et distribution.

Chapitre 3 *Méthodes et outils pour la conception de la chaîne logistique « hydrogène »*. Ce chapitre présente les méthodes et outils utilisés dans le cadre de ce travail pour la conception optimale de la chaîne logistique de l'hydrogène.

Chapitre 4 *Optimisation multi-objectif pour la chaîne d'approvisionnement « hydrogène »*. Ce chapitre est consacré à la modélisation de la chaîne logistique « hydrogène ».

Chapitre 5 *Optimisation de la chaîne logistique « hydrogène » pour les scénarios de déploiement dans la région Midi-Pyrénées*. La modélisation et l'optimisation de la chaîne d'approvisionnement

[5]Trifyl est un syndicat départemental de valorisation des déchets ménagers du Tarn. Dans sa mission de service public, elle développe le projet *production d'hydrogène à partir de biogaz* (50-100 m^3/h) pour alimenter 2 véhicules.

[6]http://www.mp-i.fr/2013/05/debat-national-transition-energetique-production-decentralisee-dhydrogene-vert-en-midi-pyrenees/

d'hydrogène vis-à-vis des caractéristiques spécifiques de la région et de ses sources d'énergie est décrite dans ce chapitre.

Chapitre 6 *Conception de la chaîne logistique « hydrogène » à l'échelle nationale*. Dans ce chapitre, l'optimisation de la chaîne d'approvisionnement « hydrogène » est appliquée au cas de la France.

Chapitre 7 Conclusions et perspectives.

Quatre annexes seront présentées à la fin de ce travail qui correspondent d'une part aux bases de données et aux résultats détaillés pour chaque étude de cas et d'autre part aux concepts mis en œuvre dans la méthodologie d'aide à la décision M-TOPSIS.

GENERAL INTRODUCTION

Hydrogen produced from renewable sources and used in fuel cells both for mobile and stationary applications constitutes a very promising energy carrier in a context of sustainable development. Nowadays, the hydrogen cost is considered as prohibitive compared to the fossil fuels used in the transportation system, but the development of some technologies associated to hydrogen coupled with high oil prices has improved its competitiveness.

A key point in the development of the hydrogen supply chain is the demonstration of feasibility of its infrastructure while many technical, economic and social obstacles must be overcome. Some strategic roadmaps were currently published about the energy potentialities of hydrogen at 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 to the hydrogen economy. The literature review of recent dedicated scientific publications, agree on the need to develop systemic studies in order to demonstrate the feasibility of the sector, 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.

In that context, this work only focuses on H_2-mobility applications. Besides its interest as a clean and economically viable fuel, hydrogen can not only be viewed as a cornerstone of the energetic system in the general context of the increased use of renewable and intermittent energies, but also as a flexible storage vector that can be used for transport and stationary applications, both on- and off-grid systems. These various applications reinforce the scope of the proposed work.

This study focuses on the development of a methodological framework for the design of a hydrogen supply chain (HSC) (production, storage and transportation). The formulation, based on mixed integer linear programming involves a multi-criteria approach where three objectives have to be optimised simultaneously, i.e., cost, global warming potential and safety risk. In the case of the environmental objective, ambitious targets are proposed in some countries: e.g. the French government adopted a Climate Plan ("*Plan climat"*) in 2004 presenting a strategy for technological research to divide by 4 the GHG emissions by 2050 compared to current levels. Several demand scenarios based on recent prospective studies will be considered on the horizon 2020-2050 in a mono- or multi-period approach, either at national or regional scale.

The different strategies that have been investigated will be specified and justified along this study. The model was designed in a generic way to be adapted to different scenarios, for example the addition of new energy sources or the modification in the geographic breakdown. The temporal aspect has an impact in the territorial features adding geographic constraints (e.g. availability of renewable resources per grid, district or region in a specific time period). In this study, two analyses have been conducted at spatial level, i.e., regional (for the Midi-Pyrenees region in France) and national (France).

The doctoral research presented in this thesis was conducted from January 2011 to January 2014 at the Laboratory of Chemical Engineering, LGC UMR CNRS 5503 INPT UPS in the Design, Optimisation and Scheduling Process team (COOP- Conception, Optimisation et Ordonnancement des Procédés) belonging to the Process Systems Engineering department. The general scope of the COOP team concerns the optimisation and design of processes.

The PhD scholarship was financially supported by CONACYT (Consejo Nacional de Ciencia y Tecnología, México). This work has already led to some publications that will be referenced in the chapters to which they are related (De-Léon Almaraz et al., 2012, 2013a, 2013b, 2014).

During this thesis work, we had the opportunity to participate in the "Green H_2 fuel" project. This study emerged as an initiative to evaluate the hydrogen economy in the Midi-Pyrénées region to enhance renewable energies and at the same time to evaluate the potential CO_2 reductions. It involved various professionals from different sectors (industry, government and academia), e.g. PHyRENEES association[7], the Regional Innovation Agency (Midi-Pyrénées Innovation-MPI)[8], WH_2[9], the Chemical Engineering Laboratory, Trifyl, etc.). The mathematical model developed in this thesis was adapted to this specific case study and the optimisation results were presented at two feedback meetings with members of PHyRENEES and MPI (12 July and 25 September 2012). In addition, the results of this project were selected to take part in the National Debate on Energy Transition (Toulouse, June 3rd, 2013).

The PhD manuscript is organised into seven chapters. A brief description of the content of each chapter is presented hereafter. A more detailed presentation will be given at the end of the first chapter:

[7] PHyRENEES Association was established on October 2007 around several partners (Ecole des Mines, Trifyl, N-GHY, Airbus, GDF INPT, ARAMIP and the General Council of the Tarn ...).

[8] MPI was created in 2006 at the initiative of the Regional Council to improve the visibility of the institutional landscape and guide companies in their innovation projects.

[9] WH_2: start-up 2011, green H_2 energy broker in France.

Chapter 1 *Motivation for the study: hydrogen as an alternative fuel for transportation*. This first chapter aims to present energy context.

Chapter 2 *Hydrogen supply chain design*. The objective of this chapter is to introduce the concept of hydrogen supply chain and its main activities, i.e., energy sources, production, storage, transportation and distribution.

Chapter 3 *Methods and tools for HSC design*. The methods and tools that are selected to develop the methodology of optimal design of a hydrogen supply chain are proposed in this chapter.

Chapter 4 *A multi-objective optimisation framework for hydrogen supply chain*. This chapter is devoted to the modelling of the hydrogen supply chain.

Chapter 5 *Hydrogen supply chain optimisation for the deployment scenarios in the Midi-Pyrénées region*. Modelling and optimisation of the hydrogen supply chain is applied to the largest region in France considering its specific features, e.g. the available renewable energy sources.

Chapter 6 *Extending the frontiers: design of a hydrogen supply chain in France*. In this chapter, a national case is considered to propose the optimal hydrogen supply chain.

Chapter 7 General conclusions and perspectives.

Four appendices are presented at the end of this work, which correspond on the one hand both to the databases and to the detailed results for each case study and on the other hand to the key concepts of the M-TOPSIS methodology.

Chapter 1

MOTIVATION FOR THE STUDY: HYDROGEN AS AN ALTERNATIVE FUEL FOR TRANSPORTATION

Résumé

Ce chapitre introductif a pour but de présenter le contexte énergétique lié au domaine du transport et les motivations qui conduisent à retenir l'hydrogène comme un vecteur alternatif d'énergie dans la transition énergétique. Nous exposons dans un premier temps la problématique liée au système de transport actuel : émission de gaz à effet de serre et effet sur le réchauffement climatique, pollution locale dans les villes et dépendance aux carburants issus de ressources fossiles. Nous présentons ensuite les alternatives aux carburants actuels comme les biocarburants ou l'hydrogène, qui sont comparés notamment en termes d'efficacité du puits à la roue. Le cas de l'hydrogène, retenu dans cette étude, fait l'objet d'une attention particulière vis-à-vis de ses atouts, des cibles à atteindre en termes de prix et de potentiel de réchauffement climatique, notamment à travers son mode de production. Les aspects liés à la sécurité et à son acceptabilité sociale sont également abordés. La problématique du déploiement de la chaîne logistique hydrogène, qui est le cœur de ce travail, est largement présentée, notamment à travers les nombreuses « feuilles de route » et scénarios du plan de transition qu'elle a suscités. L'ensemble de l'analyse justifie les motivations de ce travail dédié à la conception de la chaîne logistique de l'hydrogène mettant en œuvre une approche d'optimisation multi-objectif, et à l'étude de scénarios pertinents en vue d'une aide à la décision pour le développement de la chaîne.

Abstract

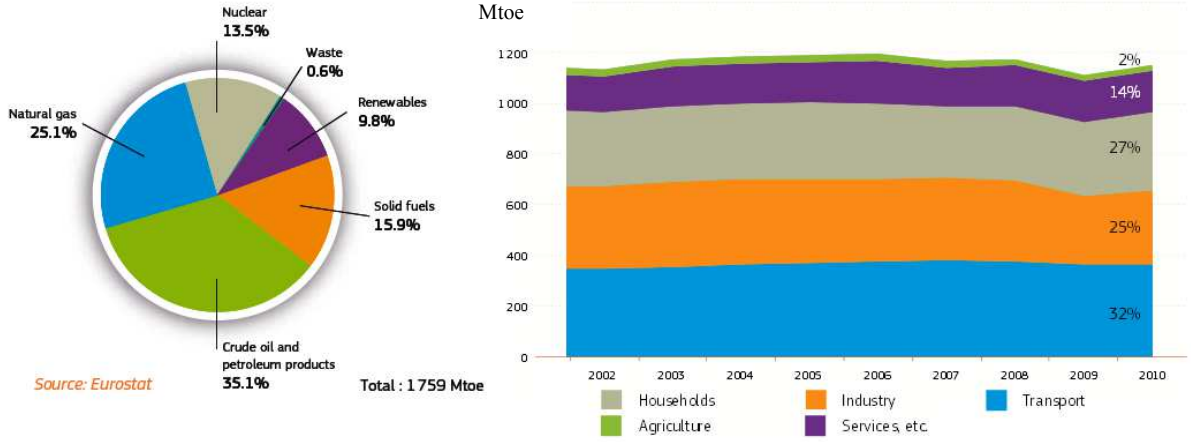
This first chapter presents the transportation energy context and the motivations to consider hydrogen as an alternative energy carrier in the transition towards a new energetic paradigm. The current transportation system is first presented with its typical features: global warming potential, air pollution in big cities and fossil dependency associated with the production and use of products such as oil and diesel. Some fuel alternatives are proposed to replace fossil products (e.g. biofuels, electricity, etc.). Particular emphasis is paid to hydrogen which is the core of this study. The different energy sources and production modes to obtain hydrogen are briefly reviewed, with specific focus on their associated efficiencies. The safety issues and the social acceptability are also briefly discussed as well as the problems associated with the start-up of a hydrogen economy and particularly those related to the lack of infrastructure. In order to overcome these barriers that have been reported in the roadmaps and energy transition plan scenarios, this work aims to model and design the hydrogen supply chain through a multi-objective optimisation framework to aid-decision making.

Acronyms

ADEME	Agence de l'environnement et de la maîtrise de l'énergie (Agency for Environment and Energy Management)
AFHYPAC	Association Française pour l'Hydrogène et les Piles à Combustible (French Association for Hydrogen and Fuel Cells)
BEV	Battery Electric Vehicle
CaFCP	California Fuel Cell Partnership
CCS	Carbon Capture and Storage
CNG	Compressed Natural Gas
DOE	Department of Energy
FCEV	Fuel Cell Electric Vehicle
GHG	Greenhouse gas
GIS	Geographic Information System
GWP	Global Warming Potential
ICE	Internal Combustion Engine
JHFC	Japan Hydrogen and Fuel Cell demonstration project
LPG	Liquefied Petroleum Gas
NEDO	New Energy and Industrial Technology Development Organisation
NIP	National Innovation Program
PEM	Proton Exchange Membrane
PHEV	Plug-in Hybrid Electric Vehicle
TOPSIS	Technique for Order Preference by Similarly to Ideal Solution
TtW	Tank-to-Wheel
WtT	Well-to-Tank
WtW	Well-to-Wheel

1.1 Introduction

Crude oil and petroleum products continue to dominate the energy mix in Europe, representing 35% (617 M tonne of oil equivalent (toe)) of the Gross Inland Consumption in 2010 (Eurostat. European Commission, 2012) (see Figure 1.1a). In the same year, transportation was the largest consumer (32%) of the total energy, followed by households and industry (see Figure 1.1b). Oil is still the largest primary fuel with more than 95% of transport energy demand (Ball and Wietschel, 2008) from which petroleum products such as gasoline and diesel are produced.



a) b)

Figure 1.1a) EU-27 Gross Inland Consumption (as % of total Mtoe) 2010
1.1b) EU-27 Total final energy consumption (1995-2010) (Eurostat. European Commission, 2012).

The main advantages of producing gasoline and diesel are related to the existing infrastructure, know-how and experience as well as a huge demand allowing efficiency improvement. Prices in fossil fuel vary in each country. The dependency in the current fossil fuel system constitutes a main issue with the antecedent of two oil crises in the 70's and 80's. Any oil supply disruption would cause tremendous impacts in fuel prices.

The use of petroleum products has also significant impacts in health and environment, especially in the big cities. Approximately, 800,000 deaths annually worldwide can be attributed to urban pollution from which a significant portion is generated by vehicles (Braun Martin, 2009). The transport sector today accounts 17% of global CO_2 emissions, with the vast majority of emissions coming from road transport. It is also responsible for 20% of the projected increase in both global energy demand and greenhouse gas (GHG) emissions until 2030 (Ball and Wietschel, 2008). As mobility is one of the major drivers of economic growth and societal development, reducing energy demand and CO_2 emissions from transport is a particular challenge. Vehicle industry is trying to improve fuel efficiency and to decrease tail pollution.

The potential economic and geopolitical implications of all these problems are triggering the search for alternative fuels such as hydrogen. To ensure energy security, a large diversified portfolio of energy sources and energy carriers[10], new propulsion systems and a more efficient energy management constitute complementary and alternative actions. This research work is devoted to explore the potential of hydrogen as an alternative fuel used for transportation. More particularly, this thesis intends to provide a comprehensive study of the feasibility of hydrogen as a transportation fuel from a supply chain point of view.

The remainder of this chapter is organised as follows. The next section is dedicated to the main issues of the current transportation system (fossil fuel dependency, air pollution and global warming) and lists some initiatives associated with climate change. Section 1.3 presents some alternatives to current fuels as compressed natural gas, biofuels, hydrogen, etc. and compares their Well-to-Wheel (WtW) efficiencies. The introduction of hydrogen as an alternative fuel is the core of section 1.4. The targets related to fuel prices and global warming potential (GWP) are presented in the same section where also safety and acceptability issues are discussed. Section 1.5 then presents the roadmaps that have been reported for hydrogen deployment. They are often used by international organisations, business and industry to address the challenges of new technologies, taking generally different approaches and varying in the depth and intensity of their analyses. They are presented at this level since they generally provide useful insights into how stakeholders envision a hydrogen economy development. For example, how hydrogen will be produced in the short, medium and long terms? How will it be distributed and stored? The second part of this section is devoted to transition plan scenarios. It has been highlighted that more precise analyses are necessary to design the hydrogen supply chain. This chapter ends with the presentation of the scientific objective and motivation of the study in section 1.6.

1.2 Main issues of the current transportation system

1.2.1 Fossil fuel dependency

There will always be considerable uncertainty concerning how much oil still exists under the Earth's surface and how much can be recovered. There is a long history of failed forecasts regarding the peaking of oil production and experience shows that reserves are usually underestimated (Ball and Wietschel, 2008). The BP Statistical Review (BP Stat, 2013) reported oil to last for approximately 53 years (see Table 1.1).

In Europe, 59% of the total energy imports consisted of crude oil and petroleum products in 2010 (Eurostat. European Commission, 2012). Moreover, there is a high geographic concentration of oil as

[10]According to ISO 13600, an *energy carrier* is either a substance (energy form) or a phenomenon (energy system) that can be used to produce mechanical work or heat or to operate chemical or physical processes.

well as a growing import dependency on few countries (i.e. Russia, Norway and Libya were the main oil suppliers for Europe in 2010, exporting almost 60% of the total oil demand).

Table 1.1 Global reserves of fossil sources at end 2012 (BP Stat, 2013).

	Reserves-to-production (R/P) ratio (years)[11]
Oil	52.9
Natural gas	55.7
Coal	109

Oil scarcity has led to make big efforts to postpone the "peak oil", for example, the recovery rate improvement in the already exploited deposits, the deep offshore production, the exploitation of extra-heavy oil reserves, or even unconventional resources, such as oil shale (*Direction générale de la compétitivité, de l'industrie et des services*, 2011).

Renewable energy seems to be a promising option to reduce the fossil fuel dependency. The fluctuating and intermittent renewable energy makes necessary to strengthen the control of energy flows between the supply and demand of electricity. The implementation of flexible and efficient storage facilities appears as a key answer to this problem. In this context, hydrogen could be produced to store energy and manage the intermittency of the renewable energy sites as a way to optimise the efficiency of the systems. As transportation uses an important ratio of the fossil sources, new propulsion systems and fuels are in R&D stage.

1.2.2 Air pollution

Some of the effects of the transport emissions are respiratory and cardiovascular diseases, damage to construction and surface materials and visibility reduction due to the smog. Besides the ecologic aspect, there is a sanitary problem to be solved. Some governments have been strongly motivated for air-quality improvement (e.g. Great Britain, Korea), and adopted comprehensive programs to reduce CO_2 through the energy tax (known as BTU tax in the US). Also some car devices have been adapted and introduced to the market to try to decrease air pollution, for example, with the use of Particle Filter (FAP)[12] in diesel vehicles, but this effort seems not to be enough to tackle all the above mentioned problems.

[11]If the reserves remaining at the end of any year are divided by the production in that year, the result is the length of time that those remaining reserves would last if production was to continue at that rate.

[12]The Particle Filter is an additional filter fitted in the exhaust system that is designed to filter out harmful soot particles from the exhaust gases and helps protect the environment. The Particle Filter is fitted exclusively to diesel engines, and reduces emissions of such particles to below the Euro V emissions regulation that came into place in 2009 of 5mg per km (Renault UK, 2013).

1.2.3 Global warming

Greenhouse gas emissions from the transport sector and from fuel production represent a major problem and are increasingly subject to regulation around the world. Since the 1970s, GHG emissions from mobility have grown by more than 120% worldwide, and most scenarios predict that this trend will continue in the future (Ball and Wietschel, 2008). Carbon dioxide is the most important anthropogenic GHG. Its annual emissions have grown between 1970 and 2004 by about 80%, from 21 to 38 giga tonnes (Gt), and represented 77% of total anthropogenic GHG emissions in 2004 as presented in Figure 1.2 (IPCC, 2007).

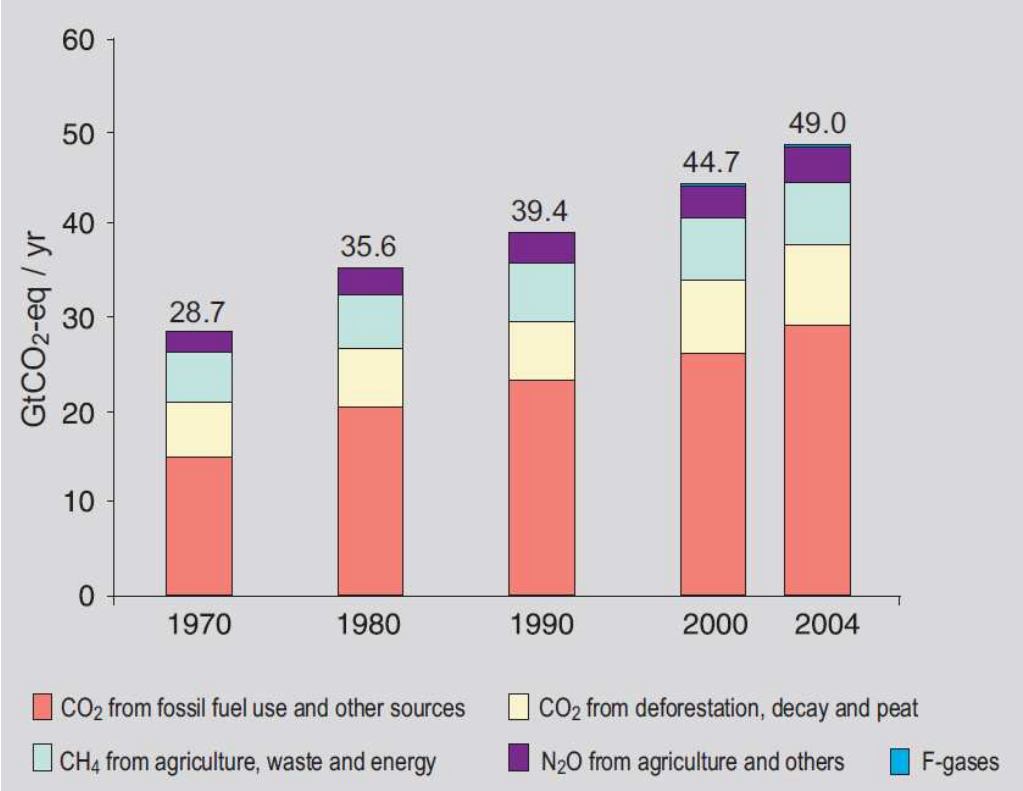


Figure 1.2 Global annual emissions of anthropogenic GHGs from 1970 to 2004 (IPCC, 2007)

The indicator of the overall effect of the process related to the heat radiation absorption of the atmosphere due to emissions of greenhouse gases is the global warming potential (GWP) (Utgikar and Thiesen, 2006) and its reference unit is the CO_2 equivalent (CO_2-equiv).

The GWP impacts all the aspects of the sustainable development. Economic and population growth in developing countries such as China, India or Brazil, cause a significant increase in energy demand (Bento, 2010) and pollution. In the future, the world could face higher costs and major risks associated with climatic change and massive movements of population (e.g. people moved by environmental reasons) (UNFCCC, 2010). Sustainable development can reduce these vulnerabilities. The increasing levels of emissions from transport suggest that stronger mitigation efforts may be necessary for this

sector. This may be difficult to accomplish for several reasons, including issues related to globalization and development, as well as the difficulty of assigning responsibility for emissions from international transport. A crucial first step in designing an efficient mitigation policy is to quantify the extent to which emissions from transport affect the climate system.

The force of the regulations should not be underestimated. The Brazilian case of support for biofuels is a good example (Bento, 2010). Although the signed Kyoto Protocol was not legally binding, some international initiatives supported this treaty. By its part, the International Energy Agency (IEA) has studied some scenarios to face the problems associated with climate change. More precisely, the scenario "*Blue Map*" is the optimistic scenario, in which global CO_2 emissions related to energy will be reduced by half by 2050, compared to 2005 levels: for the most industrialized countries, the GHG emissions are expected to be divided by four GHG by 2050. According to these projections, 53% of the observed difference is due to energy efficiency and changes in fuels. The other two main contributions come from the carbon capture and storage (CCS) and the use of renewable energy (*Direction générale de la compétitivité, de l'industrie et des services,* 2011).

Carbon taxes can also be used as a policy tool for CO_2 abatement. Despite significant price increases for some fuel types as adopted in some countries, the carbon tax effect on emissions was modest in the transport sector according to (Bento, 2010). To reduce GHG emissions, a portfolio of technologies and mitigation activities across all sectors such as improving energy efficiency, CCS and the use of renewable energies or fuels are required. Some mobility alternatives are treated in the next section.

1.3 Mobility alternatives

Nowadays, gasoline and diesel are the easiest and cheapest fuels to be produced and handled. ICEs have the potential to reduce their CO_2 footprint significantly through an average 30% improvement in energy efficiency by 2020 and the additional blending of biofuels. After 2020, however, further engine efficiency improvements are limited and relatively costly, while the amount of biofuels that will be available may be limited (McKinsey & Company, 2010).

In the near and medium term, smaller cars, more lightweight and aerodynamic construction as well as better drive train efficiency through improved conventional internal combustion engines (ICEs), hybridisation or dieselisation can all further improve the fuel economy of vehicles and help reduce fuel consumption and emissions (Ball and Wietschel, 2008). Other alternatives have been suggested to address energy-related issues, including methanol, ethanol, methane, liquefied petroleum gas, electricity and hydrogen. In order to compare some of these options, well-to-wheel (WtW) efficiency for transport fuels will be distinguished.

The WtW efficiency can be appreciated through two stages, i.e., well-to-tank (or upstream stage) and tank-to-wheel (also known as downstream stage). The well-to-tank (WtT) energy efficiency is defined as the ratio of the lower heating value of a fuel that is available for propulsion to the total energy consumed in production, handling (compression/liquefaction), distributing and refuelling. The tank-to-wheel (TtW) evaluates the vehicle/fuel combination ratio. In this section, the WtW efficiency for different fuels presented by (McKinsey & Company, 2010) is taken as a basis (see Figure 1.3).

Primary energy carrier	Fuel production		Vehicle		Well-to-wheel efficiency
Oil	Gasoline	86%	ICE	30%	25%
	Diesel	84%	ICE	35%	29%
	Power	51%	BEV	68%	31%
	Power -> H_2	34%	FCEV	56%	15%
	H_2	51%	FCEV	56%	23%
Gas	CNG	94%	ICE	30%	24%
	Diesel[13]	63%	ICE	35%	21%
	Power	58%	BEV	68%	35%
	Power -> H_2	39%	FCEV	56%	18%
	H_2	70%	FCEV	56%	31%
Coal	Gasoline[5]	40%	ICE	30%	12%
	Diesel[5]	40%	ICE	35%	14%
	Power	50%	BEV	68%	30%
	Power -> H_2	34%	FCEV	56%	15%
	H_2	41%	FCEV	56%	18%
Biomass	Ethanol	35%	ICE	30%	10%
	Biodiesel	35%	ICE	35%	12%
	Power	35%	BEV	68%	21%
	Power -> H_2	24%	FCEV	56%	11%
	H_2	31%	FCEV	56%	14%
Renewable power	Power -> H_2	100%	BEV	68%	61%
	H_2	68%	FCEV	56%	30%

Figure 1.3 FCEV well-to-wheel efficiency adapted from(McKinsey & Company, 2010)[14]

It must be highlighted that the efficiencies reported in this study are rather optimistic for all the technologies; for example, the efficiency of gas-to-power for the production stage has a favorable yield of 58% whatever the technology used. These orders of magnitudes will not be used in the

[13]Gasoline and diesel production through Fischer-Tropsch process

[14]Distribution stays for all fuels above 89% efficiency and in the retail case is 99% except for hydrogen (90%).

remaining chapters of this manuscript. Fuel cell electric vehicle (FCEV) WtW efficiency appears to be competitive with ICE, with a flexible use of feedstock, while battery electric vehicle (BEV) remains the most efficient power-train. Then, a brief description of the fossil fuels and their competitors is given below to present their main features, WtW efficiency, advantages and challenges.

1.3.1 Gasoline and diesel

The overall energy efficiency is around 25% for gasoline (McKinsey & Company, 2010) (respectively, about 29% for diesel) (see Figure 1.3). In this sense, today's vehicles are actually producing more heat than propulsion energy. Besides, higher priced, conventional oil resources can be replaced by high carbon alternatives such as oil sands, oil shale or synthetic fuels from coal and gas, which result in increasing GHG emissions unless production plants are equipped with CCS (Ball and Wietschel, 2008). They can also be replaced by the options listed below.

1.3.2 Compressed natural gas (CNG)

Natural gas achieves one of the greatest reduction in vehicle emissions of CO_2 (20–25%) (Ball and Wietschel, 2008). One example of the CNG development can be found in Europe, with reference to commercial vehicles: in 2012, Germany had some 1200 medium and heavy duty CNG trucks and 1600 CNG buses, all of them working in urban services. There are around 900 filling stations (German initiative for natural gas-based mobility, 2012). The benefits of CNG, as well as LPG (Liquefied Petroleum Gas), are unlikely to offset the costs associated with further development of the refuelling infrastructure, vehicle conversions and safety issues. In addition, in the long term, natural gas will face the same resource-economic constraints as crude oil (Ball and Wietschel, 2008).

1.3.3 Biofuels

There is also a significant push for biofuels taking place around the world. The interest in these alternatives is also motivated by energy security concerns which tend to stimulate a greater reliance on indigenous energy resources which often result in increased GHG emissions. Nevertheless, all these fuels have in common that they are simple to handle, have a high volumetric energy density, are easy to store on board a vehicle and can use the existing distribution and refuelling infrastructure (Ball and Wietschel, 2008). The biofuels are produced from biomass, which can be converted through thermal, chemical or biochemical processes. Some examples are:

- ethanol, produced from sugar or starch crops, corn and sugarcane, can be used as a fuel in its pure form (widely used in US and Brazil). WtW efficiency is 10% (McKinsey & Company, 2010);
- biodiesel, from vegetable oils and animal fats can also be used as a fuel in its pure form., with WtW efficiency of 12% (McKinsey & Company, 2010);
- biogas/bio-methanol from biodegradable waste materials is produced by anaerobic digestion process.

There is still uncertainty related to the amount of biofuels that will be available for passenger cars in the medium and long term in Europe (sustainably produced). A comprehensive analysis on the true global potential of biofuels is needed to determine both their availability and for which sectors and regions they may be most effectively used (McKinsey & Company, 2010).

1.3.4 Electric vehicles

The switch to electricity reduces the oil dependency by opening transports up to a much wider portfolio of primary energy sources of the power sector. Electric vehicles thus help reduce CO_2 emissions and local air pollution while at the same time offer a potential storage option for surplus electricity from intermittent renewable energies (Ball and Wietschel, 2008). Electric vehicles have substantially lower pollution from noise, NO_2 and particles (McKinsey & Company, 2010). They can be classified as: BEVs, FCEVs and Plug-in Hybrid Electric Vehicles (PHEVs). They have zero tail-pipe emissions while driving, resulting in significantly improving local air quality.

1.3.4.1 Battery electric vehicle (BEV)

Owing to limits in battery capacity and driving range (currently 100-200 km for a medium sized car) and a current recharging time of several hours, BEVs are ideally suited to smaller cars and shorter trips, i.e. urban driving. The most promising battery technology is the Lithium-Ion battery but some technical and economic issues, in particular the availability of lithium resources have to be analysed. If battery performance was to improve markedly and at the same time costs could be reduced, BEV could represent a complete solution to decarbonising the transport sector, thus making the discussion about other alternatives such as hydrogen largely obsolete (Ball and Wietschel, 2008). The maximum WtW efficiency is for the BEV 61% (Figure 1.3) when electricity is obtained via renewable sources and even if the power is obtained by non-renewable sources, it results the most promising option in terms of efficiency (31-35%). Yet at this time, BEVs have a shorter range than FCEVs, PHEVs and ICEs. Fast charging may become widespread, but the impact on battery performance degradation over time and power grid stability is unclear.

1.3.4.2 Plug-in electric vehicle (PHEV)

With a smaller battery capacity than BEVs, PHEVs have an electric driving range of 40-60 km. Combined with the additional blending of biofuels, they could result in emission reductions for longer trips. PHEVs have a similar range and performance to ICEs, but electric driving only applies to shorter distances, while the amount of biofuels available for longer trips is uncertain. PHEVs are more economic than BEVs and FCEVs in the short term (McKinsey & Company, 2010). However, the influence of large-scale electrification of the transport sector on the electricity system must be analysed and understood; for instance, if network extensions are necessary, this could be a major economic barrier for BEV and PHEV (Ball and Wietschel, 2008).

1.3.4.3 Fuel cell electric vehicle (FCEV)

The dominant fuel cell type is the Proton Exchange Membrane (PEM). H_2 is fuelled into the gas tanks under pressure, from 350 to 700 bars. H_2 fuel requires a purity of 99.99%; this quality level is higher compared to the level for industrial applications (99.95%) (ISO/TS 14687-2:2008 in (PHyRENEES, 2009)). The storage is made in a carbon fiber fuel tank. In fuel cells, electricity and water are usually produced from hydrogen and oxygen in an electrochemical reaction, which also releases heat. According to the American Academy of Sciences (Bento, 2010), the cost of platinum represents 57% of the final cost of the battery. In (McKinsey & Company, 2010), it is reported that 69% of the fuel cell power train cost is related to the fuel cell system and the H_2 tank and 25% to electric drive. FCEVs have a driving performance (similar acceleration), range (around 600 km) and refuelling time (< 5 minutes) comparable to ICEs. They are therefore a feasible low-carbon substitute for ICEs in longer trips. The emerging FCEV market (2010-20) requires close value chain synchronization and external stimulus in order to overcome the first-mover risk of building hydrogen retail infrastructure. The fuel cells exhaust produces zero emissions when fuelled by hydrogen. Road transport noise in urban areas would also be significantly reduced (Ball and Wietschel, 2008). Figure 1.3 shows a FCEV efficiency around 56% and H_2 could achieve 11-31% of WtW efficiency depending of the energy source. H_2 critics mainly base themselves on the energetic inferiority of hydrogen as an energy carrier compared to electricity (Haeseldonckx and D'haeseleer, 2011). However, hydrogen WtW efficiency is higher to that of gasoline in most of cases.

Even if BEV offers the best efficiency as vehicle with 68% its low km range is its main constraint associated. Then, the FCEV could be considered as a more flexible option in terms of km range at good vehicle efficiency (56%).

1.4 Hydrogen

Hydrogen occurs naturally in the form of chemical compounds, most frequently in water and hydrocarbons. It is a type of high-quality carbon-free energy carrier. Until the 1960s, hydrogen was used in many countries in the form of town gas for street lighting as well as for home energy supply (cooking, heating, lighting), and the idea of a hydrogen-based energy system was already formulated in the aftermath of the oil crises in the 1970s (Ball and Wietschel, 2008). In Europe, 80% of the total hydrogen was consumed by mainly two industrial sectors: the refinery (50%) and the ammonia industry (32%), which are both captive users (Dagdougui, 2011a). Currently only about 5% of hydrogen is considered as "marketable" and delivered elsewhere as a liquid or gas by truck or pipeline (Guillén Gosálbez et al., 2010). Hydrogen produced worldwide is about 700 billion Nm^3 per year (50 million t of H_2, enough to fuel more than 600 million FCEV) (Ball and Wietschel, 2008).

Hydrogen offers several advantages. It cannot be depleted and it can be stored over relatively long periods of time, compared to electricity. One kilogram of hydrogen is approximately equivalent to one gallon of gasoline based on lower heating value energy content (Midilli and Dincer, 2008)(Hugo et al., 2005)(Hake et al., 2006)(Heracleous, 2011)(Li et al., 2008)(Bartels et al., 2010). H_2 can be obtained from a number of primary energy sources, such as natural gas, coal, biomass and solar, wind and hydro energies, contributing towards greater energy security and flexibility (Hugo et al., 2005)(Midilli and Dincer, 2008). Another advantage is the variety of the production processes (Heracleous, 2011) and the distribution options in a variety of forms using different technologies: gaseous hydrogen, liquefied hydrogen (Li et al., 2008) and finally, it offers easy disposal and/or recycling of the reaction products (Hake et al., 2006).

Despite the potential benefits, and the previous attempts towards a hydrogen economy, its full realization faces a number of social, technical and economic obstacles. The establishment of a new hydrogen infrastructure for FCEV is difficult because no smart transition from gasoline/diesel to hydrogen can be expected due to the lack of bivalent operation modes for such vehicles (Hake et al., 2006).

Large investments are needed, these costs will play a major role on the final price of hydrogen (Bento, 2010). In many studies, the current lack of hydrogen infrastructure is noted as the most important barrier to develop the hydrogen economy (Kim et al., 2008)(Hugo et al., 2005)(Murthy Konda et al., 2011a)(Li et al., 2008). Special issues are noted in the storage-and-delivery infrastructure (Kim et al., 2008). Different configurations and options are being studied, for example, (Haeseldonckx and D'haeseleer, 2011) propose the use of existing natural gas and electricity infrastructures to power the hydrogen production units.

According to (Ball and Wietschel, 2008), the critical element is the cost development of the fuel cell propulsion system, whose forecasts are a major source of uncertainty. The end use technologies' manufacturers require a high density hydrogen demand before investing in the mass production of the end use technologies, while energy companies are hesitant to install hydrogen production, distribution and other infrastructures without having the assurance of profitable demand levels (Hugo et al., 2005)(Qadrdan et al., 2008). This problem is addressed as ''chicken and egg'' enigma, a real barrier to hydrogen economy. The introduction of any new fuel requires a significant capital investment and long-term commitment, while facing high risks of low demand, and accordingly, poor short-term returns. Timing of the investment over the next 10–30 years will be critical (Hugo et al., 2005).

The investment cost affects directly the H_2 fuel cost. The way to produce (according to a certain energy source), store and transport hydrogen will affect the CO_2 emission related to the WtT. Some questions must to be answered:

- is hydrogen competitive with current fuel prices?
- does hydrogen offer a real benefit in reduction of GWP?

Many studies and roadmaps focusing on hydrogen have been developed in which the targets to be reached for H_2 fuel price and CO_2 emissions are highlighted. These targets are briefly presented below.

1.4.1 H_2 cost

A kilogram of hydrogen has the approximate energy content of one gallon of gasoline; therefore the cost of hydrogen per kilogram is directly comparable to the gasoline cost per gallon (while there is a possibility that H_2 may receive some green tax benefits or tax exemption on environmental grounds (Murthy Konda et al., 2011a).

In US, in 2013 the prices varies from 3.00-4.00 US$/gallon (U.S. Energy Information Administration, 2013), see Table 1.2. In France, the gasoline price (unleaded 95) on July 2013 was 7.73 US$/gallon (1.55 €/L)[15] and for the Diesel 6.73 US$/gallon (1.35 €/L) (U.K. Drive Alive, 2013)[16].

Some studies have proposed or determined the hydrogen cost to be competitive in different time periods. (Ball and Wietschel, 2008) presented their targets trying to be representative for both the European Union and North America: around 2030, hydrogen costs range from 3.6–5.3 US$/kg in above mentioned regions, mainly depending on the feedstock. In the long term until 2050, hydrogen supply costs stabilize around this level, but with an upward trend due to the assumed increase in energy prices and CO_2 certificate prices.

The HyWays roadmaps (European Commission, 2008) propose that long-term hydrogen costs of 4.71-7.11 US$/kg (3.6–5.4 €/kg) can be achieved. The set of data is summarised in Table 1.3. From these data, the targets of hydrogen cost can be classified as follows, in periods 2020 and 2030, the cost must be lower than 5.3 US$/kg and in 2050 H_2 must cost less than 7.11 US$/kg.

[15] 19 March 2012 US$1.317 = 1.00 Euro.

[16] Date: July 18th 2013. The data is collected from various sources, some from official government websites, some from fuel companies' sites, and some from price comparison sites in the respective countries.

Table 1.2 Conventional fuel prices and H_2cost targets.

Year	Fuel	US$	€[6]	Reference
2013	Gasoline in US (gallon)	3.00-4.00	2.2-3	(U.S. Energy Information Administration, 2013)
2013	Gasoline in France (gallon)	7.73	5.8	(U.K. Drive Alive, 2013)
2013	Diesel in France (gallon)	6.73	5	(U.K. Drive Alive, 2013)
2020	H_2 (kg)	5.3	4	HyWays. (European Commission, 2008)
2030	H_2 (kg)	3.6-5.3	2.73-4.02	(Ball and Wietschel, 2008)
2030	H_2 (kg)	3.95	4	HyWays. (European Commission, 2008)
2050	H_2 (kg)	4-4.6	3-3.5	(Ball and Wietschel, 2008)
2050	H_2 (kg)	4.74	3.6	(Patay, 2008)
2050	H_2 (kg)	4.74-7.11	3.6 – 5.4	HyWays. (European Commission, 2008)
2050	H_2 (kg)	4.5-6.8	3.41-5.16	(Murthy Konda et al., 2011a)

1.4.2 CO_2 emissions

To get an idea of the potential CO_2 reduction achievable in the transport sector from the introduction of hydrogen vehicles, CO_2 emissions from hydrogen supply have to be compared on a WtW basis (i.e. energy source, producing, distributing and using the fuel, including primary production, extraction, transportation, refining, and finally vehicle operation) with conventional gasoline/diesel fuels. For example, in France, the WtW for an average ICE-Gasoline is 220 g CO_2/km and for the ICE-Diesel the total emissions are 196 g CO_2/km (TtW~ 188 and 176 g per km respectively)(ADEME, 2010). These numbers could then be compared to the life cycle of the FCEV-H_2 in order to better appreciate the advantages in terms of CO_2 emissions (see Table 1.3).

Table 1.3 Tank-to-wheel emission targets for vehicles 2010 and 2050 (g/km).

	Tank-to-wheel 2010 (g CO_2/km)	Tank-to-wheel 2050 (g CO_2/km)	Source
ICE Gasoline France	188.8	-	(ADEME, 2010)[17]
ICE Diesel France	176.1	-	(ADEME, 2010)
ICE Gasoline EU	~ 190	~ 100	(McKinsey & Company, 2010)
ICE Diesel EU	~ 165	~ 95	(McKinsey & Company, 2010)
FCEV	~ 120	0	(McKinsey & Company, 2010)
BEV	~ 60	0	(McKinsey & Company, 2010)
PHEV	~ 150	~ 20	(McKinsey & Company, 2010)

BEVs and FCEVs are commonly improperly considered as zero emissions (only TtW considered)[18]. GHG emissions from the life cycle of fuels for electric vehicles and FCEV must measure the upstream emissions related to the production of electricity or hydrogen. The emissions from these vehicles are thus entirely dependent on the manner in which the electricity and/or hydrogen is produced, along with

[17]Average TtW, not only for new cars.

[18]No emission from the vehicles themselves (except for water vapour in the case of FCEVs, and any emissions related to heating and cooling systems) (Institute of transportation studies (ITS UC DAVIS), 2011).

the energy efficiency of the vehicle (typically expressed in watt hours per mile or kilometre for BEVs, and miles or kilometres per kilogram for hydrogen-powered vehicles)(Institute of transportation studies (ITS UC DAVIS), 2011).

In 2009, a regulation setting binding targets on reducing the tailpipe CO_2 emissions (g/km) of new cars was brought into force within the European Union (EC Regulation No. 443/2009, 2009). This regulation sets a target for an overall average of 130 g/km tailpipe CO_2 from 2012 onwards. There are plans for further reductions of TtW emissions by 2020 to 95 g/km (equivalent to 113 g CO_2 per km – WtW-)(Boretti, 2011)(McKinsey & Company, 2010). Hydrogen should be below these targets in a WtW perspective.

1.4.3 Safety

In 1990, the International Standard Organisation (ISO) has established a technical committee to develop standards in the field of production, storage, transport and various applications of hydrogen as for example, the European Integrated Hydrogen Project (EIHP), which makes proposals for the regulation of FCEV and the hydrogen activities (CEA, 2013). Another project that works with the issues regarding safety is addressed by the European Network of Excellence HySafe on a technical level (European Commission, 2008). Hydrogen storage is regarded as one of the most critical issues, which must be solved before a technically and economically viable hydrogen infrastructure implementation. In fact, without effective storage systems, a hydrogen economy will be difficult to achieve (Dagdougui, 2011a).

To ensure the safely use of hydrogen, it must essentially prevent leakage, since hydrogen is flammable and explosive, and any "confined" situation can be dangerous. This involves the use of appropriate safety devices[19] (fans, sensors ...). A good knowledge of these dangers and their consequences is intended to implement a safe design of systems using hydrogen. Besides, hydrogen is non-toxic and is very volatile.

Although the H_2 is commonly used in industry, it is often considered as a hazardous gas. Hydrogen is actually no more dangerous than other flammable fuels such as gasoline and natural gas. Nevertheless, under specific conditions, hydrogen can behave dangerously. The burning or explosion of hydrogen causes most fatal accidents. Therefore, when hydrogen infrastructure design strategies are established, safety considerations are of paramount importance for the sustainable hydrogen economy (Kim and Moon, 2008),(Hake et al., 2006).

[19] It is difficult to detect without appropriate sensors because it is colorless, odorless and airborne flame is almost invisible.

In the transition to a hydrogen economy, the public perception of safety is a critical issue. Although the public view on hydrogen is in general positive, an early large accident could change this quickly. As the new hydrogen applications cover new operational domains, like high pressures or cryogenic temperatures, the successful and safe usage in industrial processes might not be translated directly to all these cases. All the stages of the hydrogen fuel network must be studied to try assuring the best conversion to this economy.

1.4.4 Social perception and acceptability

To better understand the term acceptability, we had an opportunity to have an interview with Christophe BESLAY, Professor in Sociology (Toulouse University), who is an expert in the field of energy and issues of acceptability. According to his experience, it does not represent a market problem by now; the real problem is the lack of political and industrial mobilization. There are technological advances which could help the hydrogen economy and also scientific and technical research is done to overpass the technical problems such those related to storage. In this moment to focus on the use and acceptability of hydrogen would be a false debate.

Government and industry must be convinced and take the first step. Communication between them is the key point to understand the benefits of this technology. The general process for the social integration of new technologies is given in three phases: the first is the stage where the manoeuvres of the major players (government and industrials) work with the strategy related to the technology. The second is the experiment period with smaller stakeholders. In this stage, it is possible to compare the design and real usage. A lot of tension between these two phases could exist. Finally the last step is the appropriation (related to use) and diffusion of innovation to the major public.

The study AIDHY/CEA (Le Duigou, 2010) conducted in 2010 was a decision support for the identification and support to societal changes brought by new hydrogen technologies. It analysed the acceptability among users and experts. According to this presentation, the public is not worried by safety issues about the use of hydrogen. Potential 77% of people said to be interested in this fuel, strong acceptability appeared in highly urban areas.

The public debates before a project on a particular topic can be convenient because the potential options must be sufficiently explained (e.g. BEV vs. FCEV); one of the challenges is to demonstrate that they are part of a long-term vision. In France, the National Debate for the Energy Transition (*"Débat national sur la transition énergétique 2013"*) allows to discuss some questions like: How can France move towards energy efficiency and energy conservation? How to achieve the energy mix targets? Which renewable energies should France rely on? These points, and others, are discussed by the civil society and experts. The Regional Innovation Agency MPI (Midi-Pyrénées Innovation)

organised this debate on June 3rd, 2013 in Toulouse, treating the "*hydrogen as fuel*" topic based on the results obtained in this work in a case study of the Midi-Pyrénées region that will be treated in the fifth chapter of this thesis.

Communication efforts will always be important in the transition phase, since each stakeholder has its own "language" and a large quantity of analysis about potential scenarios regarding the H_2 economy is mandatory. In this sense some roadmaps and transition plan scenarios have been developed all around the world but the pertinence of each study depends in the general or particular focus of the approach (for example a company study vs. a national study), the limits of the system treated, etc. The most representative works are briefly presented in the next section.

1.5 Roadmaps and transition plan scenarios

1.5.1 Roadmaps

A *roadmap* provides a blueprint (program, project) for the coordinated, long-term, public and private efforts required for hydrogen energy development: some objectives are fixed for a determined time period. The roadmaps for the hydrogen economy are widely deployed by many countries around the world. Roadmaps have been generally used to aid decision-making and business planning.

In Europe, in the *HyWays project* (2007-2008), over 50 member state (MS) workshops were conducted with key stakeholders. The HyWays combine technology databases and socio-techno-economic analyses to evaluate selected stakeholder scenarios for future sustainable hydrogen energy systems. In this project, market scenarios[20] for hydrogen end-use applications were also developed. Each country outlined its own preferences (Finland, France, Germany, Greece, Italy, the Netherlands, Norway, Poland, Spain and the United Kingdom). The HyWays project differs from other road mapping exercises as it integrates stakeholder preferences, obtained from multiple member state workshops, with extensive modelling in an iterative way. The stakeholder validation process, which takes into account country specific conditions, is a key element of the road mapping process. In Europe, the prospect of hydrogen economy plays a major role, especially because of two main conditions: the aggregation of many countries that have various specific institutional, opportunities, conditions, territorial and socio-economic barriers (Dagdougui, 2011b). Another well-known roadmap is *H_2 Mobility* (2010), fixing a plan to introduce the use of FCEV in Europe, starting in Germany and UK (Williamson, 2010) whereas H_2 Mobility France began in 2013. In this program, the main car manufacturers and gas producers are involved.

[20] The planning of scenarios can be considered as a systematic tool that supports designing the HSC. The main objective of scenarios is to think about what will be the decisions making process under a certain situation that usually cannot be determined with precision. The use of scenarios can serve as guidance for the implementation of certain policies and measures to obtain a desirable future position (Dagdougui, 2011b).

Iceland can be identified as the first hydrogen economy in the world. *The Icelandic New Energy* is a partnership that was established between the Icelandic government, Shell, Norsk Hydro, Ford and the University of Reykjavik. It is a pioneering initiative to create the first hydrogen economy in the world by 2040 (Dunn, 2000). The project aims to promote energy independence by exploiting the vast renewable resources of the island such as geothermal and hydropower. In 2003, the country inaugurated the first hydrogen station in the world to supply the three hydrogen buses that ran through the ECTOS program until the end of 2006. In 2007, a new demonstration phase began with 13 SMART-H_2 model cars and boats to hydrogen (Bento, 2010).

World Energy Network (WE-Net, 1993) established in *Japan* as the first major national program for hydrogen and fuel cells. This was made possible by cooperation between government, research institutes and industry, managed by the 'New Energy and Industrial Technology Development Organisation" (NEDO). This program had a goal planning and implementation of R&D for hydrogen technologies. In the first phase (1993-1998), the program was oriented research, and building a vision for hydrogen in Japan. In the second phase (1999-2002), the project has also been a priority for the technology demonstration and infrastructure. R&D expensed during the two phases were in the range of $200 million (Solomon and Banerjee, 2006)(Bento, 2010). In 2008, the *Japan Hydrogen and Fuel Cell demonstration project* (JHFC) was launched. The objective was to improve energy efficiency by 30% between 2003 and 2030, to reduce CO_2 emissions by 50% in 2050 as well as to decrease dependence regarding imports of oil from 47% to 40% by 2030 (from 97% to 80% in transport).

The *U.S.* Department of Energy (*DOE)* has been managing the hydrogen program in cooperation with industry, national laboratories, universities, and government agencies since 2007. The marketing decision should be taken by the industry as the competitiveness of FCEV and hydrogen. This decision is planned for 2015 subject to the achievement of technological goals (Bento, 2010)(Patay, 2008).

The National Innovation Program (NIP) is a program for the development of hydrogen and fuel cells combining industrial and German scientists, initiated in 2007 with support from the government. In the *Clean Energy Partnership*, *Germany* plans to build large-scale public stations with the goal of 2020. 1,000 stations by the German government claims invest 1.5 to € 2 billion until 2017 and hopes to have enough gas stations by 2013 to make possible to link the north and south of the country by car, about 870 km. (CEP). Berlin is the main city for this international cooperation between BMW Group, Berliner Verkehrsbetriebe BVG, Daimler, Ford, GM, Hamburger Hochbahn, Linde, Shell, StatoilHydro, Total, Vattenfall Europe and Volkswagen. The programs in Germany are run by a dedicated independent structure: *NOW GmBH* (National Organisation Wasserstoff-und Brennstoffzellentechnologie)(NOW).

Norway, Sweden and Denmark participate at the *Scandinavian Hydrogen Highway Partnership* that was founded by 133 companies, national associations and hydrogen programs in Norway (HyNor), Sweden (Hydrogen Sweden) and Denmark (HydroLink). The goal is to drive the transition in this region by the validation of the viability of the use of hydrogen in everyday life. The demonstration includes 500 hydrogen cars, 100 buses and 500 cars during the period 2012-2015. The flagship project is the establishment of hydrogen stations along the highway between the cities of Oslo and Stavanger, Norway, and widening the road to Sweden and Denmark (Scandinavian Hydrogen Highway Partnership).

In *France*, the French Association for Hydrogen and Fuel Cells (Association Française pour l'Hydrogène et les Piles à Combustible*: AFHYPAC*) started a French study on H_2 power and mobility on May 2013. This association is working with more than twenty consortium partners in the *H_2 Mobility in France* roadmap to produce a competitive implementation plan, supported by private and public hydrogen infrastructure stakeholders over the period 2015-2030. Private and public actors, regional, national and international, coordinated by the AFHYPAC and under the aegis of the Ministry of Ecology, Sustainable Development and Energy will develop a roadmap with the basis of different deployment scenarios for FCEV and refuelling stations, showing the benefits and costs of the transition data (AFHYPAC). The results will be soon published. *Seiya Consulting*[21] in partnership with the AFHYPAC organised *HyVolution*, a French event dedicated to hydrogen technology and fuel cells, (5-8 September 2013) in Albi.

The Agency for Environment and Energy Management (Agence de l'environnement et de la maîtrise de l'énergie: *ADEME*) takes part in the implementation of public policies in the areas of environment, energy and sustainable development. ADEME roadmap was lanced in 2010 where 5 strategic pillars to the vision 2020 related FCEV and H_2 were developed: a) hydrogen and renewable energy convergence; b) electro-mobility new generation; c) batteries and hydrogen for sustainable development in the cities; d) hydrogen and batteries as vectors for international growth; e) transverse support of the industry measures. The necessity of research priorities and demonstrators was clearly highlighted. By 2015, 5000 FCEV for captive fleet use and 2-5 cities equipped with fuelling stations are planned (ADEME, 2011).

At a regional level, one of the most famous H_2 plans can be found in *California*. Since 1999, demonstration projects are managed by the partnership for the promotion of hydrogen in the *California Fuel Cell Partnership* (CaFCP). This partnership was established between the company Ballard Power Systems, Daimler Chrysler and Ford Motor Company, Shell Hydrogen, and Chevron

[21] http://seiya-consulting.com/

(formerly ARCO), and the California agencies (California Air Resources Board and California Energy Commission). Its mission is to facilitate the commercialization of fuel cells for transportation. Since then, the CaFCP supported the establishment of stations and experienced more than 170 hydrogen vehicles. Stations are normally financed by the state government (Bento, 2010). More recently, two programs, California Fuel Cell Partnership and *California Energy Commission and Air Resources Board* are in effect. The former is a roadmap for fuel cell vehicles and hydrogen stations and the latter is a program of incentives for vehicles and fuelling infrastructure from state agencies (Yang and Ogden, 2013).

In the *Midi-Pyrénées* region (which has a one-tenth area of that of California), *PHyRENEES* association was established in October 2007 around several partners (Ecole des Mines d'Albi, INPT, Trifyl, N-GHY, Airbus, GDF, ARAMIP and the General Council of the Tarn). One of its missions was to contribute to a national roadmap for the development of the program « H_2 mobility » as presented in November 2012 (Dupin-Janson, 2012). French car manufacturers (Renault, PSA /Peugeot-Citroën/ and Mia Electric), Michelin for equipment and the energy actors (CEA, Air Liquide and Total) are involved in this contribution. The *Midi-Pyrénées roadmap* projects a forecast of 200 FCEV for captive fleet use in the region with 5 refuelling stations and 20 logistics handling equipment fuel cell powered by renewable hydrogen in 2015 (Grano, 2011). This plan is consistent with the ADEME roadmap. In the Midi-Pyrénées region, the first H_2 refuelling station was installed in Albi in September 2013. In the same month, a demonstration site of production of hydrogen by bio-methane started to operate in *Trifyl*[22].

In 2013, the « *Journées H_2 dans les territoires* » took place from 16 to 17 May 2013 in Albi, France. One of the main objectives of the session was to inform and try to link the National and European policies to local (regional) actions. We had the opportunity to attend this event. In France, various regions are working in roadmaps to the development of H_2 for electro-mobility, some examples are Midi Pyrénées (PHyRENEES and Midi-Pyrénées Innovation), Nord-Pas-de-Calais (Roadmap 2014-2020), Lorraine (Nancy project and Livre blanc Alphea), Pays de Loire (Navy-bus project), Bretagne, Provence-Alpes-Côte d'Azur, Franche-Comté, Rhône Alpes, Corse (Myrthe project), Nord-Pas-de-Calais and Haute-Normandie (AFHYPAC et al., 2013).

Finally, it must be highlighted that the value of the road mapping process lies in the development of the comprehensive review of the identification of the research needs, threats and opportunities (a kind of SWOT analysis) and they also establish the targets to be reached. The roadmaps show that there is a

[22] http://www.trifyl.com/

crucial need to describe more precisely the "how" and the "who" for a range of technological components involved in the whole supply chain.

1.5.2 Transition plan scenarios

Other authors/institutions have presented transition models to the future HSC. The *transition plan scenarios* are usually accompanied with the cost estimation of the hydrogen pathways and even if environmental impacts could be also estimated, they are not optimised. They report the cost for each demand scenario with various hypotheses. The objective here is not to model the hydrogen infrastructure from the mathematical viewpoint, but to understand the behaviour of the hydrogen supply chain in certain areas assuming specific scenarios. These transition models are implemented on national or/and regional scales, aggregating simultaneously territorial information and specific data such as local policies and regulations (Dagdougui, 2011b).

In (Bento, 2010), the objective is to understand what are the positive factors and the barriers in the transition from a large carbon emitter energy system based on fossil fuels to a hydrogen economy in Europe, and to figure out how it can be arranged. In this study, different demand scenarios are analysed.

A recent study entitled "*A portfolio of power-trains for Europe: a fact-based analysis*" (McKinsey & Company, 2010) provides a factual comparison of four different power-trains – BEVs, FCEVs, PHEVs and ICEs – on economics, sustainability and performance across the entire supply chain (WtW) between now and 2050, based on confidential and proprietary industry data. Various scenarios with different potential hydrogen demand behaviour (three scenarios 5, 25 and 50% at 2050) were built. The study was conducted at a continental level. This study considered the interconnection with many stakeholders of the HSC including vehicle producers (i.e. BMW AG, Daimler AG, Ford, General Motors LLC, Honda R&D, Hyundai Motor Company, Kia Motors Corporation, Nissan, Renault and Toyota Motor Corporation), industrial gas companies (Linde and Air Liquide). From 2010 to 2020, all cost and performance projections are based on proprietary industry data and on projected learning and annual improvement rates after 2020.

Transition plan scenarios can be taken as an important basis for more precise studies where the different potential activities of the network can be measured and analysed (e.g. mathematical optimisation to design the hydrogen supply chain). The different roadmaps and transition plan scenarios that already exist and that have been presented represent necessary information and can be considered as the starting point to launch more detailed analysis because of the definition of general targets and of the coordination and communication efforts from which valuable information is shared.

Table 1.4 Roadmaps and transition plan scenarios

Program or institution	Scale	Year	Description	Source
HyWays	Europe	2007-08	Some market scenarios for hydrogen end-use applications are developed (Finland, France, Germany, Greece, Italy, the Netherlands, Norway, Poland, Spain and the United Kingdom).	(Dagdougui, 2011b)(European Commission, 2008)
H_2Mobility	Europe	2010	This roadmap plans to introduce the use of FCEV in Europe, starting in Germany and UK.	(Williamson, 2010)
Université de Grenoble	Europe	2010	The objective of this thesis is to understand the positive factors and the barriers in the transition to a hydrogen economy in Europe.	(Bento, 2010)
A portfolio of power-trains for Europe: a fact-based analysis	Europe	2010	It provides a factual comparison of four different power-trains – BEVs, FCEVs, PHEVs and ICEs – on economics, sustainability and performance across the entire supply chain (well-to-wheel) between now and 2050, based on confidential and proprietary industry data.	(McKinsey & Company, 2010)
The Icelandic New Energy	Iceland	1999	This is the first hydrogen economy in the world. A partnership was established between the Icelandic government, Shell, Norsk Hydro, Ford and the University of Reykjavik. The project aims to promote energy independence by exploiting the vast RES of the island such as geothermal and hydropower.	(Bento, 2010)
World Energy Network (WE-Net) (2003) / Japan Hydrogen and fuel cell demostration project (JHFC) (2008)	Japan	2003-08	The WE-Net was the first major national program for hydrogen and fuel cells managed by the 'New Energy and Industrial Technology Development Organisation "(NEDO). The objective of the JHFC: improving energy efficiency by 30% between 2003 and 2030, reducing CO_2 emissions by 50% in 2050.	(Solomon and Banerjee, 2006) in (Bento, 2010)
Clean Energy Partnership	Germany	2007	Plans to build large-scale public stations with the goal of 2020. 1,000 stations by the German government claims invest 1.5 to € 2 billion until 2017 and hopes to have enough gas stations by 2013 to make possible to link the north and south of the country by car, about 870 km.	(CEP; NOW.)
ADEME roadmap	France	2010	By 2015, 5000 FCEV for captive fleet use and 2-5 cities equipped with fuelling stations are planned in France	(ADEME, 2011)
H_2 power and mobility	France	2013	AFHYPAC is working with more than twenty consortium partners in the H_2 Mobility roadmap to produce a competitive implementation plan, supported by private/public stakeholders over the period 2015-2030.	(AFHYPAC et al., 2013)
California Hydrogen Highway	California	1999	This partnership was established among Ballard Power Systems, Daimler Chrysler, Ford Motor Company, BP, Shell Hydrogen, Chevron, and the California agencies (California Air Resources Board and California Energy Commission). Its mission is to facilitate the commercialization of fuel cells for transportation. Stations are normally financed by the state government	(Bento, 2010)
California Fuel Cell Partnership - California Energy Commission and Air Resources Board	California	2009	The former is a roadmap for fuel cell vehicles and hydrogen stations and the latter is a program of incentives for vehicles and fuelling infrastructure from state agencies	(Bento, 2010; Yang and Ogden, 2013)
PHyRENEES	Midi-Pyrénées	2010	According to the Midi-Pyrénées roadmap, a first step will be reached in 2015: 200 FCEV for captive fleet use in the region with 5 refuelling station and 20 forklifts fuel cell powered by renewable hydrogen.	(Grano, 2011)
Scandinavian Hydrogen Highway Partnership	Scandinavia	2012	Founded by 133 companies, national associations and hydrogen national programs in Norway (HyNor), Sweden (Hydrogen Sweden) and Denmark (HydroLink). The goal is to drive the transition in this region by the validation of the viability of the use of hydrogen in everyday life. The demonstration includes 500 hydrogen cars, 100 buses and 500 cars during the special period 2012-2015.	(Scandinavian Hydrogen Highway Partnership)

The principal limitations related to these macro studies are yet the difficulty to generate specific results related to the location, size and number of production, storage or transport units and also the lack of interconnection between the different objectives. Their principal advantage is that they provide valuable information that can be used to implement scenarios of interest, thus demonstrating or not the potential of hydrogen infrastructure. They will be particularly useful to define the scenarios of interest that will be used in the implementation of this work. The main references that will serve as a useful basis are summarised in Table 1.4.

1.6 Scientific objective and motivation of the study

Driven by concerns over energy security, urban air quality and global warming potential, a transition from the current energy system has become an urgent and essential task that receives significant attention. To get the new boundaries related to transport issues, different worldwide options started to be studied, i.e. the carbon tax, the incorporation of CCS in the processes to obtain petroleum products, the improvement in the internal combustion engine efficiency, the promotion of public transport and also the development of new fuel alternatives and propulsion engines. The introduction to the market of new propulsion systems such as BEV, PHEV and FCEV can treat the abovementioned problems.

Among these options, the FCEV fuelled by hydrogen may offer benefits in terms of reducing CO_2 and harmful pollutant emissions. FCEV power trains are competitive to ICE in the WtW efficiency point of view. The use of hydrogen can also improve the security of primary energy supplies. The FCEV could be considered as a flexible option in terms of km range at good fuel and vehicle efficiencies (competitive with conventional fuels).

Hydrogen offers many advantages as a potential fuel. More precisely it is capable to treat the main energy problems presented in the first section of this chapter. Many energy sources, production processes, transportation and storage modes exist. Then, the way as hydrogen economy could be developed is very flexible. At the same time, all these options are not really interconnected and well-studied; then, the lack of infrastructure constitutes one of the main challenges in the hydrogen and FCEV path. The way as this network is developed will affect the cost, the CO_2 emissions and some safety conditions. By 2020, hydrogen should be below to 95 g/km to be competitive with ICE (Boretti, 2011)(McKinsey & Company, 2010). One of the most significant obstacles to achieve the hydrogen transition is the general perception that the cost associated to the infrastructure would be prohibitory expensive compared to the current fuels. According to the dedicated literature, H_2 cost must be lower than 5.3 US$/kg in periods 2020 and 2030, and H_2 will cost less than 7.11 US$/kg in 2050. Regarding safety, hydrogen is actually no more dangerous than other flammable fuels such as gasoline and natural gas. Nevertheless, under specific conditions, hydrogen can behave dangerously. To ensure the safely use of hydrogen, it must be essential to know how to manage the risks. In terms of acceptability

the study AIDHY/CEA found that the public is not close and/or worried about the use of hydrogen. Communication is important in the early stage, so that a large quantity of analysis and information about potential scenarios regarding the H_2 economy is mandatory.

Currently, a large amount of literature related to hydrogen can be found. The roadmaps as HyWays and H_2 mobility are guiding many projects in Europe. They establish a certain number of targets in a very general perspective. In some cases, not all the network is considered but a particular activity (e.g. to install a certain number of filling stations). Moreover, some transition plan scenarios study different ways as the hydrogen economy could be reached and they evaluate external variables as competitors and demand. It can been highlighted that a study which considers the whole hydrogen supply chain that can be shared with the government, industrials and universities seems pertinent in this stage to aid decision-making. This work lies in this perspective and the scientific objective is to develop a generic framework that can take into account the design of a hydrogen supply chain with many energy sources and that can embed the various production and storage technologies, while considering the transportation modes to link hydrogen demand to its supply. More practically, the aim is to develop an optimisation tool that could allow the generation of quantitative information when all the nodes of the supply chain are defined and integrated. The general literature survey clearly highlights that the design of the hydrogen supply chain involves a multi-criteria formulation in which cost, environmental impact and safety must be simultaneously taken into account at the earlier design stage. Particular emphasis will thus be devoted in this work to address the multi-objective formulation and solution of the design of the hydrogen supply chain.

More specifically the developed tool intends to answer the following questions:

- is hydrogen competitive with current fuel prices?
- does hydrogen offer a real benefit in reduction of GWP?
- which is the safest option for the hydrogen supply chain?
- what is the best option for production and storage of hydrogen?
- what are the most cost effective transportation modes and pathways to connect hydrogen demand with its supply?

To bring insight to this issue, this manuscript is organised as depicted in Figure 1.4.

- The supply chain management seems relevant because it integrates suppliers, manufacturers, warehouses, and stores, so that hydrogen is produced and distributed at the right quantities, to the right locations, and at the right time, in order to optimise the whole system. This approach is presented in **Chapter 2** following this chapter that positions the general energy context in the transportation sector and that justifies the interest of using hydrogen as an energy vector.

Chapter 2 also involves a brief description of the hydrogen supply chain activities. A literature review related to supply chain optimisation is then conducted. This analysis leads to propose the key points that motivated this work and that positions the proposed modelling framework based on a multi-objective approach as an original one.

- **Chapter 3** presents the modelling and optimisation methods and tools that will be used and developed throughout this work. The general methodology that will be applied at the different levels of approach and that will be tackled is developed for hydrogen supply chain deployment, either at national or regional scales.
- The mathematical model with the considered constraints and objectives is presented in **Chapter 4**. This model is applied to a case study reported in the literature survey and dedicated to Great Britain for validation purpose. This chapter compares the mono- and multi-objective approaches and clearly highlights the benefits of a multi-objective approach.
- **Chapter 5** is dedicated to the modelling and optimisation of the HSC in the Midi-Pyrénées region through the project "*Green H_2 fuel*" initiated by PHyRENEES, Midi-Pyrénées Innovation (MPI) and the LGC. The mathematical model presented in Chapter 4 is adapted to the specific features of the region and its energy sources. A mono/multi period problem is treated. Optimisation scenarios are performed first through mono-objective cases considering the three objective functions (cost, CO_2 and risk) and then the multi-objective cases are tackled using Ɛ-constraint and lexicographic methods for the optimisation stage. The so-called TOPSIS (Technique for Order Preference by Similarly to Ideal Solution) multiple criteria decision making follows the optimisation step. The geographic information system (GIS) is introduced in the last section of this chapter, technology that allows organising, analysing and mapping spatial data.
- The optimisation of the HSC is then applied to the national case of France in **Chapter 6**. The objective is twofold in this chapter: on the one hand, to examine if the methodology is robust enough to tackle a different geographic scale and second to see if the regional approach is consistent with the national scale. New data collection, demand prediction and assumptions are involved but the same model as the one applied to the Midi-Pyrénées region is used here with minor differences. In this case study, the GIS spatial tool is used before optimisation to identify the geographic items that are further used in the optimisation step. First, the mono-objective optimisation strategy is presented. Second, the multi-optimisation approach with Ɛ-constraint is analysed and discussed. Finally, a new scenario considering the decision maker preferences is described following the economic cycle.
- Conclusions and perspectives are presented in **Chapter 7**.

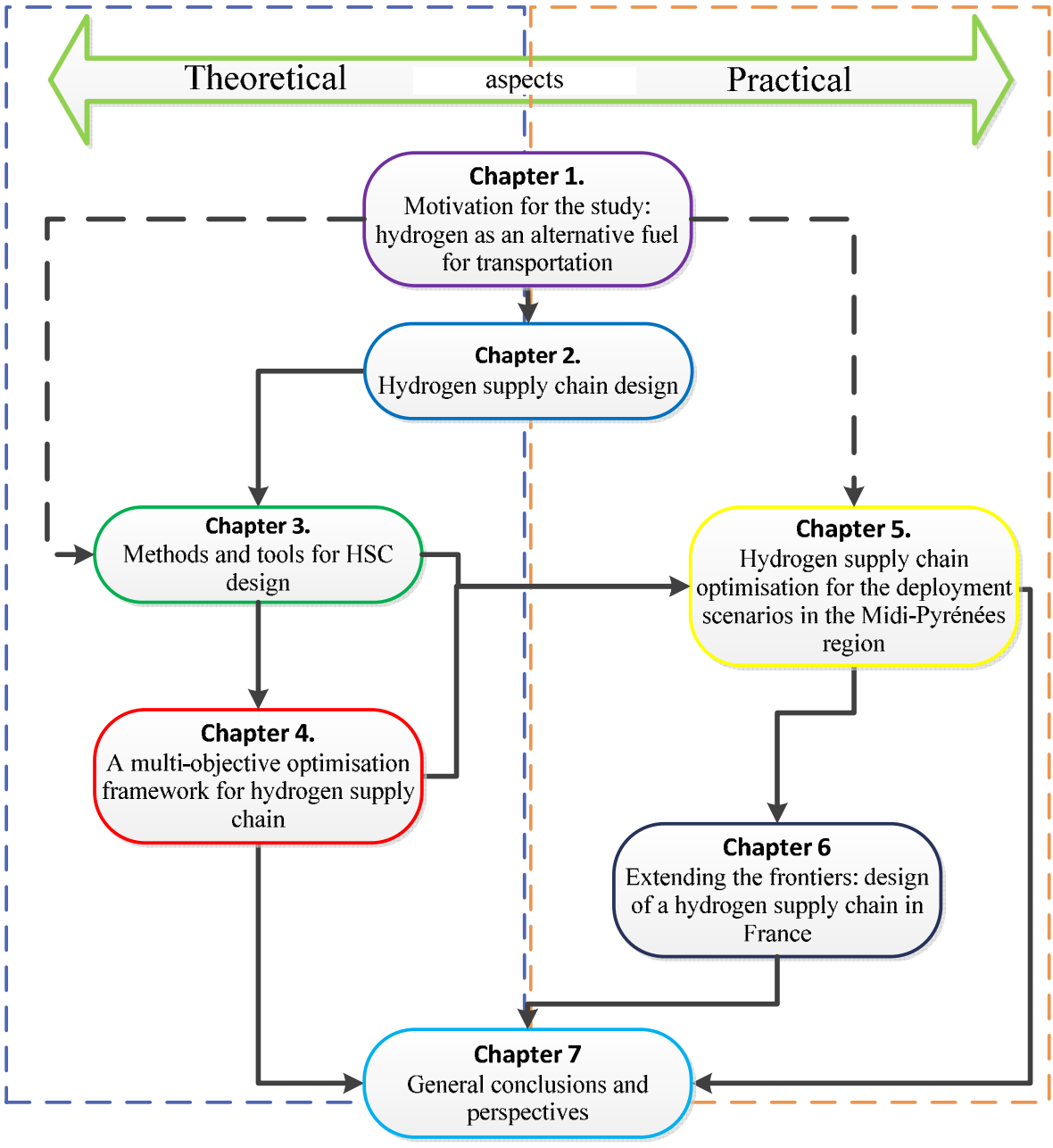


Figure 1.4 Schematic description of the manuscript

Chapter 2

HYDROGEN SUPPLY CHAIN DESIGN

Résumé

L'objectif de ce chapitre est de présenter le concept de la chaîne logistique de l'hydrogène et les principales activités qui y sont impliquées, i.e., production, stockage, transport et distribution. Elles serviront de briques élémentaires dans la modélisation globale de la chaîne et de son optimisation. Une analyse de la littérature dédiée à la modélisation de la chaîne logistique hydrogène est ensuite proposée. L'ensemble de ces éléments conduit au développement d'un modèle basé sur une formulation de type optimisation multi-objectif en variables mixtes prenant en compte trois types de critères : économique, environnemental et lié à la sécurité du procédé. Un point clé consistera à prendre en compte les aspects spatio-temporels, mono/multi-période et échelle régionale/nationale. Une attention particulière sera aussi apportée aux contraintes géographiques, à travers l'utilisation d'un outil de géolocalisation.

Abstract

The aim of this chapter is to present the concept of hydrogen supply chain with its associated activities, i.e. production, storage, transportation and distribution. These items are the elementary bricks of the global modelling the network. The current state of the art related to the hydrogen supply chain design is also presented. The formulation of a multi-objective optimisation model is then proposed taking into account economic, environmental and safety criteria. A key point concerns the consideration of spatial-temporal aspects involving either mono or multi-period approaches and different geographic scales and breakdowns. A particular attention is paid to the geographic constraints, which can be analysed through a dedicated *geographic information system* (*GIS*).

Acronyms

ASU	Air separation unit
BG	Biomass gasification
CCS	Carbon capture and storage
CG	Coal gasification
CH_2	Compressed hydrogen
CSP	Concentrating solar power
GIS	Geographic Information System
HSC	Hydrogen supply chain
LH_2	Liquid hydrogen
LP	Linear programming
MILP	Mixed Integer Linear Programming
MOREHyS	Model for Optimisation of Regional Hydrogen Supply
PEM	Proton Exchange Membrane
PSA	Pressure swing adsorption
PV	Photovoltaic
RES	Renewable energy sources
SCM	Supply chain management
SMR	Steam methane reforming
WtW	Well-to-wheel

2.1 Introduction

Chapter 1 highlighted the lack of existing infrastructure for hydrogen deployment that is largely reported in the dedicated literature. One contribution of this thesis is to model the supply chain management (SCM) for hydrogen. SCM generally uses a set of approaches to efficiently integrate suppliers, manufacturers, warehouses, and stores, so that merchandise is produced and distributed at the right quantities, to the right locations, and at the right time, in order to minimise system wide cost while satisfying service level requirements (Papageorgiou, 2009) while taking into account other constraints. As previously explained in chapter 1, the pathway towards a hydrogen economy and more particularly here towards the use of hydrogen as an energy vector must encompass a broad range of items concerning the three pillars of sustainability based on economic, environmental and social impacts. SCM models can be used to design improved business pathways which could result in reduced environmentally impact while satisfying local regulations and international treaties for greenhouse gas emissions while being also economically achievable.

The management of supply chains is a complex task mainly due to large size of the physical supply network and inherent uncertainties and decisions (Papageorgiou, 2009):

- number, size and location of manufacturing sites, warehouses and distribution centers, and the resources inside them;
- production decision related to plant production planning and scheduling;
- network connectivity (e.g. allocation of suppliers to plants, warehouses to markets, etc.);
- management of inventory levels and replenishment policies;
- transportation decisions concerning mode of transportation (e.g. road, rail, etc.) and also sizes of material shipments.

The SCM can broadly be divided into three main categories:

(i) supply chain design;
(ii) supply chain planning and scheduling;
(iii) supply chain control (real-time management).

A supply chain network refers to a network of firms engaged in manufacturing, assembly or storage of parts to create a product. The firms are grouped in nodes that represent the functionality that the finished product must perform, with the arcs between the nodes capturing the precedence constraints among them (see some examples in Figure 2.1 and 2.3). Each node typically has several ways to accomplish its function and is a potential stock point for inventory. Deciding what option should be employed at each node and where inventory should be placed among these nodes is called “supply chain configuration” (Nepal et al., 2011). These *decisions* may depend upon many factors such as lead time, cost, relationships and other constraints. The procurement nodes are those that do not have any

incoming arcs (i.e., they represent the purchase of components outside the supply chain). The assembly/manufacturing/transferring nodes represent nodes where one or more components are combined together.

Instead of selecting the lowest cost bidder as that used to be the standard industry practice in the past, companies are now considering other performance indicators to improve their systems. Cost, operability, reliability, environmental impacts, safety and social implications are all performance measures that should be considered when assessing the different pathways as viable long-term alternatives (Hugo et al., 2005)(Li et al., 2008). Research opportunities are evident in the appearance of new types of supply chain associated with sustainability and resource efficiency.

SCM can be based either on mathematical programming or on simulation techniques and their application depends on the type of problem or task. The distribution of hydrogen as a fuel for the entire population of a region, a country and a continent, will require the gradual deployment and long-term major infrastructure.

The systemic consideration of a hydrogen supply chain (HSC) in a general perspective can be divided into different phases: technologic development and/or improvement, implementation assessments, implementation phase, operation, maintenance and dismantling (Patay, 2008). Currently not all the potential technologies to be used in the HSC are mature. Studies on the design of these technologies are then required. The whole life cycle of the system is out of the limits of this thesis but a general review of the current status of such technologies is needed in order to contextualize and design scenarios that will be further used. The core of this study concerns the implementation assessment or supply chain design where different potential scenarios of the HSC are analysed at a strategic stage.

The remainder of this chapter is organised as follows; in the next section (2.2), the HSC for an industrial and mobility use is introduced. The system is represented by nodes and connections and a general HSC is displayed. Different hydrogen activities (production, storage, transportation, etc.) are involved in a HSC and will be presented. Hydrogen can be produced from both fossil and renewable resources (section 2.3). Section 2.4 reviews the different technologies related to the various sources. It is highlighted that hydrogen can provide storage options for intermittent renewable technologies such as solar and wind and might thus facilitate the large-scale introduction in the energy mix. The centralisation degree according the plant capacity is introduced, and processes such as steam methane reforming, gasification and electrolysis are presented. Finally the issue related to CO_2 capture and storage is mentioned. Hydrogen conditioning and storage are the core of section 2.5. Section 2.6 is devoted to transportation with different modes as pipeline, tube trailer and tanker truck to supply H_2 fuel to the refuelling stations (section 2.7). All these activities need to be integrated in a systematic

modelling framework that allows a more precise approach than roadmaps and planning scenarios (as previously explained in chapter 1). Then, the modelling approaches of the HSC are described in section 2.8 and a literature review is performed in section 2.9. This analysis emphasizes that achieving the potential benefits of a hydrogen system requires careful integration of production, storage and end-use components with minimised cost and maximised efficiency, and a strong understanding of environmental impact, reliability and opportunities. These positions this work in a system modelling approach based on a multi-objective optimisation framework (section 2.10). The developed system tool will provide the platform for standardised comparisons of energy systems for specific applications.

2.2 Hydrogen supply chain

2.2.1 H_2 supply chain for industrial uses

H_2 production was 90 billion Nm^3 in Europe and 7 billion Nm^3 in France in 2007 (PHyRENEES, 2009). While most of it is produced onsite for captive uses, a significant portion of H_2 produced today is a by-product in the chemical industry (e.g. chloralkali electrolysis) and, since there is no specific purpose, this is sometimes wasted, flared or treated by gas industries. The production of chlorine is a key industry. France has the second ranking place just after Germany. Three main chlorine producers share the market in 10 sites all around the country: Arkema (before Atofina), Solvay and Chloralp (exportations of 4.3 million of t in 2007).

In current schemes, the logic of industrial distribution is generally as follows: hydrogen is produced in centralised plants or produced onsite for captive uses. H_2 is obtained mainly from Steam Methane Reforming (SMR) and coal gasification and also obtained as a by-product in from the chloralkali electrolysis plants. It is used on-site or transported (short distances) by pipelines. The option to be liquefied or compressed and then transported via tube trailers or tanker trucks also exists but is less frequent. Ammonia production plants, oil processing units, methanol and metal industries are customers with high demand volume (see Figure 2.1).

2.2.2 H_2 supply chain for mobility

The hydrogen supply chain for H_2 as fuel is defined as a system of activities from suppliers to costumers. These activities are: energy source, production, storage, transportation, and dispensation of hydrogen to refuelling stations. Unlike most other fuel infrastructures, hydrogen can be produced either centrally (similar to existing gasoline supply chains) or distributed (as small scale units that can produce H_2 close to the use point in small quantities) modes at forecourt refuelling stations, therefore significantly reduces the distribution cost.

The stakeholders can be addressed as economic, social or institutional agents, business enterprises and cultural groups of en specific country or region related to the hydrogen economy as displayed in Figure 2.2.

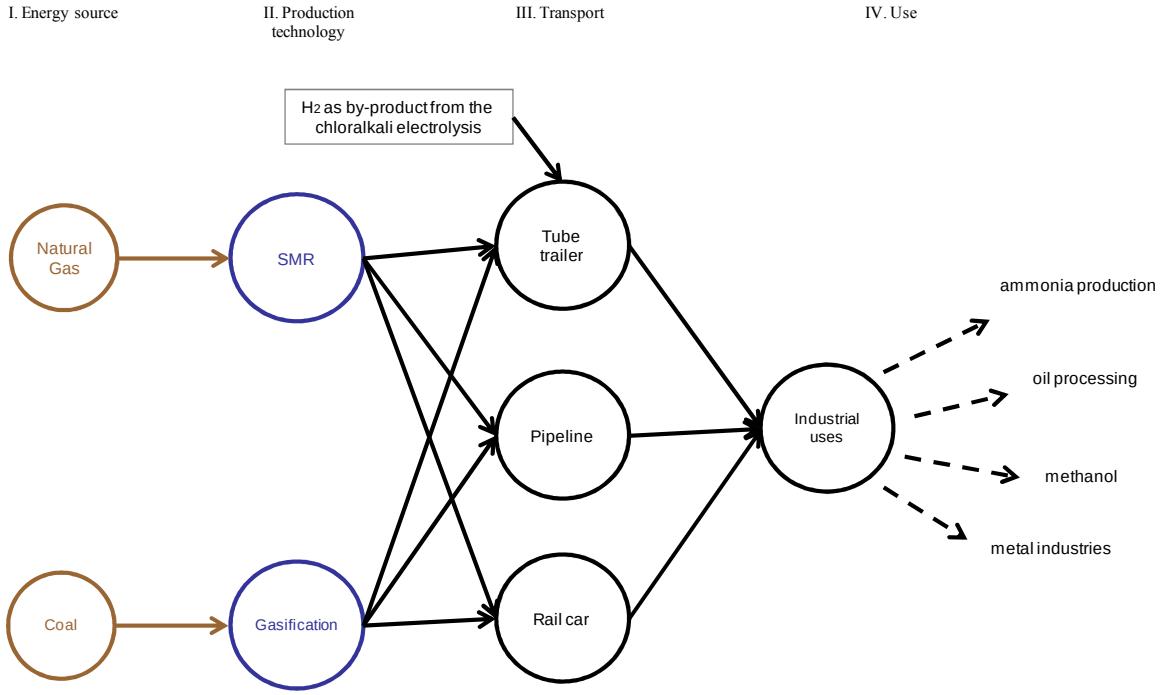


Figure 2.1 Hydrogen supply chain for captive uses

The selection of the "best" hydrogen pathway involves comparison of the various technological options in terms of multiple performance criteria, with the ultimate goal being to define a strategy whereby the infrastructure investment can be planned with confidence (Hugo et al., 2005). Several options are presented in Figure 2.3.



Figure 2.2 The hydrogen supply chain related to demand and supply with the stakeholders.

In that context, some questions arise and the scientific objective of this work is to bring them an answer:

- which is the environmental impact of the energy source used to produce H_2?
- which production option is more cost effective?
- is centralised production or decentralised production (small-scale production at local fuelling more cost effective?
- what are the most cost effective transportation modes and pathways to connect hydrogen demand with its supply?
- does the well-to-wheel (WtW) of the HSC result in less CO_2 emission than those related to gasoline and diesel?
- what is the safest configuration of the HSC and which quantitative criterion can be used to evaluate safety?

HSC modelling requires the identification of the main characteristics of its activities. A general review of the well-known options is displayed in Figure 2.3. It must be emphasized that the degree of maturity is not the same among the technologies.

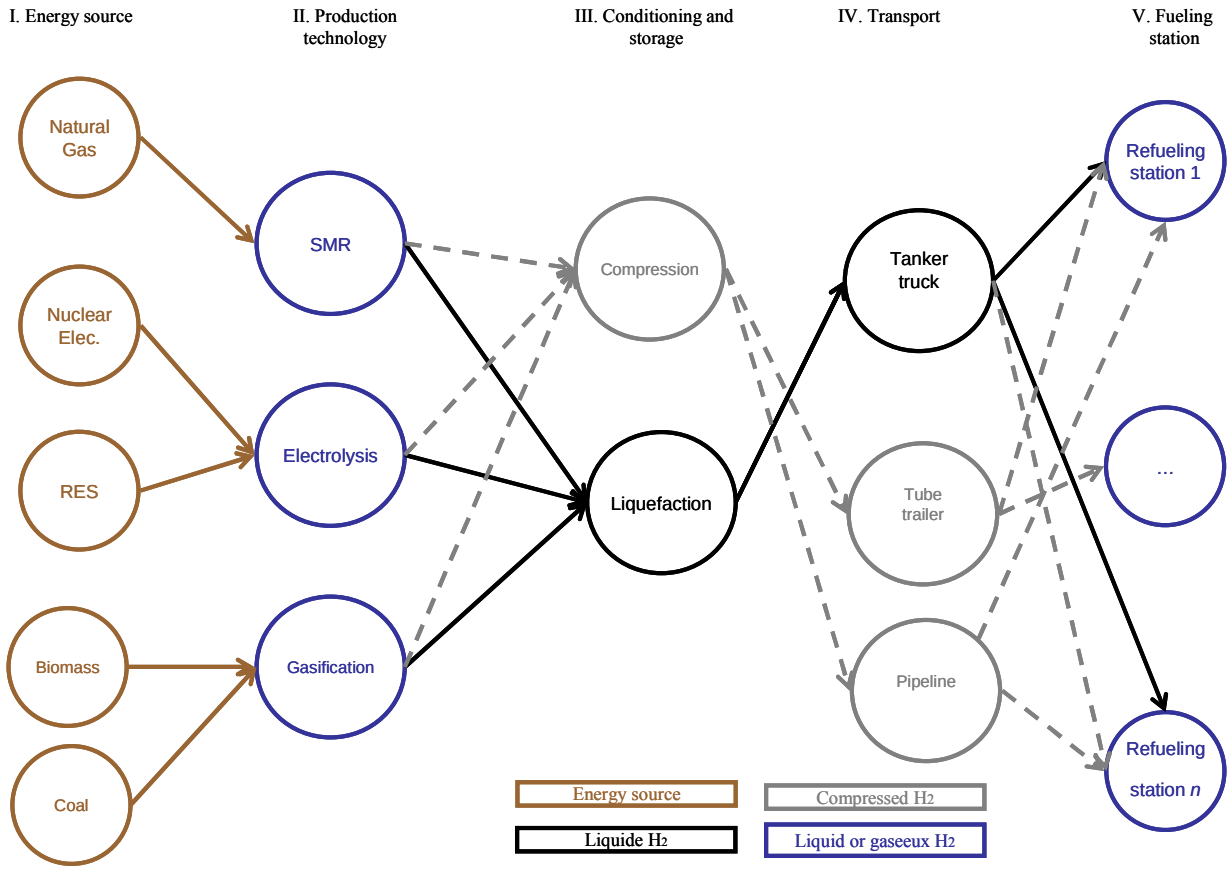


Figure 2.3 Hydrogen supply chain for mobility uses.

2.3 Energy sources

The local market conditions and availability of regional primary energy feedstock have a large impact on selection of supply chains pathways. As previously explained, hydrogen has the benefits of improving security of fuel supplies since it can be produced from diverse primary energy sources, such as fossil fuels (such as natural gas, naphtha, heavy oil, and coal) and renewable energy sources (RES) (i.e. wind, biomass, water, or solar energy). Currently, almost 95% of hydrogen is produced from fossil fuels via steam reforming, gasification and partial oxidation processes (Heracleous, 2011). According to (Murthy Konda et al., 2011a), feedstock remains the biggest contributor in the cost of H_2 fuel with 40% share.

RES are playing an ever-increasing role in European electricity generation. Their share increased from 14% in 1995 to 21% in 2010. Hydro-power plays by far the most important role in electricity generation. Nevertheless, the importance of RES other than hydro has grown considerably; in 1995 they contributed only 8% of green electricity, in 2010, solar, wind, geothermal energy and biomass had generated 43% of the electricity in the EU (see Figure 2.4) (Eurostat. European Commission, 2012).

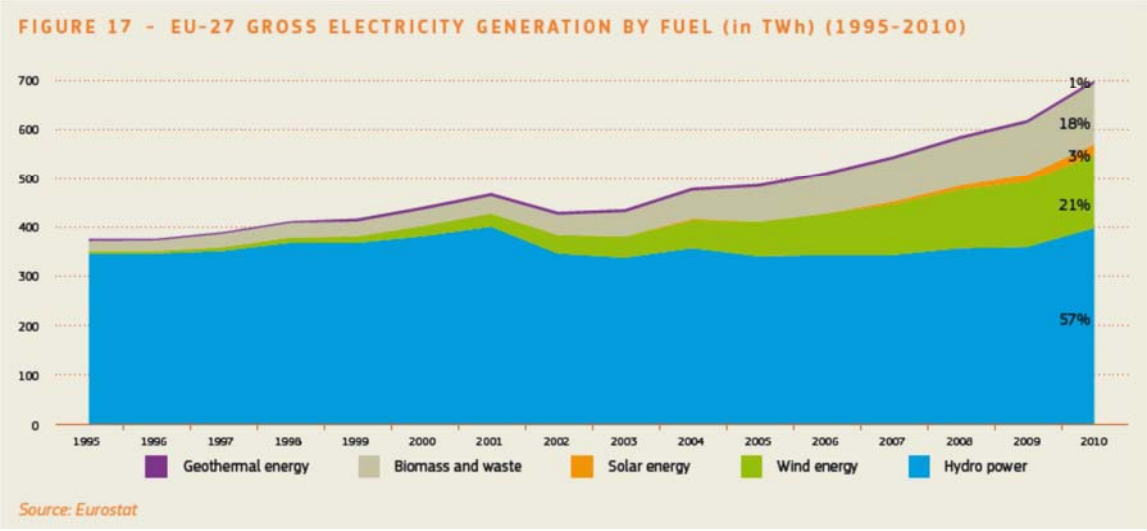


Figure 2.4 EU-27 gross electricity generation by fuel (in TWh) (1995-2010) (Eurostat. European Commission, 2012).

Concerning the evolution in the energy mix, several scenarios can be found in the literature: some are more optimistic in the rate projected for the use in the RES as (WWF, 2011) and (EREC, 2010) reports that consider a 100% production rate from RES by 2050. The Renewable Energy Association in France presented a RES roadmap for 2020 and 2030(Syndicat des énergies renouvelables, 2012). In the French energy report 2050 (Percebois and Center d'analyse stratégique., 2012), some scenarios (CEA, AREVA, Global chance, RTE, etc.) regarding the nuclear and RES are presented in Appendix C1. Some of these projections will be used in the next chapters.

2.3.1 Natural gas

Natural gas is a fuel consisting mostly of methane produced through the decay of organic materials. Further, most natural gas is obtained from wells, although it can be produced from organic waste through the use of digesters (Bartels et al., 2010). Natural gas is typically found near areas with large oil or coal reserves. Worldwide, there are 187.8 trillion cube meters of proved reserves, which is expected to last about 56 years at the current consumption rate (BP Stat, 2013). The existing natural gas infrastructures can be used to power the hydrogen production units.

2.3.2 Coal

Coal reserves are abundant and relatively well distributed globally; it will continue to play a leading role until 2050 and beyond. It should nevertheless be noted that, as pointed out by the European Directive of 2009, a key level in the short term, to reduce GHG emissions is to improve energy efficiency in end-use in different sectors: construction, transport and industry. In this regard, using coal as energy source is not without problems in that it releases carbon dioxide and other pollutants when combusted. Mining of coal causes topographical and ecological changes, especially with the mountaintop removal method used in the Appalachian Mountains. Coal gasification and carbon sequestration (see also Section 2.4.5) may be able to minimise pollutants and greenhouse gases while changes in mining practices can reduce the environmental concerns.

2.3.3 Biomass

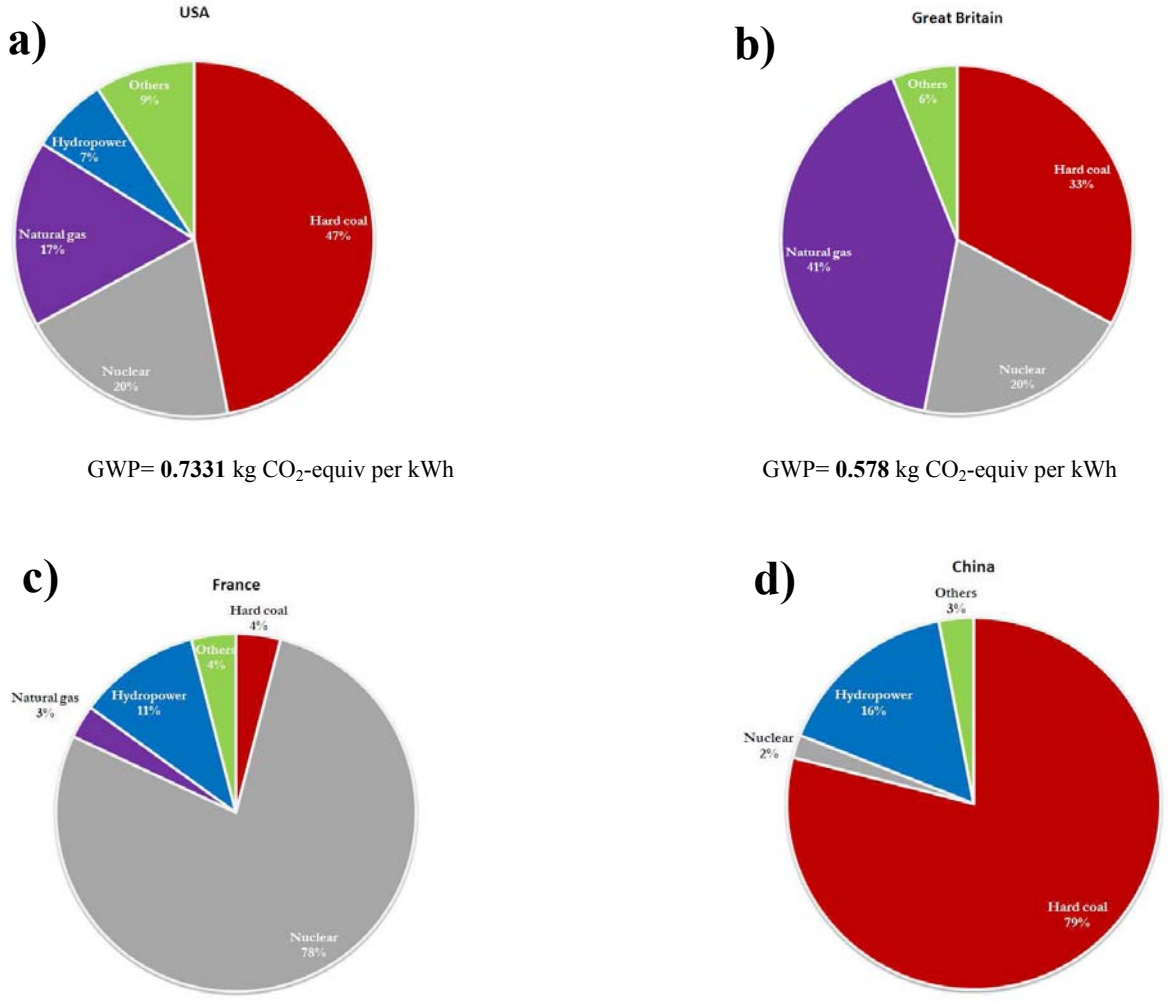
Biomass consists of biological material that can be used for industrial purposes, such as plants, wood, or waste. Biomass has historically been used as a heating fuel through the use of combustion furnaces. There are four main categories of biomass resources that have the potential to be used as a feedstock. The first is energy crops, which as the name implies are specifically grown for energy content. Examples are corn, soybeans, poplar trees, and algae. Agricultural waste is the second category, which includes crop and animal waste. The third is forestry waste from harvesting trees and clearing land, while the fourth category is industrial and municipal waste (Bartels et al., 2010).

Many countries around the world have allocated the research and development towards the hydrogen production from biomass but some limitations exist. One issue with biomass is whether there is enough land to produce the amount of fuel and food needed in the world (Bartels et al., 2010). Other limitation is that the processes of hydrogen production from biomass are still in the development stage and require a strong effort in terms of R&D and demonstration activities (Balat and Balat, 2009). Also, the characteristics of biomass are very important since they can vary greatly from location to location, seasonally and yearly. So that the hydrogen production via biomass route may not be competitive with the hydrogen production with fossil fuels (Dagdougui, 2011b). However, the waste-to-energy application has received much attention due to its potential to become a major hydrogen source.

Biomass has been by far the largest source of RES consumed in the EU. Consumption of biomass was up 13% in 2010, accounting for 69% of the total consumption of renewables. Most of this was used for power generation and in households (Eurostat. European Commission, 2012). If it is true that biomass plays a significant role in the current French energy mix, this use is mainly for combustion and heat production (*Direction générale de la compétitivité, de l'industrie et des services*, 2011).

2.3.4 Electricity as energy carrier for hydrogen production

Depending of the energy mix of each country, the use of electricity to produce hydrogen (via electrolysis) could determine the environmental impact of the H_2 fuel. For example, the French energy mix is dominated by nuclear power (78%) when the USA and China main source to produce electricity is coal, with 47% and 79% respectively, these numbers are displayed in Figure 2.5 that also shows the GWP per kWh of electricity for each particular production mix based on the Ecoinvent unit processes database with the method IMPACT 2002+ V2.10. France has the lowest GWP impact. The existing electricity infrastructures can then be used to power the hydrogen production units.



GWP= **0.7331** kg CO_2-equiv per kWh

GWP= **0.578** kg CO_2-equiv per kWh

GWP= **0.085** kg CO_2-equiv per kWh

GWP= **1.048** kg CO_2-equiv per kWh

Figure 2.5 Comparison among USA, Great Britain, France and China energy mixes (SimaPro 7.3 database consulted 28/06/2013)

H_2 can be considered as a "clean" energy carrier (if produced solely from renewable energies) and is emission-free at the point of final use (avoiding the transport-induced CO_2 emissions) (Ball and Wietschel, 2008). Through the production of H_2, the losses resulted from the intermittence of solar, wind and hydro sources can be reduced. Also, if electricity offer increases and electrolysers are installed next to the renewable energy site, no need to invest in new electric grid would be another advantage. Development of renewable sources for electricity production in the next years is uncertain and will vary depending on the regional condition and politic strategies.

2.3.4.1 Nuclear

Nuclear power could produce hydrogen by either electrolysis of water, or by direct thermal decomposition of water using heat from high temperature reactors. No greenhouse gas emissions are created directly during the generation of nuclear power. But nuclear plants depend of uranium and the world proved reserves of uranium are approximately 3,622,000 tonnes, and current annual usage is 65,000 tonnes (Bartels et al., 2010). Therefore, the world has approximately 56 years of uranium supply, assuming no new sources are found and demand remains the same. The nuclear sector has the advantage of producing a kWh with a relatively stable price.

Nuclear fission produces dangerous waste that remains highly toxic for thousands of years and there is nowhere in the world where it can be stored safely. In 2011, Germany has made important energetic strategic changes regarding the role of nuclear power following the Fukushima accident. Its *Energiekonzept* project, prior to the events of Fukushima, was already based on a halving energy demand by 2050 and substantial use of renewable energy (Percebois and Center d'analyse stratégique., 2012). Germany has established the ambitious target to abandon nuclear energy completely between now and 2022. In France, the energy mix is lead by nuclear power (see Figure 2.5c); this topic is discussed in forums as the National Debate for the Energy Transition ("Débat national sur la transition énergétique," 2013). In this country, currently there are 58 nuclear reactors that produce more than three-quarters of the electricity demand of the country. The report "Energy 2050" (Percebois and Center d'analyse stratégique., 2012) evaluates presents scenarios according to the operating life of French nuclear plants.

2.3.4.2 Solar

The sun provides an effectively supply of energy that can be used to generate electricity and heat. Today, solar energy technology contributes only to 2% of our total energy supply, but this proportion is growing fast. In the Ecofys scenario presented by (WWF, 2011), solar energy could supply around half of the total electricity, half of the building heating and 15% of the industrial heat and fuel by 2050. In this context, two technologies have reached an advanced degree of maturity: photovoltaic (PV) cells and concentrating solar power (CSP).

There are many types of PV cells produced, being more commonly silicon based. These have a quite high efficiency, but very pure silicon is needed so the manufacturing process requires a large amount of energy. Efficiencies of more than 20% (for commercialised cells) have been obtained with silicon cells already produced in mass production (EPIA, 2011). Thin film panels, which either do not require silicon or use much smaller amounts, are starting to be mass produced and commercially available. Even if thin films can be packaged into flexible and light-weight structures, the main disadvantage is their low commercial module efficiency (7-12%) which differs of the record lab efficiency, e.g. for the cooper, indium, gallium, (di) selenite/ (di) sulphide (CIGS) and cooper, indium, (di) selenite/ (di) sulphide (CIS) offer a record commercial efficiency of 12.1% and a record lab efficiency of 20.3% (EPIA, 2011) (Pérez Gallardo, 2013). Among commercial photovoltaic technologies, concentrating photovoltaic (CPV) has the highest solar energy-to-electricity conversion efficiency; in (Vossier et al., 2012), efficiencies over 40% resulted from CPV technology. One obvious drawback of solar power is that the supply varies. PV cells do not function after dark and are less efficient on cloudy days.

CSP uses mirrors or lenses to focus the sun's rays onto a small area where the heat can be collected for example to heat water, which can be used to generate electricity via a steam turbine or for direct heat. The central location is best in hot deserts. This is both an advantage (because the visual impact is minimised) and a disadvantage (because very long cables are required for transit to the point of consumption). The overall system efficiency depends on the efficiencies of the receiver, storage system, turbines, etc. The work of (Ortega et al., 2008) presents an overall efficiency comparison among different technologies for a 50 MWe plants: parabolic trough oil (14%), central receiver system (CRS) + steam (13.6%) and CRS+ molten salts (14%). According to (Montenon, 2013), this technology is stable and has an efficiency over 20% with the advantage to produce at night periods. Recently, ambitious projects are in development, the PEGASE (Production of Electricity from Gas and Solar Energy) project was leaded by CNRS-PROMES (2006-2013) in partnership with the General Council of Pyrénées Orientales (CG 66). This project aims to set up and test a high performance solar plant prototype based on a Combined Cycle Gas Turbine added to a solar receiver, on the site of the old central tower in Thémis France. High conversion efficiency and low cost of electricity are expected (30% conversion efficiency sun / electricity through a combined cycle -gas + steam turbine-)(PROMES-CNRS)

Several different technologies can be used for solar energy to hydrogen conversion. One approach involves electrolysis of water by using PV or CSP with a thermal power cycle. Another approach uses a thermo-chemical process to break water into hydrogen and oxygen by using high-temperature heat from concentrating solar energy (Bartels et al., 2010).

2.3.4.3 Wind

Wind turbines are typically constructed in large groups of individual wind turbines in order to form a large wind farm (Bartels et al., 2010). On-shore wind has now reached a certain maturity, even if the intermittent nature of the production makes it difficult integration into power grid systems, and the technical improvements are mostly incremental. However, off-shore wind power has emerged recently (the first field of 500 MW in 2003 in Denmark), but faces some technical barriers: keeping equipment in harsh environments (saline, weather) and grid power connection (*Direction générale de la compétitivité, de l'industrie et des services*, 2011).

Wind-to-hydrogen may allow wind energy to be harnessed in areas without electrical transmission capacity, or it could provide an energy storage medium for the intermittent wind resource in order to provide a more constant renewable electricity supply (Bartels et al., 2010).

2.3.4.4 Hydro

Hydropower is currently the world's largest renewable power source. Large-scale hydropower plants store water in a reservoir behind a dam, and then regulate the flow according to electricity demand. Hydropower can provide a relatively reliable source of power on demand. The Ecofys scenario reflects a relatively small increase in hydropower. In this scenario, hydropower would provide 12% of the electricity in 2050 compared with 15% today (WWF, 2011). Nowadays, highly efficient turbines that generate electricity by spinning water are installed. Small hydropower, defined by installed capacity of up to 10 MW, is the backbone of electricity production in many countries in the European Union (EREC, 2010). Small hydropower is based on a simple process, taking advantage of the kinetic energy and pressure freed by falling water or rivers, canals, streams and water networks.

Regarding the type of operation, hydropower can be classified as *run-of-river* or *pumped hydro*. Run-of-river stations have no reservoir capacity, so that the water coming from upstream must be used for generation at that moment, or must be allowed to bypass the dam. Pumped hydro produces electricity to supply high peak demands by moving water between reservoirs at different elevations.

2.4 Production

In this section, the production technologies and the centralisation levels are briefly analysed. Steam methane reforming and gasification have been largely mentioned in the literature and currently they can be used to mass production. Electrolysis is a promising route to obtain H_2 especially from renewable sources such as wind, solar and hydro.

2.4.1 Centralisation degree

To classify the degree of centralisation of the HSC two categories will be used either centralised or decentralised (on-site) units. A centralised production option would be analogous to current gasoline supply chains, where the economies of scale are capitalised upon within an industrial context and large quantities are produced at a central site and then distributed (Hugo et al., 2005)(Murthy Konda et al., 2011a). Centralised plants promise higher hydrogen production efficiency but also some difficulties are associated in high-volume hydrogen to be transported.

Decentralised production consists in small regional plants or even local filling stations that could generate hydrogen. While hydrogen generation efficiency for decentralised is lower than those for centralised plants, losses in hydrogen transport can make such a scheme more efficient (Kim et al., 2008)(Haeseldonckx and D'haeseleer, 2011). There is a tendency in the literature to argue that decentralised production plants could overcome many of the infrastructural barriers facing a transition to hydrogen (Ball and Wietschel, 2008). Most studies consider the decentralised route as the key to by-passing the infrastructural problem (Haeseldonckx and D'haeseleer, 2011). A decentralised approach often results in higher costs as efficiencies are generally lower and because on-site production facilities are often dimensioned to cover peak demand (especially when no storage is foreseen or possible). However, a further increase of demand will require larger pipelines, which thus implies new investment costs (Haeseldonckx and D'haeseleer, 2011).

2.4.2 Steam methane reforming

Most of the hydrogen (97%) is made by steam reforming of natural gas also known as SMR (Koroneos et al., 2004). SMR is used in the chemical and petro-chemical industries; it is currently the cheapest production method and has the lowest CO_2 emissions of all fossil production routes (Ball and Wietschel, 2008).

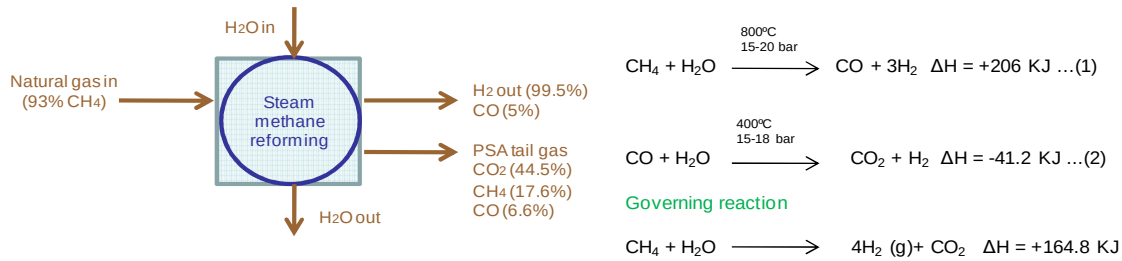


Figure 2.6 Steam methane reforming block diagram and governing reaction.

The main steps during the production of hydrogen from natural gas are (Hajjaji, 2011): a) production of the synthesis gas, b) conversion of carbon monoxide to hydrogen (Water Shift Gas) and c) purification.

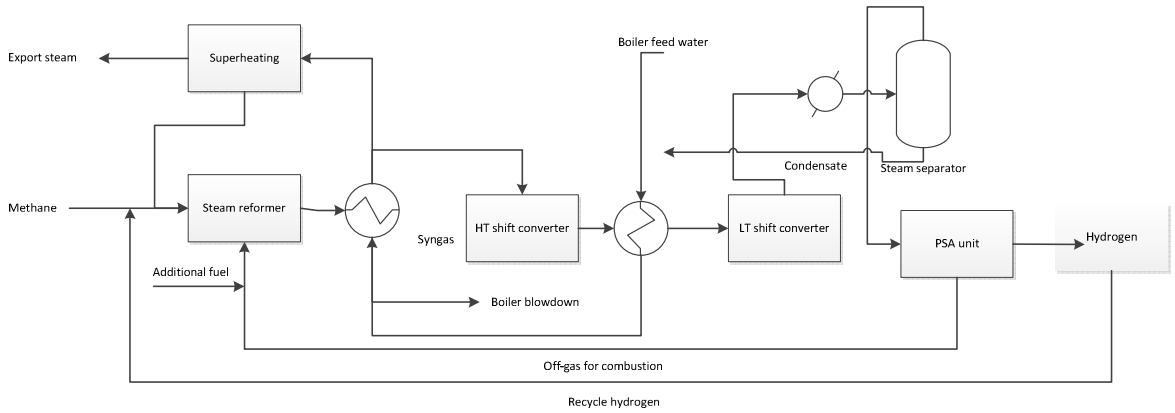


Figure 2.7 Simplified process flow diagram for hydrogen production by steam methane reforming (Rajesh et al., 2001).

The first stage (Figure 2.6 and 2.7)is a catalysed endothermic reaction between methane (natural gas) with water vapour at high temperature (steam reforming) to produce synthetic gas, which mainly consists of carbon monoxide and hydrogen along with some water, carbon dioxide, and methane (Bartels et al., 2010). During steam reforming hydrocarbons are catalytically split in the presence of steam at temperatures of 800–900◦C (Landucci et al., 2007). Then, carbon monoxide is converted to carbon dioxide following the exothermic shift reaction. In the purification stage pressure swing adsorption (PSA) is the prevailing process (Koroneos et al., 2004) in which the reactive gas mixture, containing methane and hot steam, is fed to the tube side of a catalytic furnace reactor. Since the reaction is endothermic, the combustion of methane with air in the furnace side of the reactor provides the required reaction heat. The exhausted beds are regenerated via hydrogen washing, so even if a high purity product is obtained, about 25% of hydrogen is lost. The hydrogen-enriched purge gas is recycled to the furnace side of the reactor and burned together with the combustion methane (Landucci et al., 2007).

2.4.3 Biomass and coal gasification (BG/CG)

Biomass gasification for hydrogen production, still at an early stage today, is expected to become the cheapest renewable hydrogen supply option in the coming decades although biomass has restricted potential and competes with other biofuels as well as heat and power generation (Ball and Wietschel, 2008). The biomass gasification process is explained according the NREL report (National Renewable Energy Laboratory, 2011) in three main types of processes: fixed bed (downdraft and updraft), fluidized bed (bubbling fluidized bed, circulating fluidized bed) and entrained flow gasifiers.

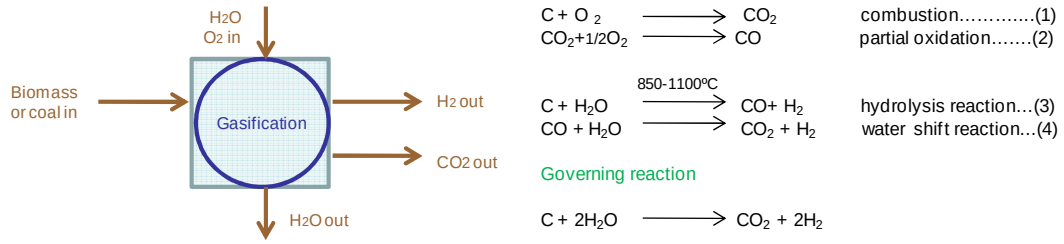


Figure 2.8 Gasification block diagram and governing reaction.

Each type can use one or a combination of gasification agents, including steam, air, and oxygen, to promote conversion. Gasification is an endothermic process and requires a heat source to promote reaction (Figure 2.8). Indirect gasification typically uses steam and direct gasification uses high-pressure air or oxygen as agents. Indirect gasifier temperatures are 750°–900°C and produce syngas, char, and tars. One disadvantage of this approach is that a char combustor, a steam reformer, and an extra compressor are needed to boost the syngas pressure before the acid gas is cleaned up. During direct gasification, biomass under pressure in the presence of oxygen and steam produce medium thermal energy syngas and heat via an exothermic process. The heat is captured in the gasifier and combined with oxygen to maintain temperatures of 850°–1100°C. One disadvantage of this process is that it needs an expensive air separation unit (ASU) for oxygen supply (see Figure 2.9).

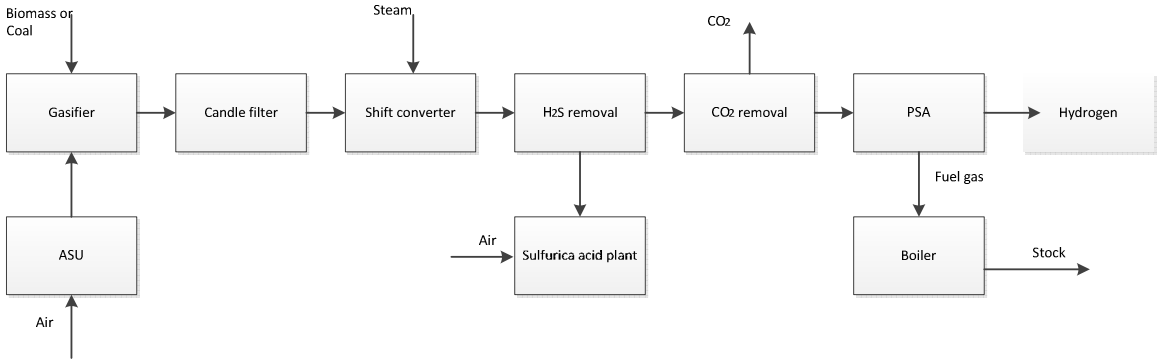


Figure 2.9 Simplified process flow diagram for H2 production by gasification (NETL, 2007)

2.4.4 Water electrolysis

Water electrolysers can be divided into two categories, alkaline and proton exchange membrane (PEM) electrolysers. According to (Ball and Wietschel, 2008), electrolysis processes are more expensive than SMR and only applied if high-purity hydrogen is required but a recent work (Bartels et al., 2010) reports that H_2 production from electrolysis may become economically competitive because fossil fuel feedstock costs also increase, and technological advancements decrease the cost of alternative energy types (Murthy Konda et al., 2011a). Significant cost reductions are also expected for many materials, and catalysts and cell components used in PEM electrolysers could benefit from large scale production of PEM fuel cell of similar concept and design (Grigoriev et al., 2009).

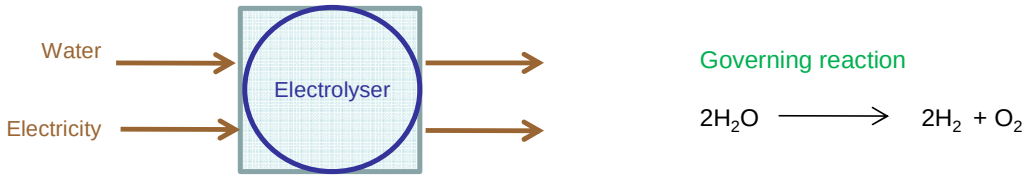


Figure 2.10 Electrolysis block diagram and governing reaction.

The governing reaction of electrolysis is shown in Figure 2.10. PEM technology provides an example of ‘‘zero-gap’’ configuration, in which electrodes are in direct contact with the surface of the ion exchange membrane. This cell concept offers some significant advantages compared to more conventional ‘‘gap-cells’’: (i) no circulating electrolyte is required, pure water being the only reactant supplied to the anodes; (ii) gaseous products H_2 and O_2 are produced at the backside of the interpolar field, offering the possibility of reducing ohmic drops and increasing current densities. As a result, low energy consumption (4.0–4.2 kW/Nm^3 H_2) and high hydrogen purity (>99.99%) are obtained (Grigoriev et al., 2009)(Dagdougui, 2011a). The flow chart of an electrolyser unit is presented in Figure 2.11.

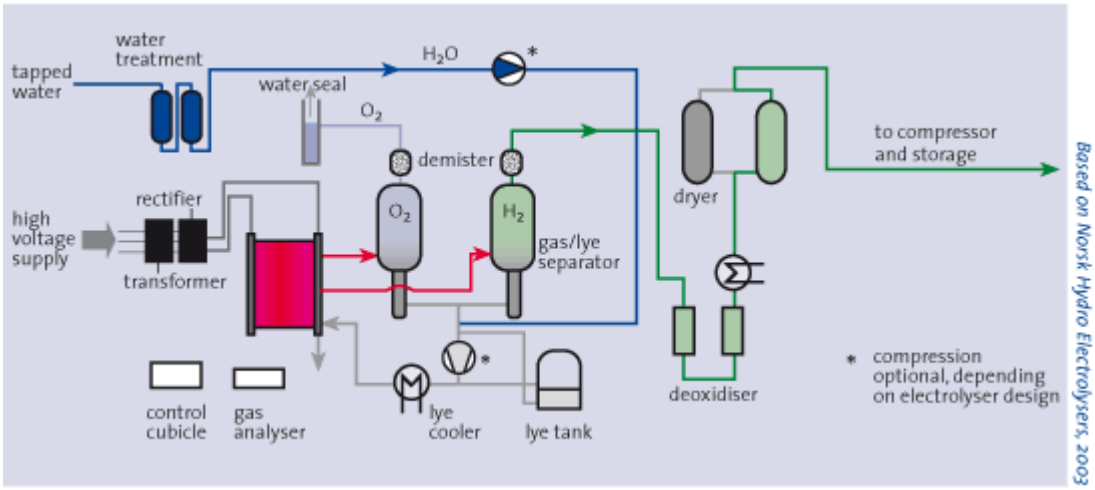


Figure 2.11 Flow chart of an electrolyser unit (Making-hydrogen.com, 2013).

PEM electrolysis is a viable alternative for generating hydrogen from RES. As long as electricity comes from a clean source, electrolysis is a clean process. But producing hydrogen via electrolysis and then using hydrogen to produce electricity again is associated with considerable losses (Hake et al., 2006). In addition, a PEM electrolyser can deliver hydrogen at high pressure, which will in turn be attractive for the application where hydrogen needs to be transported or stored (injected to a hydrogen tank or a pipeline network or be transferred to the liquefaction process). A power consumption of 52.5 kWh/kg is used by the PEM (which is equivalent to about 75% in efficiency) (Dagdougui, 2011a).

2.4.5 Carbon capture and storage (CCS)

H_2 supply chains offer the possibility of capturing most of the CO_2 emissions (~90%) and sequestering them (Murthy Konda et al., 2011a). CCS is an energy intensive and costly process involving several steps: CO_2 capture, pressurisation, transportation and final disposal into geological formations or in aquifers (Haeseldonckx and D'haeseleer, 2011)(*Direction générale de la compétitivité, de l'industrie et des services, 2011)*. There are three main technology options for CO_2 capture and storage: pre-combustion capture, post-combustion capture, and oxy fuel combustion.

2.4.5.1 Pre-combustion capture

Pre-combustion capture processes can be used in coal or natural-gas based plants. The fuel is reacted first with oxygen and/or steam and then further processed in a shift reactor to produce a mixture of H_2 and CO_2. The CO_2 is captured from a high-pressure gas mixture that contains between 15% and 40% CO_2 (Haeseldonckx and D'haeseleer, 2011)(*Direction générale de la compétitivité, de l'industrie et des services*, 2011).

2.4.5.2 Post-combustion capture

The post-combustion process is commercially applied to produce high-purity CO_2 from the exhaust of coal and gas fired boilers, furnaces and turbines. The CO_2 is captured typically through the use of solvents and subsequent solvent regeneration, sometimes in combination with membrane separation (*Direction générale de la compétitivité, de l'industrie et des services*, 2011)(Haeseldonckx and D'haeseleer, 2011). The basic technology, using mono ethanolamine, has been used on an industrial scale for decades, but the challenge is the massive up scaling for power plants and to recover the CO_2 with a minimum energy penalty and at acceptable cost. At present, the largest operating unit has a capacity of 800 t CO_2/day. To put this into perspective, large coal-fired units produce up to roughly 10,000 t CO_2/day (Haeseldonckx and D'haeseleer, 2011).

2.4.5.3 Oxygen combustion

In this technology the fuel is combusted using (nearly) pure oxygen, which is produced by a cryogenic ASU, although new technologies such as ion transport membranes are being worked on. The flue gas, containing primarily CO_2, is partially recycled to the boiler to control the combustion temperature. The main advantage of oxy fuel combustion is that it enables nearly 100% CO_2 capture (Haeseldonckx and D'haeseleer, 2011).

After the CO_2 is captured via physical absorption, it is compressed to supercritical pressure at 15 MPa, which permits efficient pipeline transmission of the CO_2. Energy use and CO_2 emissions from CO_2 sequestration are assumed to be predominately associated with compression (Johnson et al., 2008).

2.5 Hydrogen conditioning and storage

Hydrogen is a very low density gas (0.08988 kg/Nm^3 at 273°K) (Patay, 2008). The physical limits for the storage density of compressed and liquid hydrogen have more or less been reached, while there is

still potential in the development of solid materials for hydrogen storage, such as systems involving metal hydrides (Ball and Wietschel, 2008). Designing tanks both compact, lightweight, safe and cheap is crucial since this is the possibility of making hydrogen storage particularly attractive compared to electricity (CEA, 2013).

Hydrogen contains a lot of energy per unit of weight while the content of energy per unit of volume is quite low. This poses a potential problem in terms of storing large amounts of hydrogen. The traditional means of storage such as pressure tanks and cryogenic tanks have improved dramatically, and a number of new storage technologies are currently under development. The least complex method of storing pure hydrogen is as a compressed gas in a high-pressure cylinder (Dagdougui, 2011a). The lack of storage implies that enough production capacity needs to be installed in order to cover the peak demand for hydrogen (Haeseldonckx and D'haeseleer, 2011).

2.5.1 Liquefaction

Liquefaction can greatly increase the volumetric density of hydrogen, as compared to compressed gas, but the liquefaction process itself is very capital and energy intensive (Johnson et al., 2008). Hydrogen liquefaction and use of liquid hydrogen is usually practiced only when high storage density is required, for example, in aerospace applications (Dagdougui, 2011a). But H_2 can also be liquefied for being transported in larger volumes by cryogenic trucks. It is then about 800 times denser than the gaseous state where, a priori, the obvious interest of this liquid for storage and transportation. However, a certain level of cryogenic technology is needed to be implemented, either to liquefy or to keep in the liquid state (Patay, 2008). The extensive isolation technology and fuelling process, as well as the loss of hydrogen by evaporation effects during storage periods are further disadvantages of liquid hydrogen (LH_2) storage system (Hake et al., 2006).

The first liquefaction of hydrogen was obtained by James Dewar in 1898. The process was improved a few years later by the method of Georges Claude (the founder of Air Liquide) which improves the compression refrigeration machine designed by Linde (AFH2, 2011). Hydrogen is after helium, the most difficult gas to liquefy. A temperature of 20.3°K or -253°C is required. It is not obtained only by supplying cold gas but by the combined effect of cooling and clean the adiabatic expansion of the gas after it has been previously compressed (AFH2, 2011).

The electricity use in a liquefier (kWh/kg H_2) is estimated as a function of size with a minimum electricity use of around 9 kWh/kg H_2 for the most efficient, large liquefiers (Johnson et al., 2008) compared to 4.1 kWh/kg H_2 needed for compression (Grol et al., 2005).

There are currently around thirty liquefaction units worldwide (see an example in Figure 2.12). Their daily productions range from a few tonnes to 54 tonnes for the largest (Sacramento, USA, Union

Carbide). World production of LH_2 would reach 355 tonnes. The majority (84%) of this production lies in the USA: its main use is the petrochemical industry (33.5%) followed by aerospace applications (18.6%) (e.g. the first factory was built for the Apollo program in 1960) (AFH2, 2011).

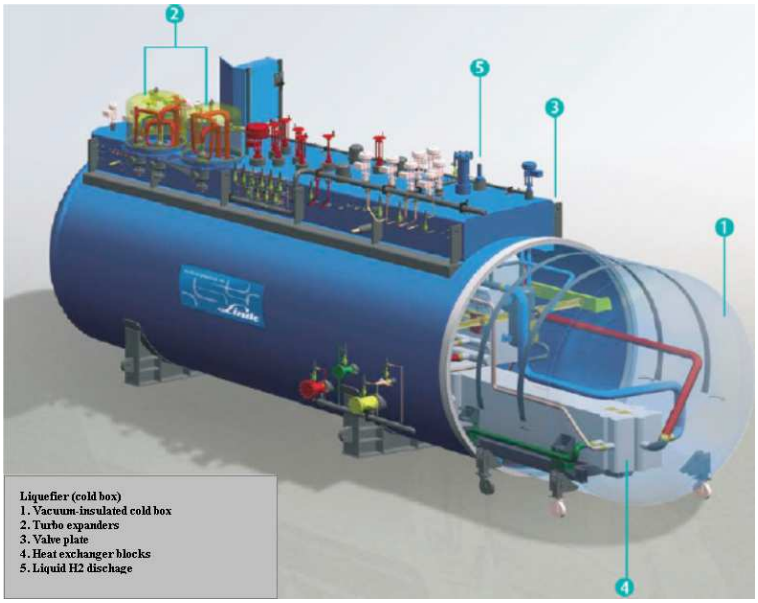


Figure 2.12 Liquefier Linde in Leuna, Germany (2008) (AFH2, 2011)

The liquefaction system can turn the hydrogen gas to medium pressure liquid hydrogen. A condenser can be located on the same site a production unit. It is designated hereafter as "liquefier attached". If not attached, a condenser can be located anywhere in the country. Each of liquefier can supply several filling stations (Patay, 2008).

2.5.2 Liquid H_2 storage

Like all liquids at low temperature, called cryogenic liquids, liquid hydrogen is stored in cryostats containers double insulation whose purpose is to limit the inevitable heat outside contributions. The former is a thermal insulation barrier against the flow of heat by direct conduction, provided by the vacuum maintained in the double wall of the cryostat. The latter, against the flow of heat by radiation is provided by a multi-reflecting sheet metal disposed in the space between the walls. A cryostat is not sealed so that a continuous evolution of hydrogen gas (precisely vapour hydrogen), which avoids excessive pressure increase. This constant evaporation, which corresponds to a weight loss of 0.5 to 1% per day depending on the technology used, is one of the major disadvantages of storing hydrogen in its liquid form (AFH2, 2011). Liquid hydrogen plays an important role during the transition phase (until 2030) and in connecting outlying areas, such as along motorways or in rural areas (Ball and Wietschel, 2008). The works of (Almansoori and Shah, 2006)(Almansoori and Shah, 2009) concluded that from an economical viewpoint, designing a liquid hydrogen based supply network is extensively cheaper than designing a gaseous-based network.

2.5.3 Compression

The production of hydrogen and conversion to gaseous form is less expensive than producing it and converting to liquid form. However this difference in production costs does not come close to bridge the gap of higher transportation cost of gaseous hydrogen compared to liquid hydrogen (Ingason et al., 2008).

The conditioning system can turn the medium pressure hydrogen gas to a high pressure hydrogen gas or compressed hydrogen (CH_2). Currently, 200 or 350 bar pressure bottles are distributed in the industry and developments now concern tanks can withstand pressures of 700 bar (CEA, 2013). A conditioning center can be located on the same site a production unit. It is designated hereafter as "attached conditioning center". If not attached, a conditioning center can be located anywhere in the country. Each conditioning centers can supply several groups of filling stations (Patay, 2008).

2.5.4 Gaseous H_2 storage

The required space of gaseous storage could be an important issue. Given the fact that large storage facilities can only maintain pressures up to 12-16 bar, this means that up to 1 million m^3 of space is required for storage capacity for 10 million Nm^3 H_2 (Haeseldonckx and D'haeseleer, 2011). In addition, storing such large quantities of hydrogen also brings along serious safety issues. Large hydrogen storage facilities are unlikely to be located near densely-populated areas.

The risk of leakage of hydrogen must also be considered in light of flammable and explosive nature of the gas under certain conditions. However, due to the small size of the molecule, hydrogen is able to penetrate many materials, including certain metals. It weakens, moreover, some making brittle. The study of high-pressure storage is therefore essentially to test the resistance of materials to hydrogen pressure. These materials must be resistant but relatively light (mobility requires). The metal tanks currently used, still prove expensive and heavy in relation to the amount of gas they can take. Non-metallic tanks but most of polymeric materials (non-load-bearing non-metal liner axial and hoop wrapped with resin-impregnated continuous filament[23]) are being developed to address these constraints (CEA, 2013).

[23]One of the most advanced lightweight storage systems for the case of compressed gas consists of a vessel, which is actually an advanced composite tank using a non-load-bearing metallic. The plastic liner axial and hoop wrapped with resin-impregnated continuous filaments is another advanced vessel (Tzimas et al., 2003)

2.5.5 Metal hydrides

An alternative to the traditional storage methods (liquid and gas) is proposed through the use of advanced solid materials. Certain materials absorb hydrogen under moderate pressure at low temperatures, forming reversible hydrogen compounds called hydrides. This type of hydrogen storage is often called "solid" hydrogen storage since hydrogen becomes part of the solid material through some physicochemical bonding (Dagdougui, 2011a). This kind of storage works like a sponge; it absorbs H_2 and stocks it. Is therefore recovered at the outlet of H_2 gas, high purity, low pressure. For use in cars, it will be compressed to 700 bar (350 bar or, depending on the model selected), and put in the filling station. This technology is well adapted for on-site applications. More information about this kind of storage can be found in ("McPhy - Solid hydrogen storage").

2.6 Transportation

Conceptually, transportation is divided into two parts: transmission and distribution. Transmission refers to H_2 transportation from a plant to other regions without-plant units and distribution refers to H_2 transportation to the refuelling stations from a plant or regional conditioning center in any region (Murthy Konda et al., 2011a).

There are various methods for transporting hydrogen, but choosing the best one depends on different parameters such as the distance of the demand center from the production site (Ball and Wietschel, 2008)(Qadrdan et al., 2008), the amount of transferred hydrogen, and the existing infrastructure such as natural gas pipeline, road, and rail (Qadrdan et al., 2008).

Note also that the choice of transportation mode is correlated with the architecture of the distribution network. Indeed, a supply chain including liquid hydrogen requires trucks, while a supply chain not including condensers or compressors requires pipelines (Figure 2.13)(Patay, 2008).

Since the volumetric energy density of H_2 is low, transportation costs can be significant (Ball and Wietschel, 2008)(Murthy Konda et al., 2011a)(Almansoori and Shah, 2006). For (Ball and Wietschel, 2008), as transport is so expensive, hydrogen should be produced close to the user centers.



Figure 2.13 Tanker truck, tube trailer and cylinder trailer (Patay, 2008)

The costs could be considerably reduced if the natural gas pipeline could be adapted to hydrogen. As hydrogen can diffuse quickly through most materials and seals and can cause severe degradation of steels, mainly due to the embrittlement, the use of existing natural gas pipelines could be problematic and has to be investigated on a case-by-case basis. Coating or lining the pipelines internally, or adding minor amounts of oxygen could solve the problems in using existing long-distance transmission pipelines made from steel. In addition, valves, manifolds, and in particular compressors would need to be modified, as they are optimised to work under a certain range of conditions, such as gas composition (Ball and Wietschel, 2008). Another possibility could be to blend hydrogen with natural gas up to a certain extent and either separate the two at the delivery point, or use the mixture, e.g. in stationary combustion applications (Ball and Wietschel, 2008)(Li et al., 2008).

2.6.1 Pipeline

Pipelines have been used to transport hydrogen for more than 50 years (Ball and Wietschel, 2008). The longest hydrogen pipeline in the world to supply chemical and petrochemical industries (about 1050 km in France, Germany and the Benelux countries) is operated by Air Liquide (CEA, 2013). The United States has more than 720 km of hydrogen pipelines concentrated along the Gulf Coast and Great Lakes, the estimation of the capital cost of hydrogen transmission pipelines range from 200,000 to 1,000,000 US$/km (Dagdougui, 2011a).

From a production unit, the gas is transported through a transmission line medium pressure (100 bar)(Patay, 2008)(Haeseldonckx and D'haeseleer, 2011). This means that less space is required to store the same amount of hydrogen. In addition, as hydrogen is stored throughout the entire pipeline network, there are no large concentrations of hydrogen at the same location, improving the overall safety. The exact amount of hydrogen that can be stored, depends on the maximum and minimum pressure, the hydrogen flow and the length and diameter of the pipeline (Haeseldonckx and D'haeseleer, 2011).

Pipelines for medium and large fuelling stations may become relevant once a significant market penetration of hydrogen vehicles has been achieved, but these are mostly used for local distribution in highly populated areas and for large-scale interregional energy transport according to the HyWays roadmap (European Commission, 2008). In (Ball and Wietschel, 2008), a pipeline network could be constructed after 2030 when the potential demand can justify the high investment.

2.6.2 Tube trailer

From a conditioning center, compressed hydrogen is being transported at around 200 bar by tube trailers according to Praxair. With the appearance of decentralised, regional production, tube trailers use is a solution for the transition phase towards the use of pipelines (European Commission, 2008).

Commercial tube trailers are well established. Generally, transporting CH_2 over the road in high-pressure tube trailers is expensive and used primarily for short distances; it becomes cost-prohibitive when transporting farther than about 321 km from the point of production in the study of (Dagdougui, 2011a). Compressed gas truck delivery is not considered as a long-term delivery solution because their low hydrogen capacity would necessitate too many deliveries (Yang and Ogden, 2013).

2.6.3 Tanker truck

From the liquefaction unit, LH_2 is transported by tanker trucks (cryogenic liquid hydrogen tankers) (Patay, 2008). This transportation mode is the most economical pathway for medium market penetration (Dagdougui, 2011a). They could transport relatively large amounts of hydrogen and reach markets located throughout large geographic areas. Fourty ton trucks can carry 3500 kg of LH_2. So that, the transport of liquid hydrogen is limited by volume, not by weight (Bossel, 2006).

2.7 Refuelling stations

At the end of the chain, the hydrogen fuel must be distributed to end users. This distribution is in refuelling stations. Research has shown that drivers would be willing to switch to another fuel only if the new fuel is available at approximately 15-25% of the existing retail stations (Haeseldonckx and D'haeseleer, 2011). The problem of refuelling stations installation could face two scenarios:

- Scenario 1: conversion of existing gasoline/diesel stations to hydrogen stations. This scenario has been implemented assuming that oil companies will represent one of the major stakeholders of hydrogen production.
- Scenario 2: installation of new hydrogen stations.

The development of refuelling stations does not seem to represent specific technical problems. Currently, 208 refuelling stations already exist in the world ((Avere France, 2012) consulted 16/08/2013), established principally in the United States, Japan, Germany and Iceland. However, it will take time for these stations to cover a whole country, which could hinder the development of hydrogen in transport. To overcome this difficulty, some car manufacturers plan to use current fuels and hydrogen (hybrid cars) (CEA, 2013).

(Patay, 2008) identified four types of refuelling stations according to their main mode of supply, allowing the filling station vehicles equipped with tanks for hydrogen gas at high pressure to about 700 bar[24] (a priori these tanks will be dominant in the market):

[24] In cases where the FCEV has 350 bar onboard storage tanks, H_2 has to be compressed up to 400 bar before being dispensed (Murthy Konda et al., 2011a)

- Type 1. Stations receiving liquid hydrogen require evaporation and compression facilities
- Type 2. Stations receiving compressed hydrogen (200 bar) from tube trailers require a high compression unit (400-700 bar)
- Type 3. Stations with a piped gaseous H_2 supply require a high compression unit (from 100 to 400-700 bar)
- Type 4. Stations with on-site H_2 production by small electrolysis units require compression (from 15 to 400-700 bar)

Hydrogen refuelling stations must be as safe as gasoline stations. The main safety aspects at the user interface are related to the risk associated with a potential ignition of a hydrogen leakage at the station or at the vehicle. Hydrogen refuelling station may be a complex architecture since; it must include additional devices that are essential to deliver the hydrogen to customers, such as compressor unit that is required to compress hydrogen to a required pressure. Refuelling station risk must be well evaluated and the code and standards for safety must be updated in order to take into account hydrogen features. Safety issues may affect the public perception of installing a hydrogen refuelling station, especially for those that live close to the facility (Dagdougui, 2011a).

The items that have presented in the previous sections, energy sources-production technologies-storage-transportation-refuelling, constitute the elementary building bricks of the supply chain. In what follows, the review of HSC modelling is proposed to position this work.

2.8 Modelling approaches

A literature review shows that the most common approach in designing and modelling the HSC are the optimisation methods through mathematical models. As opposed to simulation based approaches these models utilize formal optimisation techniques to allow advanced decisions to be captured and to provide comprehensive integrated solutions recommendations (Hugo et al., 2005). The aim of such methods is to find out 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 computer to analyse the problems (Hillier and Lieberman, 2001).

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, transportation (Dagdougui, 2011b). This approach matches with the previous definition of the HSC explained in the section 2.1.

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 strategic, tactical or operational aspects,
- temporal dimension for example either static or dynamic,
- type of data (i.e. deterministic, stochastic),
- type of approach (optimisation, simulation),
- horizon time (short, medium or long term),
- geographic dimension according to the problem definition.

The use of mathematical programming for designing a supply chain, consists of three major steps as reported in (Grossman et al, 2000; Boix, 2011):

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 optimisation criteria which are expressed as mathematical functions, and
    b) the constraints which can be either of equality or inequality type.
iii. The resolution of the mathematical model to determine one or more optimal solutions.

There are also geographic tools to design the HSC. The Geographic Information System (GIS) is a package that can be usefully integrated with a modelling system for supply chain management. The typical GIS contains an extensive database of geographic census information plus graphical capabilities of displaying maps with overlays pertaining to the company's supply chain activities (Shapiro, 2001). Besides the use of GIS, additional enhancements could be projected by coupling the GIS component to an additional mathematical model thus leading to an integrated approach. This coupling could favour the exploitation of two different decision support systems. It must be highlighted that by contrast to the mathematical optimisation approaches, the spatial or GIS based approach cannot be considered as a general methodology for finding the optimal HSC configuration. In fact, the results of the approach are depending on national or regional specific conditions, that are strongly related to the local territorial conditions, such as transportation network, population, available resources, local policies and others (Dagdougui, 2011b).

2.9 Literature review

In the mathematical formulation, Mixed Integer Linear Programming (MILP) approaches have been widely used. (Almansoori and Shah, 2006) have clearly introduced a general model that determines the optimal design of a network (production, transportation and storage) for vehicle use where the network is demand-driven. The model was applied to a Great Britain case study. The same authors

extended the model in 2009 (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 refuelling stations and local distribution of hydrogen minimising the total daily cost.

(Hugo et al., 2005) developed an optimisation-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 H_2 configurations. This model has been extended and considered as a basis for other works such as Li et al. (Li et al., 2008) for the case study in China. At the same time in Iran, a model for investigation of optimal hydrogen pathway and evaluation of environmental impacts of hydrogen supply system was examined by (Qadrdan et al., 2008). Another study also considered hydrogen from water, using electricity from hydro and geothermal power in Iceland for exportation (Ingason et al., 2008).

Several perspectives of the HSC have been integrated in (Kim et al., 2008) models as deterministic vs. stochastic approach to consider demand uncertainty in the new model. The model they proposed determines a configuration that is the best for a given set of demand scenarios with known probabilities. The stochastic programming technique used is based on a two-stage stochastic linear programming approach with fixed recourse, also known as scenario analysis. A strategic design of hydrogen infrastructure was later developed to consider cost and safety using multi-objective optimisation where the relative risk of hydrogen activities is determined by risk ratings calculated based on a risk index method (Kim and Moon, 2008).

(Patay, 2008) has developed a strategic and tactical model for the French territory and Benelux region in cooperation with Air Liquide Company. In this thesis, the demand and energy costs are exogenous parameters given the uncertainty on these parameters for a long-term horizon. This work studies the transportation and distribution nodes taking into account an economic criterion. The multi-period model is to scale the infrastructure in each time period of a time horizon (horizon year 2050). The originality of (Patay, 2008) problem results from the time horizon considered and the dynamic dimension, as well as the size of the supply chain considered.

(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 to develop an efficient solution method that overcomes the numerical difficulties associated with the resulting large scale MILP.

(Sabio et al., 2010) also developed an approach, which allows controlling the variation of the economic performance of the hydrogen network in the space of uncertain parameters examined the case study of Spain.

More recently, (Murthy Konda et al., 2011a) considered the technological diversity of the H_2 supply pathways together with the spatial-temporal characteristics to optimise a large-scale HSC. They calculate the transportation costs based in (Almansoori and Shah, 2006) and (Almansoori and Shah, 2009) approaches. The original models are modified (e.g., inclusion of existing plants, capacity expansion and pipeline features) and analysis is extended to incorporate the computation of delivered cost of H_2, well-to-tank emission and energy efficiency analyses. In (Haeseldonckx and D'haeseleer, 2011), the objective is not only to find the optimal set of activated hydrogen production plants but also to implement a hydrogen infrastructure optimisation algorithm that has to decide which hydrogen-production plants will be invested in and which plants will not.

The thesis work of (Dagdougui, 2011a) describes the risk hazards (delimitation and explanation of potential risks in some parts of the hydrogen infrastructure: pipeline and storage tank) to demonstrate the consequence of hydrogen accident in case of a future infrastructure operation. The risk is integrated into the HSC to minimise the global risk to population and environment. The model is applied to regional case studies to 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 minimisation of the cost of installation of new onsite hydrogen refuelling stations, the cost of conversion of existing gasoline to hydrogen stations and the cost of transporting hydrogen fuel to offsite stations is done. The objective of this work was to develop a decision support system for the localization of hydrogen refuelling stations taking into account the potential of production within a specific boundary region.

(Sabio et al., 2011) take into account eight environmental indicators in a two-step method based on a combination of MILP multi-objective optimisation with a post-optimal analysis by Principal Component Analysis (PCA) to detect and omit redundant environmental indicators.

More recently,(Liu et al., 2012) focuses on the analysis of hydrogen demand from hydrogen FCEVs in Ontario, Canada, and the related cost of hydrogen. Three potential hydrogen demand scenarios (2015-2050) are considered. Costs associated with the hydrogen production (electrolysis), storage (LH_2 and CH_2) and distribution (tanker truck and pipeline) were also calculated. A sensitivity analysis was implemented to investigate the uncertainties of some parameters on the design of the future hydrogen infrastructure.

Finally,(Yang and Ogden, 2013) describes the development and use of a hydrogen infrastructure optimisation model using the H2TIMES modelling framework to analyse hydrogen development in California to 2050. H2TIMES is a quasi-spatial model that develops the infrastructure to supply hydrogen fuel in order to meet demand in eight separate California regions in a least cost manner subject to various resource, technology and policy constraints. H2TIMES uses modelling to identify the least-cost method of meeting the exogenously-specified regional H_2 demand and minimise the discounted total system cost over the modelling horizon subject to the various policy and resource constraints specified in the model using linear programming (LP) and MILP.

It can be highlighted that several mono-objective optimisation approaches have been developed or extended as in (Qadrdan et al., 2008)(Almansoori & Shah, 2006, 2009, 2012; Ball et al., 2006; Hugo et al., 2005; Kamarudin et al., 2009; Kim et al., 2008)(Patay, 2008)(Liu et al., 2012)(Yang and Ogden, 2013). In these studies, the cost is the objective to be minimised. Multi-objective optimisation studies are relatively scarce and criteria to be analysed are based on economic and environmental performances; some examples are presented in (Guillén Gosálbez et al., 2010)(Hugo et al., 2005)(Li et al., 2008)(Sabio et al., 2011): minimising the expected total discounted cost and the associated financial risk (Sabio et al., 2010) and minimising the total cost of the network and the total relative risk of the network (Kim and Moon, 2008)(Dagdougui, 2011a).

Literature review reveals that few researchers have used the spatial dimension to construct the infrastructure for hydrogen. Some examples of geographic approaches include the study of (Ball et al., 2006) who developed the MOREHyS (Model for Optimisation of Regional Hydrogen Supply) approach of 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 trade-offs between hydrogen production and electricity generation within a country-specific context (high degree of regionalization)(Ball et al., 2006).

(Johnson et al., 2008) used also GIS for modelling regional hydrogen infrastructure deployment using detailed spatial data and applied the methodology to a case study of a potential coal-based hydrogen transportation system in Ohio with CCS. The objective in this work was to optimise hydrogen infrastructure design for the entire state. The MARKAL model has been applied to the UK and developed a GIS based spatial model to represent the layout of hydrogen infrastructure (Yang and Ogden, 2013).

In the case of the mathematical works, they are limited to a 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. Moreover, the multi-period issue is not systematically tackled in all the reported works. Finally, the spatial or GIS based approach cannot be considered as a general methodology for finding the optimal HSC configuration but it can be coupled to mathematical programming to design the HSC.

2.10 Discussion and work orientation

As highlighted in chapter 1, the scientific objective of this thesis is to design of a HSC for fuel use in the horizon time 2020-2050 considering national and regional scales with three performance indicators: cost, environmental impact and safety, these criteria will be formulated and explained in the chapter 4.

Mathematical programming provides a way of describing a problem and the methods to solve it. The work reported in (Almansoori and Shah, 2006) constitutes a consistent way to model the typical items of the supply chain and its interconnection in a mono-objective way considering only minimising the cost. The underlying idea of our work is to extend the model to new constraints and objectives related to environmental and safety aspects in order to treat the multi-objective problem. In the model developed by (Almansoori and Shah, 2006), the problem corresponds to a location routing type to design at a strategic level the HSC in a static mono-period mode using deterministic data with extrapolation for the long term scenario defined to the year 2050 to treat a national case. The problem is referred as MILP with minimisation of the total daily cost.

The problem strategy will include different spatial-temporal scales, the mono- and multi-period formulation for time horizon and will be able to embed national and regional cases. The objective is to propose a generic framework that can also take into account the geographic and infrastructure constraints through the use of a GIS.

In this chapter, the concept of SCM was introduced and defined as the tool to be used to model the hydrogen network to analyse the relevance of the infrastructure necessary to be established to cover a defined demand of hydrogen fuel. This study lies in a strategic phase, i.e. supply chain design. The HSC for fuel application results in a more complex network than that for on-site industrial applications. A HSC involves energy sources, production, storage, transportation, and supply of hydrogen to the refuelling stations. Obviously, the individual component models form the framework by which these system designs can be formulated and evaluated. The resulting network would heavily depend on the country/region-specific conditions. All the items of the HSC that will be used in the following will be presented in the dedicated chapters.

Indeed, some technologies that are considered in the literature as possible technologies are only at the stage of development and technical and/or economic viability is not proven or available (for storage via metal hydrides)**.** This explains why they have not been considered. Sequestration and capture methods could be used to reduce emissions, but will induce additional costs. Pipelines will not considered in this work because pipelines may become relevant once a significant market penetration of hydrogen vehicles and they have a high capital cost associated. The following chapter presents the methods and tools that will be used in this work.

Chapter 3

METHODS AND TOOLS FOR HSC DESIGN

Résumé

Ce chapitre présente les méthodes et outils utilisés dans le cadre de ce travail pour la conception optimale de la chaîne logistique de l'hydrogène. Il doit être considéré comme un complément méthodologique pour les chapitres 4, 5 et 6. En effet, la formulation détaillée des problèmes qui seront traités dans la suite sera explicitée au fur et à mesure. Les aspects principaux abordés ici concernent le choix de la stratégie d'optimisation dans un cadre mono et multi-objectif et d'une méthode d'aide à la décision pour générer une solution de compromis à partir de l'ensemble des solutions issues du front de Pareto. L'utilisation consécutive des techniques d'optimisation et d'aide à la décision permet de déterminer le type, le nombre, la capacité de traitement des unités de production, de stockage et de transport au sein de la maille retenue lors de la discrétisation du territoire. Pour positionner géographiquement les sites et les voies d'acheminement, l'utilisation complémentaire d'un logiciel de géolocalisation est proposée.

Abstract

This chapter presents the methods and tools used in this work for the hydrogen supply chain design. It should be seen as a methodological supplement to chapters 4, 5 and 6. The detailed problem formulation will be treated gradually in the following chapters. The main issues addressed here concern the choice of the optimisation strategy in mono and multi-objective frameworks as well as decision-aid methods to find a trade-off solution from the Pareto front. Consecutive use of optimisation and decision making techniques can determine the type, number and capacity of production plants, storage and transportation units within a specific territorial breakdown. The spatial design is performed using the ArcGIS® software to locate sites and routes.

Acronyms

HSC	Hydrogen supply chain
LP	Linear Programming
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Nonlinear Programming
MCDM	Multi-criteria Decision Making
ELECTRE	Elimination and Choice Translating Reality
TOPSIS	Technique for Order Preference by Similarly to Ideal Solution
M-TOPSIS	Modified TOPSIS
RHS	Right-hand-side
AUGMECOM	Augmented ε-constraint method

3.1 Introduction

This work deals with the analysis and design of the HSC for fuel use by the horizon time to 2050 at national and regional scales with three performance indicators: cost, environmental impact and safety. The decisions that would be made in the model are the following. 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 kind of energy sources and production technology constitute the best choice? What 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.

The ultimate practical goal of this research will be to develop a prototype to guide decision-makers in their strategic choices in the market positioning of hydrogen fuel.

Let us remember that a model is a description of a system by a theory or by a symbolic language with which the world of the objects, also a system can be expressed (Monsef, 1996). In the case of HSC, the basic structure definition is the base of modelling that allows quantifying, visualizing and simulating different scenarios. The HSC can be modelled according different perspectives, so that conceptual, operation, mathematical and graphical models can be distinguished (Prawda, 2004).

This chapter presents the different approaches that can be tackled in order to choose the methods to be used for the abovementioned problem and justifies the selected ones that will be utilized throughout this manuscript. The reader must be aware that this short chapter constitutes a companion paper to the following chapters of this manuscript. The objective is to propose the guidelines of the methodological choices that emerge as the best options for solution strategies. Yet, some of the formulations describing the problems are out the scope of this chapter and will be explained in the dedicated chapters.

This chapter is divided into 8 sections. Section 3.2 first presents the description of some optimisation frameworks according to the type of problem (e.g. linear, nonlinear) and some significant solution strategies that can be used. As highlighted in the section 2.9 of the previous chapter, the HSC problem can be viewed as an optimisation problem with both integer (number of production plants, storage facilities and transport units) and continuous variables (e.g. hydrogen production and flow rates). The formal presentation of all the constraints and criteria that will be involved in the whole problem will be performed in the following chapter and will demonstrate that the problem can be expressed as a linear one. Section 3.3 distinguishes the mono- and multi-objective formulations. Section 3.4 focuses on multi-objective optimisation methods since they are well suited to the HSC problem. Special attention is paid to the chosen techniques. Section 3.5 reviews the approaches for decision support orientation based on multicriteria decision aid following the multi-objective optimisation step. More

practically, the algorithm, solver and software issues are discussed in section 3.6. In the section 3.7, we examine how the HSC design optimisation framework can be linked with a spatially-detailed infrastructure model. This analysis leads us to implement the spatial design of the HSC using ArcGIS® software. Finally, this chapter ends with the methodological framework that will be used in this study.

3.2 Optimisation frameworks

Some of the most common optimisation frameworks for capturing problems are summarised in Figure 3.1. There can be classified as either *linear or non-linear programming*.

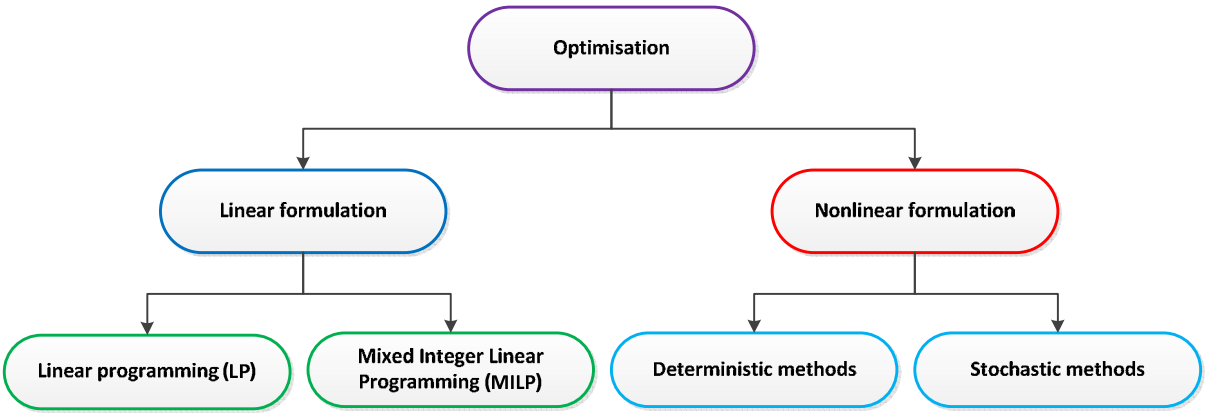


Figure 3.1 Classification of the main optimisation methods (adapted from Garcia et al., 2005).

3.2.1 Linear formulation

Linear formulation is used to obtain an optimal solution to problems where the mathematical functions in both the objective function and the constraints are all linear functions (Hillier and Lieberman, 2001). These methods can be Linear Programming (LP) or Mixed Integer Linear Programming (MILP) depending of the kind of the involved variables.

LP models are used for the efficient allocation of limited resources in known activities in order to meet the desired goals (for instance maximising profits or minimising 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. 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). In the case of both integer and continuous variables, the problem is referred as a mixed-integer linear programming one.

The MILP method consists of maximising or minimising 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 in particular binary 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 behaviours of reality. Many practical optimisation problems lead to consider 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:

Min $cx + dy$
subject to
$Ax + By \geq b$
$L < x < U$
$y = \{0,1,2,..\}$

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 $y=\{0,1,2,..\}$ represents the integer variables.

Various advantages of linear modelling can be found (Boix, 2011):
a) short resolution time compared to other methods,
b) a quick and almost automatic convergence towards a global optimum,
c) the initialization phase is not necessary (as in the case of nonlinear models).

3.2.2 Nonlinear formulation

The nonlinear formulation can be tackled by two main methods, either deterministic or stochastic algorithms procedures. In the *non-linear deterministic models*, no randomness is associated. Then, given a particular input, a deterministic algorithm will obviously produce 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 and constraints. The use of MINLP is a natural approach of formulating problems where it is necessary to simultaneously optimise the system structure (discrete) and parameters (continuous). MINLP problems are precisely so 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 non-convex (and even convex) nonlinear programs (Bussiec and Pruessner, 2003).

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, distances and then fall into probabilistic approaches and scenarios (Patay, 2008). Metaheuristics cannot guarantee to obtain an optimum. The stochastic methods are divided into neighbourhood techniques such as Simulated Annealing, Tabu Search and evolutionary algorithms comprising genetic algorithms, evolutionary strategies and evolutionary programming (Tabkhi, 2007).

The formulation of all the constraints and criteria that will be involved in the whole HSC problem will be the core of the following chapter and will demonstrate that the problem can be expressed as a linear one. This is consistent with the results of the literature review performed in chapter 2.

3.3 Mono- and multi-objective optimisation frameworks

3.3.1 Mono-objective optimisation

Mono-objective problems usually take into account economic aspects such as cost minimisation, and then a myopic optimal solution can be found because this formulation is very far of real problems where many objectives need to be considered at the same time. The mono-objective formulation can be written as follows (Bierlaire, 2006) (Boix, 2011):

$$\text{Min } f(x)$$
$$g(x) \leq 0$$
$$h(x) = 0$$

where f is a function $R^{n1} \times [0,1]^{n2}$ dans R, $g(x) \in \Re^m$, $h(x) \in \Re^p$.

Here, $f(x)$ is the objective function; vectors g(x) and h(x) are respectively m inequality constraints and p equality constraints. This set of constraints defines a restricted search space for the optimal solution. Optimisation problems are linear or nonlinear depending on the type of equations they contain and by continuous or discrete variable type, as explained in the previous sections.

3.3.2 Multi-objective optimisation

In multi-objective problems, it is not possible to find a unique optimal solution but a compromise among various objectives, since there is a conflict among antagonist criteria. The general formulation of a multi-objective optimisation problem is:

$$\text{Min}\left[f_1(x), f_2(x), \ldots, f_k(x)\right]$$
$$g(x) \leq 0$$
$$h(x) = 0$$
$$x \in S$$

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

Such an optimisation scheme is implied when there is a conflict between two or more objectives, even if the most profitable infrastructure may not be necessarily the least environmentally damaging. Because of this trade-off, there is not a single solution to this class of problem but has a set of non-dominated 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 any improvement in one objective leads to the worsening of at least one other objective. As it was abovementioned, the HSC problem involves three objectives to be minimised (cost, environmental impact and risk criterion). Multi-objective methods are briefly described in the next section.

3.4 Multi-objective optimisation methods

Several solution methods have been developed for multi-objective optimisation problems. In these methods, the concept of optimality is replaced with that of efficiency or Pareto optimality. The efficient (or Pareto optimal, non-dominated, non-inferior) solutions are the solutions that cannot be improved in one objective function without deteriorating their performance in at least one of the rest. Weakly efficient solutions are not usually pursued in multi-objective problems because they may be dominated by other efficient solutions (Mavrotas, 2009, 2007). These methods can be classified as the *a priori*, *a posteriori* and *hybrid* methods (based on Collette and Siarry, 2003) including scalar, interactive, fuzzy and meta-heuristic methods (see *Figure 3.2*).

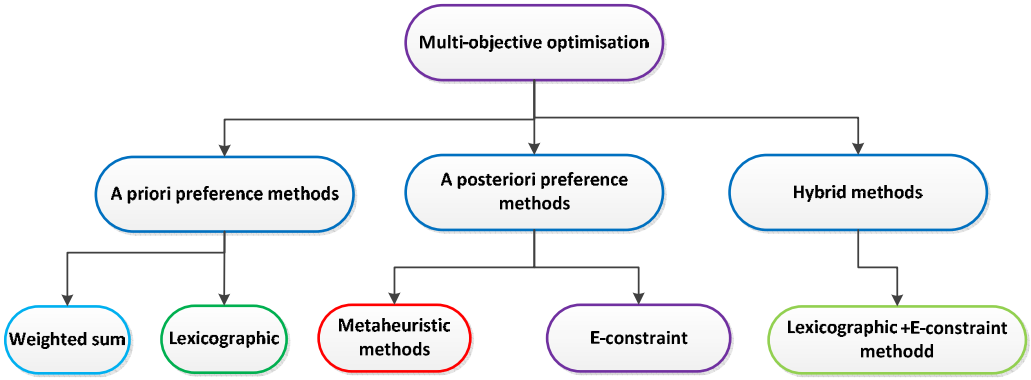


Figure 3.2 Multi-objective optimisation methods

3.4.1 A priori preference methods

With these methods, the decision maker defines the trade-off to be applied (preferences) before running the optimisation method. The aggregative methods belong to this family (where 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) or an approximation of it. Hence, the most preferred solution is "most preferred" in relation to what he/she has seen and compare so far (Mavrotas, 2009, 2007).

3.4.1.1 Weighted sum

The goal of the weighted sum is to transform the problem so that it turns into a mono-objective optimisation problem, for which there exist various methods of solution. 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, we obtain a new, unique objective function. The weighting factors are assigned a priori, then is modified to obtain the Pareto front, with all non-dominated 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)(Boix, 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 optimised. The problem is stated as follows:

$\min (w_1 \times f_1(x) + w_2 \times f_2(x) + \ldots + w_p \times f_p(x))$

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.

3.4.1.2 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 optimisation process starts minimising the most important objective and proceeds according to the assigned order of importance of the criteria. An alternative is to select randomly an objective when there is no more rank available. One disadvantage of this method is that it tends to favour 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:

$$\text{Lexmin}\{f_1(x), f_2(x), \ldots, f_r(x)\} \quad (3.1)$$

subject to

$$g(x) \leq 0$$
$$h(x) = 0$$

In order solve (3.1), the following procedure known as the sequential method is adopted. First, minimise $f_1(x)$, and determines an optimal solution x* ($f_1(x^*) = \beta 1$). Next, the problem is solved minimising $f_2(x)$ subject to $f_1(x^*) = \beta 1$, and so on at the *q* iteration:

$$\text{Lexmin}\{f_q(x): f_i(x) \leq \beta_i, i=1,\ldots,q-1\} \quad (3.2)$$

subject to

$$g(x) \leq 0$$
$$h(x) = 0$$
$$x \in S$$

If either (3.2) has a unique optimum or q = r, then the optimal solution to (3.2) is a pre-emptive optimum. Otherwise, one proceeds to iteration q + 1 (Khorram, 2010).

3.4.2 A posteriori preference methods

With these methods, the decision maker chooses the solution by examining solutions computed by the optimisation model. Methods which belong to this family produce, at the end of the optimisation, a trade-off surface (Collette and Siarry, 2003). This kind of methods produce many solutions when only one will be chosen by the decision maker, it is possible to consider that a lot of time is invested to find the Pareto front. But also, the value of using this kind of methods within a multi-criteria optimisation 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 trade-off solutions and not to present only one single "best" alternative. From the set of alternatives, the decision maker can then further investigate interesting trade-offs and ultimately select a particular strategy that satisfies his/her willingness to compromise (Hugo et al., 2005)**.** In 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.

3.4.2.1 Metaheuristic methods

Metaheuristic methods can be used as a non-aggregative approach. They are particularly useful to treat problems known as "black box" ones where no mathematical property of the problem is known (Boix, 2011). This category includes the 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 of the type of linear constraints and the deterministic input data (the balance equations must

be satisfied with a small tolerance, gap<0.001%). Another main drawback of these methods is that they could consume a large computation time (Boix, 2011).

3.4.2.2 The ε-constraint method

In the ε-constraint method, introduced by (Haimes et al., 1971) all but one objective are converted into constraints by setting an upper or lower bound to each of them, and only one objective is to be optimised (Liu and Papageorgiou, 2013).

By varying the numerical values of the upper bounds, a Pareto front can be obtained. ε-constraint fits in the family of "*a posteriori*" approach with aggregation using constraints in a decoupled method (Collette and Siarry, 2003). This method present 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 to a corner solution (extreme solution), thus generating only efficient[25] extreme solutions. Yet, the ε-constraint method alters the original feasible region and is able to produce non-extreme efficient solutions. An additional advantage of the ε-constraint method is that we can control the number of the generated efficient solutions by properly adjusting the number of grid points in each one of the objective function ranges.

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

min $f_1(x)$

subject to

$f_2(x) \leq e_2$

$f_3(x) \leq e_3$

$f_p(x) \leq e_p$

$x \in S$

By parametrical variation in the right-hand-side (RHS) of the constrained objective functions (e_i) the efficient solutions of the problem are obtained. This method is yet easy to implement but 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 e (Liu and Papageorgiou, 2013), the main difficulty of this method lies in determining Nadir points (where 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, 2009, 2007), presented in the next section.

[25] A feasible solution $x^* \in S$ is called efficient or Pareto optimal if there is no other $x \in S$ such that $f(x^*) < f(x)$ and $f(x^*) \neq f(x)$(Khorram, 2010).

3.4.3 Hybrid methods

A recent work (Mavrotas, 2009, 2007) shed new light on determining Nadir points combining the ε-constraint method with the lexicographic one. Also (Liu and Papageorgiou, 2013), noted that for some multi-objective optimisation problems, the decision makers do not have preference to any objective, i.e., all the objectives are equally important. In this case, it is crucial to generate a fair solution, in which all normalised objective function values are as much close to each other as possible. In order to generate such solutions, the lexicographic can easily be coupled to the ε-constraint method to create a hybrid method which could result in fair solutions.

The AUGMECON method (Mavrotas, 2009, 2007) is an effort to effectively implement the ε-constraint method for producing the 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 optimisation of the *p* objective functions). In a minimisation 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 optimisation of the objective functions are efficient solutions. In order to overcome this limitation, the AUGMECON method propose the use of lexicographic optimisation for every objective function in order to construct the payoff table with only efficient solutions. A simple remedy in order 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 minimisation objective functions) bound. Values worse than the reservation value are not allowed.

3.4.4 Choice of the multi-objective optimisation method

The weighted-sum method was not selected in this work because some preliminary optimisation runs lead to Pareto fronts with a too low density of solutions. The lexicographic method minimising the most important objective and then proceeding according to the assigned rank of importance of the criteria can be an interesting option because of its simplicity and computational efficiency but its efficiency is better when coupled to another method to obtain the Pareto Front. As reported in the literature survey, the original HSC model has been defined as a deterministic MILP, involving a large number of inequality constraints and equality ones (mass balances that must be rigorously solved). These are the main reasons to discard metaheuristic methods. The main difficulty related to the ε-constraint method lies in determining Nadir points (where the criteria take their worst values) but the work of (Mavrotas, 2009, 2007) shed new light on this problem combining this method with the lexicographic one which can easily be coupled to the , ε-constraint method to create a hybrid method which could result in fair solutions. Then, lexicographic, ε-constraint and hybrid "lexicographic+ ε-constraint" methods are explored in this study and will be used in the following chapters to tackle the different case studies.

3.5 Multi-Criteria Decision Making (MCDM): decision aid methods

The "classical" multi-objective methods previously presented are based on the *domination relation* and leads to a set of compromise solutions that have been filtered through the optimisation process. The problem is now to the select the best choice among these compromise solutions. This can be performed by use of a multi-criteria decision making methods (Boix, 2011; Bonnin, 2013; Hernandez-Rodriguez, 2011; Morales Mendoza, 2013; Ouattara, 2011; Pérez Gallardo, 2013). In the case of the decision aid methods, they consider the *order relation* between various elements. With the order relation it is possible to obtain a set of solutions (with a partial order relation) or one and only one solution (with a complete order relation). The other major difference is that the decision aid methods work only with discrete sets of points. These methods can treat choice, sorting and arranging methods (Collette and Siarry, 2003). A variety of methods exists (Morales Mendoza et al., 2011). For the sake of illustration, the methods of ELECTRE, TOPSIS and M-TOPSIS are briefly presented.

3.5.1 ELECTRE

The ELECTRE (Elimination and Choice Translating Reality); method was introduced by Roy in 1968 (Roy, 1968). The basic concept of the ELECTRE method is to deal with "outranking relations" by using pair wise 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 counter-part of the concordance index. 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 favourable ones. This method is especially convenient when there are decision problems that involve a few criteria with a large number of alternatives saving much time.

3.5.2 TOPSIS

TOPSIS (Technique for Order Preference by Similarly to Ideal Solution) was developed by Hwang and Yoon in 1981 (Hwang, and Yoon, 1981) as an alternative to the ELECTRE method and can be considered as one of its most widely accepted variants. 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. This approach is used for four main reasons (García-Cascales and Lamata, 2012):

a) TOPSIS logic is rational and understandable;
b) the computation processes are straight forward;
c) the concept permits the pursuit of the best alternatives for each criterion depicted in a simple mathematical form;
d) the importance weights are incorporated into the comparison procedures.

However, the TOPSIS method presents certain drawbacks. One of the problems related to TOPSIS is that it can cause the phenomenon known as rank reversal (García-Cascales and Lamata, 2012). In this phenomenon, the alternative order of preference changes when an alternative is added to or removed from the decision problem. To deal with this problem, the method M-TOPSIS is proposed.

3.5.3 M-TOPSIS

Ren et al (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) at first; and then, the $D^+ D^-$ plane is constructed. D^+ is the *x*-axis and D^- is the *y*-axis (see Appendix D). The point (D^+_i,D^-_i) represents each alternative (i = 1, 2 . . . , n). The point A (min(D^+_i), max(D^-_i)) is the "optimised 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.

3.5.4 Choice of the MCDC

A comparative study on the application of MCDM methods for design purpose in Process Systems Engineering problems can be found in (Azzaro-Pantel and Zaraté, 2009) and (Morales Mendoza et al., 2011). Several works have used these methods for multi-objective problems (Boix, 2011; Hernandez-Rodriguez, 2011; Ouattara, 2011; Pérez Gallardo, 2013) (Bonnin, 2013; Morales Mendoza, 2013). Based on these results, our choice fell on the TOPSIS and M-TOPSIS methods.

3.6 Algorithm and software

The GAMS environment, which offers a wide variety of optimisation procedures and allows using different solvers has been used in this study. GAMS has many updates and a wide range of solvers available, it can treat the problems of large sizes. In addition, complex models can be written compactly and changes in the program are relatively simple to make. Model coding is generic and can easily change the solver depending on the nature of the problem (linear, nonlinear, continuous, mixed) without changing its formulation. This software had been widely used (Almansoori and Shah, 2012, 2009, 2006; Boix, 2011; Guillén Gosálbez et al., 2010; Kim et al., 2008; Sabio et al., 2010; Tabkhi, 2007).

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.

Besides all the advantages previously described, the base model (Almansoori and Shah, 2006) was coded in GAMS using the CPLEX solver. The same solver choice can thus be useful at preliminary validation step and has thus been adopted in this study.

3.7 Spatial-based approach

This work pretends to use real-world data from GIS databases along with an optimisation model MILP. The ArcGIS® software (developed by ESRI, Environmental Systems Research Institute) is a GIS used to organise, analyse and map spatial data. A typical GIS project contains an extensive database of geographic information, graphical capabilities of displaying maps with overlays pertaining to the company's supply chain activities (Shapiro, 2001). Literature review shown in chapter 2 reveals that few researchers have used the spatial dimensions to build the infrastructure of HSC. Some examples of geographic approaches include the studies (Ball et al., 2006; Dagdougui, 2011a; Johnson et al., 2008).

It must be highlighted that by contrast to the mathematical optimisation approaches, a spatial or GIS-based study cannot be considered as a general methodology for the design of the optimal HSC. In a GIS analysis project, an analyst faces a variety of tasks that can be grouped into four basic steps (Booth and Mitchell, 1999):

1. to convert a question, such as "where is the best place for a new production plant?" or "how many potential refuelling stations are near a particular energy source?" into a GIS database design and an analysis plan. This involves breaking the question into logical parts, identifying what layers of data will be needed to answer each part and developing a strategy for combining the answers to each part of the question into a final answer.
2. to create a database that contains the geographic data required to answer the questions. This may involve digitizing existing maps, obtaining and translating electronic data from a variety of sources and formats, making sure the layers are of adequate quality for the task, making sure the layers are in the same coordinate system and will overlay correctly, and adding items to the data to track analysis result values. Personal workspaces of file based data and personal geo databases are used to organise project GIS geo databases.
3. to analyse the data. This usually involves overlaying different layers, querying attributes and feature locations to answer each logical part of the question, storing the answers to the logical parts of the question, and retrieving and combining those answers to provide a complete answer to the question.
4. to communicate the results of the analysis. Maps, reports, and graphs are all used, often together, to communicate the answer to the question.

Figure 3.3 shows how the model is integrated in a flow chart. In the optimisation model, the territory under study for HSC implementation will be divided into grids, regions or districts in which the

number, size and type of production and storage units have to be determined with the considered objective functions and constraints. Models of hydrogen delivery need distances over the road network between the supply points, the production and conditioning sites and the demand centers. To calculate the delivery distances over the road network, an average distance between the main cities is considered in the optimisation model. Yet, it does not allow locating precisely the involved units and delivery paths because only potential site could be proposed. The energy sources maps are produced using the GPS coordinates in Arc Map 10.2. In the case of roads and geographic breakdown, maps from the national geographic institute are used. Shortest path routing will be performed. The data was then entered into the GAMS model. The input data to be used in the GAMS MILP model is as follows:

- energy source location
- initial conditioning centers and production plants.
- distances between main cities (national roads; intracity delivery of hydrogen is not consider in this work)
- refuelling stations

The engineering-technical, financial and environmental data as well as demand are embedded in the model as input parameters (calculated in excel). Results are exported to Excel and new layers are created in ArcGIS® 10.2 to display the HSC locating the new production and storage sites defining also the flow rate links. We use diverse layers and constrains previously defined for a specific case study (see chapter 6 section 6.2) to create the maps or snapshots, we manually select the potential locations following the geographic restrictions.

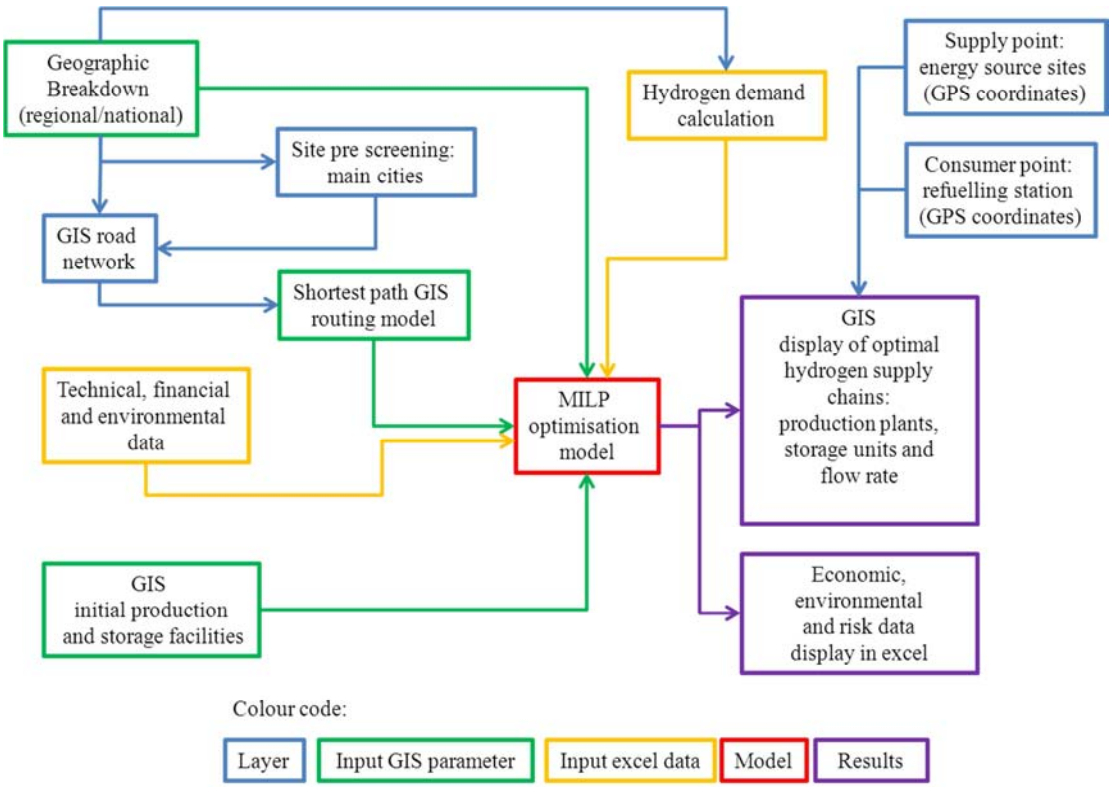


Figure 3.3 Model flow chart

3.8 Conclusions

To summarise the scope of this thesis, the four main stages of our approach are presented. The study involves data collection and mono-objective optimisation in a preliminary stage to allow the application of multi-objective methodologies. These are then followed by the use of a MCDM. These stages are briefly explained and will be followed in the case studies treated in chapters 4-6.

A. Data collection. In this stage, the potential technologies are reviewed, the geographic breakdown is defined and the databases using technical, financial and environmental information are also created. The geographic database can be created by ArcGIS®.
B. Mono-objective optimisation. The mathematical model described in (Almansoori and Shah, 2006) work addressed the optimal design of a steady-state HSC network with cost as an optimisation criterion. This model served as a validation step in the GAMS environment with the CPLEX solver. The model was extended to the consideration of safety and environmental criteria.
C. Multi-objective optimisation. When the minimal values of each objective function are found, it is possible to generate a pay-off table through lexicographic optimisation. This way the utopia and nadir points are also found and it is possible to create the Pareto Front via ε-constraint method.
D. MCDM. The last step consists in the choice of the best compromise option. For this purpose, the widely used M-TOPSIS methodology and the comparison of mono- and multi-objective optimisation results are analysed. Depending on the case study, the geographic constraints motivate the utilisation of a specific tool as ArcGIS® to map the HSC.

Chapter 4

A MULTI-OBJECTIVE OPTIMISATION FRAMEWORK FOR HYDROGEN SUPPLY CHAIN

Résumé

Ce chapitre est consacré à la modélisation de la chaîne logistique « hydrogène ». Elle est basée sur une formulation de type programmation linéaire en variables mixtes dans une approche multi-objectif et mono-période. Les trois critères impliqués sont explicités et concernent le prix de revient de l'hydrogène, l'impact sur le réchauffement climatique et un indice de risque. Le problème multi-objectif est résolu par la mise en œuvre d'une méthode lexicographique et d'une méthode ε-contrainte. L'ensemble des solutions du problème est visualisé à travers un front de Pareto, correspondant à différentes stratégies de conception. La méthode M-TOPSIS est ensuite utilisée comme outil d'aide à la décision pour trouver la solution qui offre le meilleur compromis. Le modèle est appliqué à une étude de cas en Grande-Bretagne issue de la littérature spécialisée, qui sert de référence pour comparer les approches mono- et multi-objectif. Les résultats obtenus dans les deux cas diffèrent par le degré de centralisation du réseau et par le type de technologie de production.

Abstract

This chapter is focused on the design of a hydrogen supply chain based on mixed integer linear programming used to find the best solutions for one time period in a multi-objective optimisation problem in which three objectives are involved, i.e., cost, global warming potential and safety risk. 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 is then implemented to find the best solution through an M-TOPSIS analysis. The model is applied to the Great Britain case study previously treated in the dedicated literature. Mono and multicriteria optimisations exhibit some differences concerning the degree of centralisation of the network and the selection of the production technology type.

Nomenclature

Abbreviations

FMEA	Failure Modes and Effects Analysis
GB	Great Britain
GWP	Global warming potential
HSC	Hydrogen supply chain
LCA	Life Cycle Assessment
LH_2	Liquid hydrogen
MILP	Mixed Integer Linear Programming
SMR	Steam methane reforming
TDC	Total daily cost

Indices

g: grid squares *g* and *g':* grid squares such that $g' \neq g$
i: product physical form
l: type of transportation modes
p: plant type with different production technologies
s: storage facility type with different storage technologies

Parameters

α	Network operating period (days per year)
β	Storage holding period-average number of days worth of stock (days)
β_g	Adjacency level weight factor of a region *g* in which the route is located
$AD_{gg'}$	Average delivery distance between *g* and *g'* by transportation *l* (km per trip)
CCF	Capital change factor -payback period of capital investment (years)
DT_{ig}	Total demand for product form *i* in grid *g* (kg per day)
DW_l	Driver wage of transportation mode *l* (dollars per hour)
FE_l	Fuel economy of transportation mode *l* (km per liter)
FP_l	Fuel price of transportation mode *l* (dollars per liter)
GE_l	General expenses of transportation mode *l* (dollars per day)
$GWProd_p$	Production GWP by plant type *p* (g CO_2-eq per kg of H_2)
$GWStock_i$	Storage global warming potential form *i* (g CO_2-eq per kg of H_2)
$GWTrans_l$	Global warming potential of transportation mode *l* (g CO_2 per ton-km)
LUT_l	Load and unload time of product for transportation mode *l* (hours per trip)
ME_l	Maintenance expenses of transportation mode *l* (dollars per km)
$PCapmin_{pi}$	Minimum production capacity of plant type *p* for product form *i* (kg per day)
$PCapmax_{pi}$	Maximum production capacity of plant type *p* for product form *i* (kg per day)
PCC_{pi}	Capital cost of establishing plant type *p* producing product form *i* (dollars)
$Qmax_{il}$	Maximum flow rate of product form *i* by transportation mode *l* (kg per day)
$Qmin_{il}$	Minimum flow rate of product form *i* by transportation mode *l* (kg per day)
RL_g	Risk level of the grid *g* (units)
RP_p	Risk level of the production facility *p* (units)
$RR_{gg'}$	Road risk between grids g and g' (units)
RS_s	Risk level in storage facility *s* (units)
RT_l	Risk level of transportation mode *l* (units)
$SCapmin_{si}$	Minimum storage capacity of storage type *s* for product form *i* (kg)
$SCapmax_{si}$	Maximum storage capacity of storage type *s* for product form *i* (kg)

SCC_{si}	Capital cost of establishing storage type *s* storing product form *i* (dollars)
SP_l	Average speed of transportation mode *l* (km per hour)
TMA_l	Availability of transportation mode *l* (hours per day)
TMC_{il}	Cost of establishing transportation mode *l* for product form *i* (dollars)
$TCap_{il}$	Capacity of transportation mode *l* transporting product form *i* (kg per trip)
UPC_{pi}	Unit production cost for product *i* produced by plant type *p* (dollars per kg)
USC_{si}	Unit storage cost for product form *i* at storage type *s* (dollar per kg-day)
W_l	Weight of transportation mode *l* (tons)
WFP_g	Weigh factor risk population in each grid (units)

Variables

Continuous variables

D^I_{ig}	Imported demand of product form *i* to grid *g* (kg per day)
D^L_{ig}	Demand for product *i* in grid *g* satisfied by local production (kg per day)
FC	Fuel cost (dollars per day)
FCC	Facility capital cost (dollars)
FOC	Facility operating cost (dollars per day)
GC	General cost (dollars per day)
GWPTot	Total global warming potential of the network (g CO_2-eq per day)
LC	Labour cost (dollars per day)
MC	Maintenance cost (dollars per day)
PGWP	Total daily GWP in the production facilities *p* (g CO_2-eq per day)
P^R_{pig}	Production rate of product *i* produced by plant type *p* in grid *g* (kg per day)
P^T_{ig}	Total production rate of product *i* in grid *g* (kg per day)
$Q_{ilgg'}$	Flow rate of product *i* by transportation mode *l* between *g* and *g'*(kg per day)
SGWP	Total daily GWP in the storage technology *s* (g CO_2-eq per day)
S^T_{ig}	Total average inventory of product form *i* in grid *g* (kg)
TCC	Transportation capital cost (dollars)
TDC	Total daily cost of the network (dollars per day)
TGWP	Total daily GWP in the transportation mode *l* (g CO_2-eq per day)
TOC	Transportation operating cost (dollars per day)
TotalRisk	Total risk of this configuration (units)
TPRisk	Total risk index for production activity *p* (units)
TSRisk	Total risk index for storage activity *s* (units)
TTRisk	Total risk index for transport activity (units)
$V_{ilgg'}$	Artificial variable with values between 0 and 1

Integer variables

NP_{pig}	Number of plants of type p producing product form *i* in grid *g*
NS_{sig}	Number of storage facilities of type *s* for product form *i* in grid *g*
$NTU_{ilgg'}$	Number of transport units between *g* and *g'*

Binary variables

$X_{ilgg'}$	1 when the product form *i* is to be transported from grids *g* to *g'*
Y_{ig}	1 if product form *i* is to be exported from grid *g* or 0 otherwise
Z_{ig}	1 if product form *i* is to be imported into grid *g* or 0 otherwise

4.1 Introduction

The aim of this chapter is to present the multi-objective framework that has been adopted in this work for hydrogen deployment in a mono-period problem. This work led to two publications (De-León Almaraz et al., 2012)[26] and (De-León Almaraz et al., 2013a)[27].

The remainder of this chapter is organised as follows; Section 4.2 is dedicated to problem formulation. Section 4.3 presents the general structure of the hydrogen supply chain. The mathematical model is the core of section 4.4 and considers demand, production, transportation and storage constraints. The formulation of the criteria that are considered in this work, i.e., cost, global warming potential and risk objectives is described in sections 4.5 to 4.7. Section 4.8 is dedicated to the solution strategy: first the mono-objective problem is solved and will serve as a reference case, then, the lexicographic and Ɛ-constraint methods are used to solve the multi-objective problem. The multi-criteria decision-making process that is used to select the best compromise among the optimisation results is then presented. This chapter ends with the validation of the proposed model in an academic case study of Great Britain (Almansoori and Shah, 2006) in section 4.9: the geographic breakdown is given in grid squares and only steam methane reforming and gasification are evaluated in this first case study. The obtained results between the mono- and multi-objective approaches are finally analysed and discussed in section 4.10 and 4.11.

4.2 Methodology

In this section, the main principles of the proposed methodology are presented. Firstly, the problem statement, assumptions and objectives are defined with the associated decision variables. The hydrogen supply chain (HSC) is then presented to establish the general structure of the network. The problem dimension is examined to compare mono- and multi-criteria approaches. Finally, the solution strategy phases are also developed.

4.2.1 Problem statement

As aforementioned, current designs of the HSC reviewed in the dedicated literature are generally based to a multi-objective strategy with two criteria, either cost-environment or cost-safety. A three-

[26]De-León Almaraz, S., Azzaro-Pantel, C., Montastruc, L., Pibouleau, L., Senties, O.B., 2012. Design of a hydrogen supply chain using multiobjective optimisation, in: 22nd European Symposium on Computer Aided Process Engineering. Elsevier, pp. 292–296.

[27]De-León Almaraz, S., Azzaro-Pantel, C., Montastruc, L., Pibouleau, L., Senties, O.B., 2013a. Assessment of mono and multi-objective optimization to design a hydrogen supply chain. Int. J. Hydrog. Energy 38, 14121–14145.

criteria optimisation model is proposed here considering the interconnection of social, economic and environmental impacts. Their relationship will result in the global balance of the system.

4.2.2 Objective

This work is focused on the design of a three-echelon HSC (production, storage and transportation), considering the minimum cost, the lower environmental impact and the lower safety risk. The model is validated through a well-known example concerning Great Britain and presented in (Almansoori and Shah, 2006) and results for mono-objective optimisations will be compared with the multi-objective solution.

4.2.3 Given data

Problem data involve hydrogen demand data (each grid has its own deterministic demand), techno-economic, environmental and risk data of the components in the HSC (they are presented in detail in Appendix A1).

4.2.4 Design decisions

Design decisions are based on the number, type, capacity, and location of production and storage facilities. More precisely, they involve the number and type of transport units required as well as the flow rate of hydrogen between locations. Cities or grids are also considered.

4.2.5 Operational decisions

Operational decisions concern the total production rate of hydrogen in each grid, the total average inventory in each grid, the demand covered by imported hydrogen and the H_2 demand covered by local production.

4.2.6 Assumptions

- A deterministic demand of hydrogen for the transportation system (particular-light cars and buses) is considered;
- A mono-period problem is assumed.
- Relative risk of production plant, storage facilities and transportation modes are assumed not to change under the various demand scenarios.
- The model is assumed to be demand driven.

4.3 Formulation of the HSC

4.3.1 General structure of the HSC

In this formulation, hydrogen can be delivered in specific physical form *i*, such as liquid or/and gaseous, produced in a plant type with different production technologies *p* (i.e. steam methane reforming (SMR), biomass or coal gasification); distributed by a specific type of transportation modes *l* going from the location *g* to *g'* referred as grid squares; such that g' is different than g; this grid squares are obtained by dividing the total area of the country or region into n grid squares of equal

size, a general HSC is shown in Figure 4.1. This supply chain is demand driven and it is a reverse logic network because we assume there are no flows from the market to the facilities or suppliers.

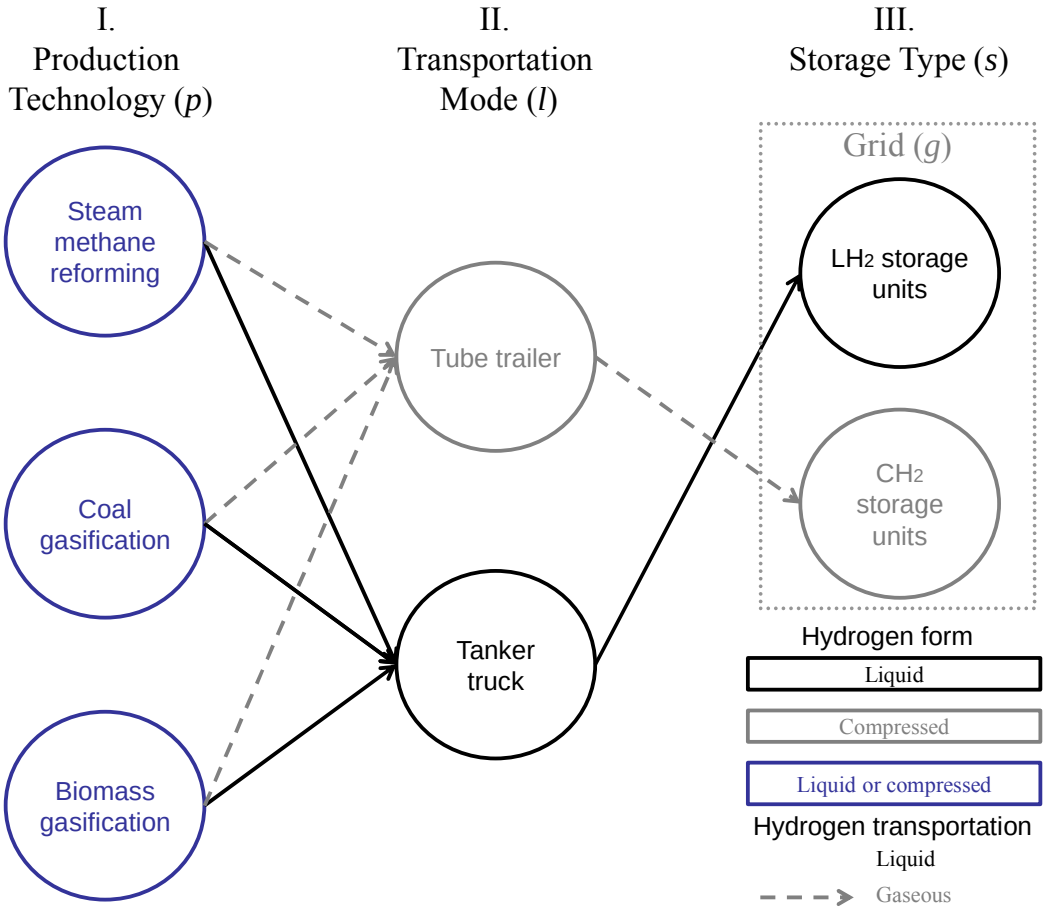


Figure 4.1 The HSC treated by (Almansoori and Shah, 2006)

4.3.2 Supply chain decision database

Several data are necessary to design the HSC as the base investment and operational costs for a given facility that will be used for extrapolation purpose, the throughput associated with a given technology, the quantities of input and output products associated with unit operations of the transformation types, etc. The whole list is presented in Appendix A1.

4.3.3 Model variables

The definition of continuous, integer and binary variables is necessary for the mathematical formulation of the HSC (detailed classification is shown in the nomenclature section of this chapter). The problem is then captured in a mixed-integer linear programming (MILP) framework. All continuous and integer variables must be non-negative. Output data will include optimal locations and capacities of new facilities, levels for transformation and process activities at each facility, outbound flows of finished products from production facilities to markets, etc.

4.4 Mathematical model

The model presented in this work has been inspired by the previous approach of Almansoori and Shah (2006, 2009 and 2012) dedicated to the optimal total daily cost of the HSC through mixed-integer linear programming (MILP). The safety study takes into account the work of Kim and Moon (2008 and 2011). Environmental impact calculations have also been introduced. Even the original model can be found in the bibliography it is important to write it here in order to show the main changes and the introduction of new constraints, also with the intention to easily appreciate the different constraints features (i.e. equality or inequality, binding and nonbinding).

4.4.1 Demand constraints

As previously mentioned, each grid has its own deterministic demand. This demand must be fulfilled eventually by production facilities established within a particular grid, i.e., local production, or by importing products from other neighbouring grids. Therefore, the demand satisfied by local production of a product form *i* in grid *g* (D^L_{ig}) is expressed by the following constraint:

$$D_{ig}^{L} \le P_{ig}^{T} \quad \forall i,g \tag{4.1}$$

On the other hand, the demand for a product form *i* in grid *g* satisfied by neighbouring grids (D^I_{ig}) is equal to the total flow imported to that grid by all types of transportation modes ($Q_{ilg'g}$):

$$D_{ig}^{I} = \sum_{l,g'} Q_{i\,lg'g} \quad \forall i,g; g \neq g' \tag{4.2}$$

The total grid demand (D^T_{ig}) must equal the demand satisfied by the local production plus the demand imported from other grids:

$$D_{ig}^{T} = D_{ig}^{L} + D_{ig}^{I} \quad \forall i,g \tag{4.3}$$

4.4.2 Production facilities constraints

A total mass balance on a grid must be written to determine the total daily production rate of a particular grid. Since we assume a steady-state operation, the sum of the total flow rate of each product entering grid *g* ($Q_{ilg'g}$) plus the total production rate of the same grid (P^T_{ig}) must equal the total flow rate leaving this grid ($Q_{ilgg'}$) plus the total demand required by grid *g* itself (D^T_{ig}):

$$P_{ig}^{T} = \sum_{l,g'} \left(Q_{i\,lg\,g'} - Q_{i\,lg'g} \right) + D_{ig}^{T} \quad \forall i,g \tag{4.4}$$

The total production rate of a product form *i* in grid *g* is equal to the production rate of all plants of type *p* established in that same grid:

$$P_{ig}^{T} = \sum_{p} PR_{pig} \quad \forall i,g \tag{4.5}$$

The production rate of a product form *i* produced by any plant of type *p* in grid *g* (PR_{pig}) cannot exceed certain limits. Thus, there is always a maximum production capacity for any product ($PCap_{pi}^{max}$).

Moreover, there is often a minimum production rate ($PCap_{pi}^{min}$) that must be maintained while the plant is operating:

$$PCap_{pi}^{\min} NP_{pig} \le PR_{pig} \le PCap_{pi}^{\max} NP_{pig} \quad \forall p,i,g \tag{4.6}$$

Constraint (4.6) means that the maximum daily production rate of product form *i* produced by plant type *p* is constrained by the number of production facilities NP_{pig}. Likewise, the total production rate of each product form *i* in grid *g* (P^{T}_{ig}) cannot exceed certain limits. Therefore, P^{T}_{ig} is bound between the minimum and maximum production capacities of all plants that are established in this particular grid:

$$\sum_{p} PCap_{pi}^{\min} NP_{pig} \le P_{ig}^{T} \le \sum_{p} PCap_{pi}^{\max} NP_{pig} \quad \forall i,g \tag{4.7}$$

4.4.3 Transportation constraints

There must be a continuous flow of product between different grids in order to satisfy the required demand. The flow of a product form *i* from grid *g* to a different grid *g'* will only exist if the transportation mode is established. Thus, there is always a minimum and a maximum flow rate of products (Q_{il}^{min} and Q_{il}^{max}) needed to justify the establishment of a transportation mode between two grids in the network:

$$Q_{il}^{\min} X_{i\lg g'} \le Q_{i\lg g'} \le Q_{il}^{\max} X_{i\lg g'} \quad \forall i,l,g,g';g \ne g' \tag{4.8}$$

Flow of a product form *i* between different grids can only occur in one direction. This is because if a grid can only satisfy its needs by importing from other grids it would not make sense for that grid to export to other grids:

$$X_{i\lg g'} + X_{i\lg' g} \le 1 \quad \forall i,l,g,g';g \ne g' \tag{4.9}$$

A particular grid can only import product from neighbouring grids or export product to other grids, or neither but not both for the same reason stated earlier:

$$Y_{ig} \ge X_{i\lg g'} \quad \forall i,l,g,g';g \ne g' \tag{4.10}$$

$$Z_{ig} \ge X_{i\lg' g} \quad \forall i,l,g,g';g \ne g' \tag{4.11}$$

$$Y_{ig} + Z_{ig} \le 1 \forall i,g \tag{4.12}$$

4.4.4 Storage facilities constraints

An important issue in the operation of this network is the ability of the storage facilities to hold the product for a certain period of time in order to accommodate for any demand and supply fluctuations. Therefore, storage facilities could be built either locally within a specific grid next to the production

facility—if established—or outside the grid boundary away from the production source. During steady-state operation, the total inventory of a product form *i* in grid *g* (S^T_{ig}) is equal to a function of the corresponding demand (D^T_{ig}) multiplied by the storage period (β), days of cover:

$$S_{ig}^{T} = \beta D_{ig}^{T} \ \forall i, g \quad \textbf{(4.13)}$$

The parameter β is introduced to cover fluctuations in both supply and demand as well as plant interruptions. The capacity of each storage facility of type *s* storing product form *i* ($SCap_{si}^{max}$) cannot exceed certain limits. This consideration will guarantee that the total inventory of each product in each grid will be bound within certain limits:

$$\sum_{s} SCap_{si}^{\min} NS_{sig} \le S_{ig}^{T} \le \sum_{s} SCap_{si}^{\max} NS_{sig} \ \forall i, g \quad \textbf{(4.14)}$$

4.4.5 Non-negativity constraints

All continuous and integer variables must be non-negative:

$$D_{ig}^{L} \ge 0 \ \forall i, g \quad \textbf{(4.15)}$$

$$D_{ig}^{I} \ge 0 \ \forall i, g \quad \textbf{(4.16)}$$

$$NP_{pig} \ge 0 \ \forall i, p, g \quad \textbf{(4.17)}$$

$$NS_{sig} \ge 0 \ \forall i, s, g \quad \textbf{(4.18)}$$

$$P_{ig}^{T} \ge 0 \ \forall i, g \quad \textbf{(4.19)}$$

$$PR_{pig} \ge 0 \ \forall i, p, g \quad \textbf{(4.20)}$$

$$Q_{i \lg g'} \ge 0 \ \forall i, l, g, g'; g \ne g' \quad \textbf{(4.21)}$$

$$S_{ig}^{T} \ge 0 \ \forall i, g \quad \textbf{(4.22)}$$

4.5 Cost objective

The total daily cost (*TDC*) of the network is determined in the same way as in the linear model of (Almansoori and Shah, 2006). The TDC ($ per day) of the whole HSC is a function calculated by the addition of four main costs:

4.5.1 Facility capital cost

The facility capital cost is related to the establishment of production plants and storage facilities at candidate locations. It is calculated by multiplying the number of new plants and new storage facilities by their capital cost as follows:

$$FCC = \sum_{i,g} \left(\sum_{p} PCC_{pi} NP_{pig} + \sum_{s} SCC_{si} NS_{sig} \right) \quad \textbf{(4.23)}$$

4.5.2 Transportation capital cost

One modification was made to the original model (Almansoori and Shah, 2006). It consists in the way to calculate the number of transport units (*NTU*) because it did not take an integer value. Values of transportation capital cost (*TCC)* and transportation operating cost (*TOC)* were lower than the real cost considering integer values. Equations 4.24 and 4.25 were added to the model and Eq.(4.26) is modified to allow rounding the *NTU* value.

$$V_{ilgg'} \geq 0 \quad \forall i,l,g,g' \tag{4.24}$$

$$V_{ilgg'} \leq 1 * X_{ilgg'} \quad \forall i,l,g,g' \tag{4.25}$$

where $V_{ilgg'}$ is a continuous variable with values between 0 and 1 related to the binary value of $X_{ilgg'}$ which takes the value of 1 when the product form *i* is to be transported from grids *g* to *g'*.

Then $NTU_{ilgg'}$ depends significantly on the average distance travelled between different grids ($AD_{gg'}$), the capacity of a transport container ($TCap_{il}$), the flow rate of products between various grids ($Q_{ilgg'}$), the transportation mode availability (TMA_l), the average speed (SP_l), and loading/unloading time (LUT_l) . Finally, the $V_{ilgg'}$ is added and an integer value is found.

$$NTU_{ilgg'} = \left(\frac{Q_{ilgg'}}{TMA_l TCap_{il}} \left(\frac{2AD_{gg'}}{SP_l} + LUT_l \right) \right) + V_{ilgg'} \tag{4.26}$$

It can be noted from equation (4.26) that $AD_{gg'}$ is multiplied by two to account for the return journey. Finally, the transportation capital cost is given by the following equation:

$$TCC = \sum_{i,l,g,g'} NTUgrid_{ilgg'} xTMC_{il} \tag{4.27}$$

4.5.3 Facility operating cost

The facility operating cost is related to the cost required to operate the production plants and storage facilities efficiently. It is obtained by multiplying the unit cost of production and storage by the corresponding amount of production and storage:

$$FOC = \sum_{i,g} \left(\sum_{p} UPC_{pi} PR_{pig} + \sum_{s} USC_{si} S_{ig}^{T} \right) \tag{4.28}$$

4.5.4 Transportation operating cost

The transportation operating cost consists of fuel, labour, maintenance, and general costs. The daily fuel cost contributes significantly to the total operating cost. It is a function of daily fuel usage and fuel price:

$$FC = \sum_{i,l,g,g'} FP_l \left(\frac{2AD_{gg'} Q_{ilgg'}}{FE_l \, TCap_{il}} \right) \tag{4.29}$$

where the first and second terms of the multiplication in equation (4.29) represent fuel price and daily fuel usage, respectively. The daily labour cost associated with transporting the hydrogen between different grids is given as a function of the total delivery time and driver wage:

$$LC = \sum_{i,l,g,g'} DW_l \left(\frac{Q_{i\,l\,g\,g'}}{TCap_{il}} \left(\frac{2AD_{gg'}}{SP_l} + LUT_l \right) \right) \quad \textbf{(4.30)}$$

Again, the first and second terms of the multiplication in equation (4.30) represent driver wage and total delivery time, respectively. The maintenance cost includes general maintenance of the transportation systems. It is a function of the total daily distance driven and the cost per unit distance travelled:

$$MC = \sum_{i,l,g,g'} ME_l \left(\frac{2AD_{gg'} Q_{i\,l\,g\,g'}}{TCap_{il}} \right) \quad \textbf{(4.31)}$$

The general cost consists of transportation insurance, license and registration, and outstanding finances. It depends on the number of transport units and the corresponding expenses:

$$GC = \sum_{i,l,g,g'} GE_l \left(\frac{Q_{i\,l\,g\,g'}}{TMA_l\, TCap_{il}} \left(\frac{2AD_{gg'}}{SP_l} + LUT_l \right) \right) \quad \textbf{(4.32)}$$

Finally, the total transportation operating cost is equal to the sum of fuel, labour, maintenance and general costs:

$$TOC = FC + LC + MC + GC \quad \textbf{(4.33)}$$

4.5.5 Objective function 1

The *TDC* represents the cost expressed in $ per day of the entire HSC where *FCC* is the facility capital cost ($), *TCC* is the transportation capital cost ($), α is the network operating period (days per year) related to the capital charge factor (*CCF*, in years). Then, the facility operating cost (*FOC*, $ per day) and the transportation operating cost (*TOC*, $ per day) are also associated in Eq. 4.34.

$$TDC = \left(\frac{FCC + TCC}{\alpha . CCF} \right) + FOC + TOC \quad \textbf{(4.34)}$$

The addition of new constraints to find global warming potential and safety risks values are necessary to implement the proposed multi-objective approach. The definition of the additional objective functions considered is presented below.

4.6 Global warming potential (GWP) objective

The total daily production GWP (*PGWP*, in g CO_2-eq per day) is associated with the production rate of product type *i* produced by each plant of type *p* in grid *g* (PR_{pig}, in kg per day) and the total daily GWP in the production facility type *p* (GW_i^{prod}, in g CO_2-eq per kg):

$$PGWP = \sum_{pig} (PR_{pig} GW_i^{prod}) \quad \textbf{(4.35)}$$

The total daily storage GWP (*SGWP*, in g CO_2-eq per day) is given by Eq. (4.36) where the PR_{pig} is related to the total daily GWP for the storage technology (GW_i^{stock}, in g CO_2-eq per kg):

$$SGWP = \sum_{pig} (PR_{pig} GW_i^{stock}) \quad \textbf{(4.36)}$$

The total daily transport GWP (*TGWP*, in g CO_2-eq per day) is determined as follows:

$$TGWP = \sum_{i\lg g'} \left(\frac{2AD_{\lg g'} . Q_{i\lg g'}}{TCap_{il}} \right) GW_i^{Trans} . W_l \quad \textbf{(4.37)}$$

where the average delivery distance between *g* and *g'* by transportation mode *l* (km $trip^{-1}$) is multiplied by the flow rate of product form *i* transported by the mode *l* between *g* and *g'* and divided by the transportation capacity for product form *i* (kg $trip^{-1}$). These three terms allow the computation of the number of km per day that must be run to cover the demand taking into account the round trip. Finally those terms are related to the global warming potential (GW_i^{Trans}, in g CO_2-eq per tonne-km) associated to the transportation mode *l* and its weight (W_l, in tons).

Eqs. (4.35), (4.36) and (4.37) enable the calculation of the total GWP (*GWPTot*, in g CO_2-eq per day) as indicated by:

$$GWPTot = PGWP + SGWP + TGWP \quad \textbf{(4.38)}$$

4.7 Safety objective

Kim and Moon (Kim and Moon, 2008)(Kim et al., 2011) developed expressions to evaluate the total risk of production and storage facilities (*TPRisk* and *TSRisk* respectively) as well as the total transport risk (*TTRisk*) where the relative risk of hydrogen activities is determined by risk ratings calculated based on a risk index method. The *TPRisk* is calculated as follows:

$$TPRisk = \sum_{pig} \left(NP_{pig} . RP_p . WFP_g \right) \quad \textbf{(4.39)}$$

where NP_{pig} is the number of plants of type *p* producing product form *i* in grid *g*, RP_p is the risk level of the production facility *p* and WFP_g is the population weight factor in *g* in which a production or storage facility is located. The *TSRisk* is related to the number of storage facilities of type *s* for products form *i* in grid *g* (NS_{sig}), the risk level in storage facility *s* (RS_s) and the WFP_g as indicated by:

$$TSRisk = \sum_{sig} \left(NS_{sig} . RS_s . WFP_g \right) \quad \textbf{(4.40)}$$

The *TTRisk* is associated with the number of transport units from g to g' ($NTU_{ilgg'}$) in each grid, the safety risk level of transportation mode l (RT_l) and the road risk between grids g and g' ($RR_{gg'}$). The equation adopted in what follows is:

$$TTRisk = \sum_{ilgg'} NTU_{ilgg'} . RT_l RR_{gg'} \quad \textbf{(4.41)}$$

By combining Eqs. (4.39), (4.40) and (4.41), the total relative risk (*TR*) is given by:

$$TR = TPRisk + TSRisk + TTRisk \quad \textbf{(4.42)}$$

4.8 Solution strategy

4.8.1 Problem dimension

The mono-objective problem dimension treated in (Almansoori and Shah, 2006) was compared with the multi-objective approach considered in our work to analyse the statistics and main differences (see Table 4.1). The problem was solved minimising TDC for both cases but the new constraints presented in section 4.6 and 4.7 were added for the multi-objective case. Then, the number of constraints was doubled and similar results were observed for the number of integer and continuous variables. The computational time increased by a factor of 37% in the multi-objective case optimising the TDC when the GWP and risk are constraints. The model dimension involves 12464 constraints and 6242 variables (among them, 2516 are integer).

Table 4.1 Statistics for Mono- and multi-objective approaches.

Type of optimisation	Mono-objective	Multi-objective
Number of constraints	6197	12464
Number of integer variables	1326	2516
Number of continuous variables	1369	3726
CPU time (s)	717	987
Optimal gap (%) 0,01%		

In a preliminary phase, each mono-criterion problem was optimised separately to analyse how its optimal values are decreased when making a multi-criteria optimisation.

4.8.2 Mono-objective optimisation and lexicographic optimisation

The geographic area (country or region) to be studied is selected and divided in grids or sub-regions. The possible configurations of the HSC to be located in that place are defined (such as product physical form, viable production processes, transportation type, etc…). The mathematical model is then formulated within the GAMS 23.9 (Brooke et al., 1988) environment and solved using CPLEX. Each independent objective function is to be minimised using a lexicographic optimisation strategy that produces only efficient solutions when all the objectives are considered.

(Mavrotas, 2009) proposes the use of lexicographic optimisation for every objective function in order to construct the pay-off table with only efficient solutions. A simple remedy in order 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 minimisation objective functions) bound. Practically, the lexicographic optimisation is performed as follows: an objective function (of higher priority) is first optimised, obtaining min TDC=*z1**. Then, a second objective function is optimised (total GWP) by adding the constraint TDC=*z1** in order to keep the optimal solution of the first optimisation, in order to obtain min GWP= *z2**. Subsequently, the third objective function is optimised by adding the constraints TDC=*z1** and GWP= *z2** in order to keep the previous optimal solutions and so on until all the objective functions are treated in a more general case involving more objective functions.

4.8.3 Solution phase: multi-objective optimisation

The pay-off table designed from the application of the lexicographic optimisation allows defining the solution. In this approach which tries to minimise all objective functions, the optimal values represent the lower bounds (utopia points) of each objective in the feasible space and the nadir points are relative to values corresponding to the upper bounds on the Pareto surface, and not in any feasible space (values worse than the reservation value are not allowed).

The tri-objective optimisation problem is solved by implementing the ε-constraint method. Once the epsilon points (intermediate equidistant grid points) are defined, the objective function TDC has to be minimised. The GWP and TR objective functions are then transformed into inequalities constraints.

The global model can be formulated in a more concise manner as follows:

Minimise {TDC}

Subject to:

$h(x,y)= 0$

$g(x,y)\leq 0$

$x\in R^n, y\in Y=\{0,1\}^m, z\in Z^+$

$Risk \leq \varepsilon_n (n = 0,1,2,..., N)$

$TotalGWP \leq \varepsilon_m (m = 0,1,2,..., M)$

Demand satisfaction
Overall mass balance
Capacity limitations
Distribution network design
Site allocation
Cost, environmental and risk correlations
Non-negativity constraints

The objective of this formulation is to find values of the operational $x\epsilon R^n$, and strategic $y\epsilon Y=\{0,1\}^m$, $z\epsilon Z^+$ decision variables, subject to the set of equality h(x,y)= 0 and inequality constraints g(x,y)≤ 0. In this model, the continuous operational variables concern decisions dedicated to production, storage and transportation rate, whereas the discrete strategic variables capture the investment decisions such as the selection of activity types and transportation links.

All costs, emissions and risk equations occur as linear functions of the associated decision variables levels. That means the production, storage and transportation costs, GWP and safety risk levels are

linear values of the associated decision variables. The solution consists of a Pareto front composed of solutions that represent different possibilities of supply chain configurations.

4.8.4 *Multiple Choice Decision Making (MCDM)*

An M-TOPSIS (*Modified Technique for Order Preference by Similarity to Ideal Situation* (Ren et al., 2007)) analysis is carried out on the Pareto front with the same weighting factor for the cost, safety and environmental criteria since it is particularly efficient to avoid rank reversals (unacceptable changes in the ranks of the alternatives (Maleki and Zahir, 2012)) and to solve the problem on evaluation failure that may occur in the original TOPSIS version.

4.9 Case study (Great Britain)

A general HSC is presented in Figure 4.1, where the hydrogen form could be liquid or gaseous and some transportation modes and storage facilities are available. A case study of Great Britain (GB) treated by (Almansoori and Shah, 2006) has also been analysed to illustrate the main capabilities of the new proposed model. GB is divided into 34 grid squares of equal size. Three different production processes are evaluated: SMR, biomass and coal gasification. Hydrogen has to be liquefied before being stored or distributed. Liquid hydrogen (LH_2) is stored in super-insulated spherical tanks then delivered via tanker trucks. (Almansoori and Shah, 2006) estimated the total hydrogen demand in Great Britain as a function of the total number of vehicles, average total distance travelled and vehicle fuel economy (see Appendix A.1.1). The estimated demand is assumed to supply private-and-light goods vehicles and buses at 2002 levels. This is based on the assumption that 100% of the abovementioned vehicles would be powered by proton exchange membrane fuel cells (13392 tons per day). Four cases will be analysed (see Table 4.2) and compared with those of the *base case* (Almansoori and Shah, 2006). *Case 1* consists in the minimisation of the total daily cost both with a variant approach to compute NTU and a more recent solver version, CPLEX 12 versus CPLEX 9 as the approach used in (Almansoori and Shah, 2009). *Case 2* minimises the total Global Warming Potential (CO_2 emissions) of the network. *Case 3* is devoted to the minimisation of safety risk. Finally, Case 4 concerns the simultaneous optimisation of the three-abovementioned criteria.

Table 4.2 Different case studies and objectives to be analysed.

Minimisation of	Total daily cost	Global warming potential	Total risk
Base case	X		
Case 1	X		
Case 2		X	
Case 3			X
Case 4	X	X	X

4.9.1 Techno-economic data

A large amount of input data is required to solve the problem. All the techno-economic parameters (i.e., minimum and maximum production and storage capacities, average delivery distance between grids and capacity of each transportation mode, etc.) are defined in Appendix A1.

4.9.2 Environmental data

As new constraints are integrated to the model, new data was collected to compute the emission of each activity of the supply chain. It must be emphasized that an exhaustive Life Cycle Assessment (LCA studies the impact and effects of a product from the purchase of the raw material until its utilization and elimination. ISO 14040) was not performed. Only CO_2 emissions relative to production, storage and transportation were evaluated. Strømman and Hertwich in (Rivière, 2007) reported that the GWP for the SMR (without CO_2 capture and depository) process was of 10100 gCO_2-equiv per kg H_2 produced. The same indicator results in 10540 gCO_2-equiv per kg when hydrogen is produced via coal gasification (underground mined coal) (Grol et al., 2005). Biomass gasification leads to 3100 gCO_2-equiv per kg (Utgikar and Thiesen, 2006). After liquefaction process, H_2 storage in spherical tanks results in 5251 gCO_2-equiv per kg H_2 according to the Detailed California Modified in 2009 (*Detailed California Modified GREET Pathway for Compressed Gaseous Hydrogen from North American Natural Gas*, 2009) including manufacture, construction facilities, fuel consumption, flare combustion and methane venting. Moreover, an amount of 62 g CO_2-equiv per ton-km is emitted by tanker truck transportation (McKinnon and Piecyk, 2011) and the weight of the transportation taken into account is 40 ton (AFH2, 2011).

4.9.3 Safety data

The evaluation of the safety risk takes as parameters three indicators, i.e., the risk level of each activity, the population weight factor and the adjacency level in transportation links**.** For the risk level of each activity (H_2 production-storage facilities and transportation units), (Kim and Moon, 2008) and (Kim et al., 2011) have developed a risk assessment methodology through the hazard identification using the failure modes and effects analysis (FMEA) and the consequence-likelihood analysis to complete the risk evaluation (each hazard is plotted on a frequency vs. consequence matrix (risk binning matrix), that indicates its level of risk as high, moderate, low, or negligible).

The risk-binning matrix in (Kim and Moon, 2008) summarises the individual risk and relative risk level according to its remark raking and is taking into account for our data base. All hydrogen activities considered are marked as Levels II–IV according to harmfulness for people, the environment and facilities. The acceptance criterion of these levels is described in Appendix A.1.5. A risk level III corresponds to SMR, tanker truck and liquid storage. Values for biomass and coal gasification were not found, then, they were assumed to have the same risk level as SMR.

The population risk weight factors for each grid are classified in Table 4.3, i.e., when the population of a particular grid is over 2 million, we assume that this region has a score of 5, from 1 to 2 million the score is 4 and so on. According to this classification, a higher weighting rate for grids corresponds to a higher population density.

Table 4.3 Relative impact level of grids based on the population density.

Population level (persons per grid)	Grids
Level 1 (under 2.5^{E+05})	2,5,8,9,12,16,20,21,26,34
Level 2 (2.5^{E+05}-5^{E+05})	1,3,4,6,7,15,30,31,32,33
Level 3 (5^{E+05} -1^{E+06})	10,11,17,19,25,27
Level 4 (1^{E+06} – 2^{E+06})	13,22
Level 5 (over 2^{E+06})	14,18,23,24,28,29

The adjacency level in transportation links was calculated as a function of the crossed grids or those close to the road. If hydrogen is transported through some intermediate grids, the impacts on these regions must be taken into account as indicated in the following equation:

$$RR_{gg'} = \sum_{g} (RL_g + \beta_{g2} RL_{g2} + \beta_{g3} RL_{g3} + \ldots + RL_{g'}) \quad \textbf{(4.41)}$$

where subscripts g and g' represent the first and last regions and g_1, g_2, .., g_n represent the intermediate regions through which hydrogen is transported; β_g is the weight factor that indicates the adjacency level of a region in which the route is located. It takes a rating value between 0.1 and 1.0 according to the adjacency level. For a transiting grid, the value is 1, for a close region, the value is 0.5, this value is multiplied by the risk level of the grid (RL_g) classified according to the grid size -by population density- (i.e., small=1, medium=2 or large=3). This calculation is detailed in the method proposed by (Kim et al., 2011). Due to the geographic division of the original case study (Almansoori and Shah, 2006), some difficulties were encountered to precisely locate the roads. The following method was then adopted: if hydrogen produced in region 1 is transported to region 33, this transportation arc has to penetrate nine grids (g1, g4, g7, g10, g13, g17, g23, g28 and g33) and is close to four grids (g2, g3, g18 and g22); applying Eq.4.41, the external effect factor of the transportation arc from region 1 to 33 is 25.5 (see Appendix A.1.6). Appendix A.1.4 shows the total relative risk matrix for impact on city transportation between grids. The highest risk line is the hydrogen transportation from grid 31 (565) and the lowest risk line concerns hydrogen transportation from grid 17 (335). If decision-makers design the hydrogen supply chain by considering only transportation safety, it is safer to completely avoid transportation from grid 31.

4.10 Results and discussion

The different stages of the proposed methodology were developed and applied in the abovementioned case study. In this section, the results and corresponding configurations are analysed and discussed in detail. In a preliminary phase, the three criteria were optimised separately to analyse how their optimal

values decrease when making a multicriteria optimisation. The ε-constraint method is applied and the best compromise solution is then chosen from the Pareto front via M-TOPSIS.

4.10.1 Preliminary phase. Mono-objective optimisation and lexicographic optimisation

The preliminary phase allowed finding the pay-off table through lexicographic optimisation (see section 4.9). Thus, it is possible to obtain as the solution that minimises TDC as the one that corresponds to point that is a non-dominated solution also for Total GWP and Total Risk. The optimisation runs were performed for *cases 1*, *2* and *3* where cost, CO_2 emissions and safety risk are to be minimised. The results of each independent optimisation can be seen in Table 4.4. The optimisation runs were implemented with a Pentium (R) Dual-core CPU E6600 @ 3.06 GHz processor machine.

Table 4.4 Comparison between conventional (mono-objective) and lexicographic optimisation results

	(a) Pay-off table obtained by a conventional MILP optimiser			(b) Pay-off table obtained by the lexicographic optimisation		
Case	1	2	3	1	2	3
Minimise	TDC	GWP	TR	TDC[28]	GWP[1]	TR[1]
Total network cost (M$ per day)	**64.57**	135.92	77.57	**64.57**	132.05	73.65
Total GWP (10^3 ton CO_2-equiv per day)	205.86	**111.85**	203.35	205.86	**111.85**	205.6
Total Risk (units)	10,363	6005	**5970**	10,292	5970	**5970**

TDC: total daily cost

GWP: global warming potential

TR: total risk

Following the conventional optimisation we first calculate the pay-off table by simply calculating the individual optima of the objective functions. The conventional MILP optimiser will produce the pay-off table shown in Table 4.4 (a). However, it is almost sure that a conventional MILP optimiser will calculate the solution of the first point and will stop the searching giving this solution as output. In order to avoid this situation, the lexicographic optimisation of the objective functions is performed and the results are shown in Table 4.4 (b).

It can be highlighted that the optimal solution obtained through conventional optimisation of TDC (TDC=64.57 $ per day, Total GWP=205.86 thousand tons CO_2 per day and Total risk=10363 units) is a dominated solution in the problem due to alternative optima resulted through the lexicographic optimisation (TDC=64.57 $ per day, Total GWP=205.86 10^3 tons CO_2 per day and Total risk=10292 units) the total risk is decreased by 71 units. The same analysis can be made for the two other objective functions. The bold characters in Tables 4.4, 4.5 and 4.6, are relative to the values of the optimised criterion for the mono-objective optimisation and in the case of the lexicographic

[28] This criterion is the first optimised through the lexicographic approach for this case.

optimisation are related to the first optimised objective (higher priority). Information concerning the decision variables is presented in Table 4.5. The values of flow rates between grids, total production and storage per day in each location can be found in Appendix A.2.1. All the mono-objective cases are analysed in the next section.

Table 4.5 Mono-objective and lexicographic optimisation results of the hydrogen supply chain.

Case	Base case [17]	1	2	3
Minimise	Cost[29]	Cost[30]	GWP[2]	Risk[2]
Number of production facilities	28	28	47	47
Number of storage facilities	265	265	265	265
Number of transport units	-	171	3	3
Capital cost				
Plants and storage facilities (M$)	47,310	47,310	98,694	57,475
Transportation modes (M$)	80.22	85.50	1.50	1.50
Total daily capital cost (M$ per day)[31]	43.28	43.28	90.13	52.49
Operating cost				
Plants and storage facilities (M$ per day)	21.16	21.16	41.92	21.16
Transportation modes (M$ per day)	0.126	0.126	0.001	0.001
Total operating cost (M$ per day)	21.29	21.29	41.92	21.16
Total cost				
Total network cost (M$ per day)	64.57	**64.57**	132.05	73.65
Production facilities (10^3 t CO_2-equiv per day)	-	135.27	41.52	135.27
Storage facilities (10^3 t CO_2-equiv per day)	-	70.33	70.33	70.33
Transportation modes (10^3 t CO_2-equiv per day)	-	0.261	0.002	0.002
Total GWP (10^3 t CO_2-equiv per day)	-	205.86	**111.85**	205.60
Transportation modes risk	-	4557	40	40
Production facilities risk	-	580	775	775
Storage facilities risk	-	5155	5155	5155
Total risk (units)	-	10292	5970	**5970**

4.10.1.1 Base case and case 1 (minimal TDC)

The results obtained in *case 1* are in agreement with the *base case* (Almansoori and Shah, 2006). The minimal number of 28 production plants is obtained with SMR technology dispersed throughout GB territory. Production of LH_2 via SMR has also been found in previous works (Sabio et al., 2011)(Kamarudin et al., 2009), with cost as an objective function. The number of storage units is 265 when adopting the same value for demand and with a storage period of 10 days. *Case 1* involves 171 tanker trucks to cover the demand between grids which represents a transportation capital cost of 85.5M$ as compared with 80.2M$ in (Almansoori and Shah, 2006) where the number of transport units is not reported. Transportation costs (i.e., fuel, labour, maintenance and general costs) are directly influenced by the number of trips, trip distances and number of transport units for each case. Among all the case studies, the higher transportation cost is observed for *case 1* when minimising TDC: less plants are installed but more transport units are required to cover all the national demand,

[29] Mono-objective optimisation.
[30] This criterion is the first optimised through the lexicographic approach for this case.
[31] Assuming a capital charge factor-payback period of capital investment of 3 years and the network operating value in 365 days per day. Demand 13 392 360 kg per day.

consequently, the transportation operating cost is also higher and the network results in a centralised HSC with the minimal total daily cost for the network of 64.57 M$. The configurations that can be obtained are presented in Figures 4.2 and 4.3 and exhibit low differences in the distribution links and liquid hydrogen amounts to be transported between *base case* and *case* 1. The minor variations that can be observed could be attributed to the solver version. In *case 1*, less distribution links are found but the amount of LH_2 transported keeps the same value. The imported part of demand of LH_2 between grids and the flow rates is listed in Appendix A.2.1.

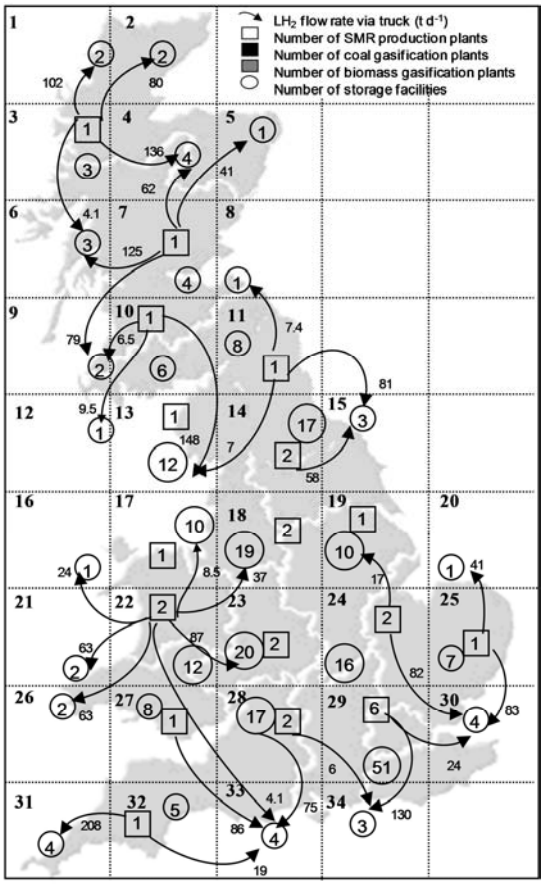


Figure 4.2 Network structure of liquid hydrogen produced via medium-to-large SMR plants, stored in medium-to-large storage facilities, and distributed via tanker trucks. Cost minimisation (Almansoori and Shah, 2006).

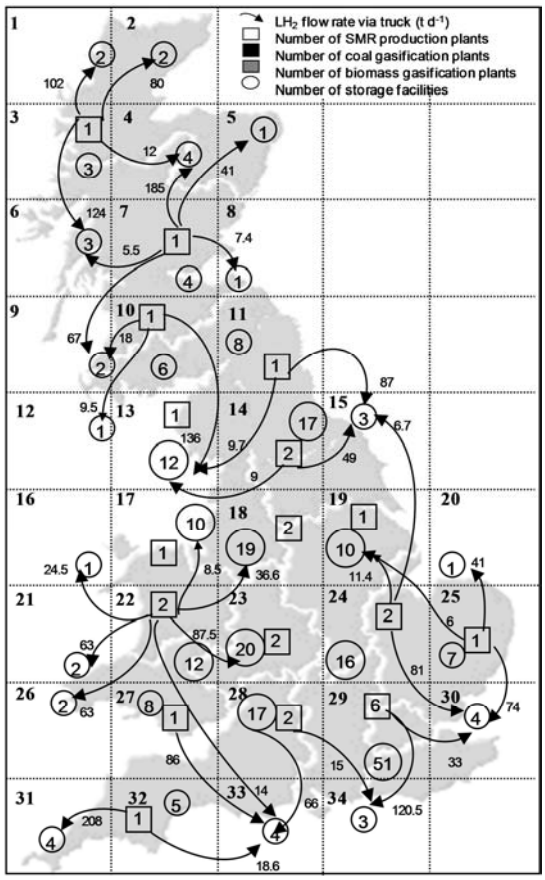


Figure 4.3 Network structure of liquid hydrogen produced via medium-to-large SMR plants, stored in medium-to-large storage facilities, and distributed via tanker trucks for the case 1 (cost minimisation).

4.10.1.2 Case 2 (minimal GWP)

Case 2 is relative to the minimisation of the global warming potential. Minimal total GWP resulted in 111.85 10^3 of tons CO_2 per day in which the main contribution is given by the liquid storage process (62%), followed by the amount emitted by the production facilities (37%) and a minimal impact of transportation (only three tanker trucks are considered in this network). In the case of storage facilities, the solver does not change the amount of facilities installed since there is only one size of

storage tank, so that the optimisation is only performed with the number of production facilities and transportation units as significant decision variables. The number of production plants increase considerably (from 28 plants in *case 1* to 47 in this case) and all of them are biomass gasification facilities.

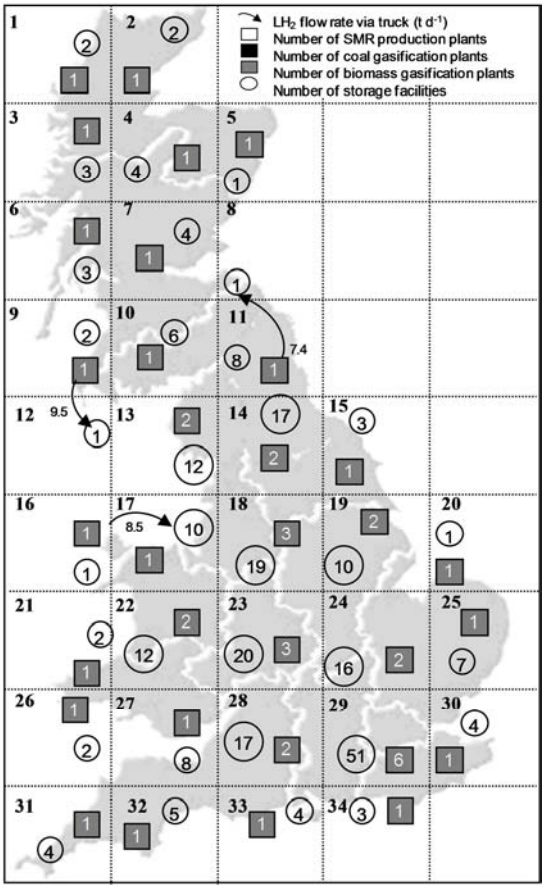


Figure 4.4 Network structure of liquid hydrogen produced via medium-to-large biomass gasification plants, stored in medium-to-large storage facilities, and distributed via tanker trucks for the case 2 (CO_2 minimisation).

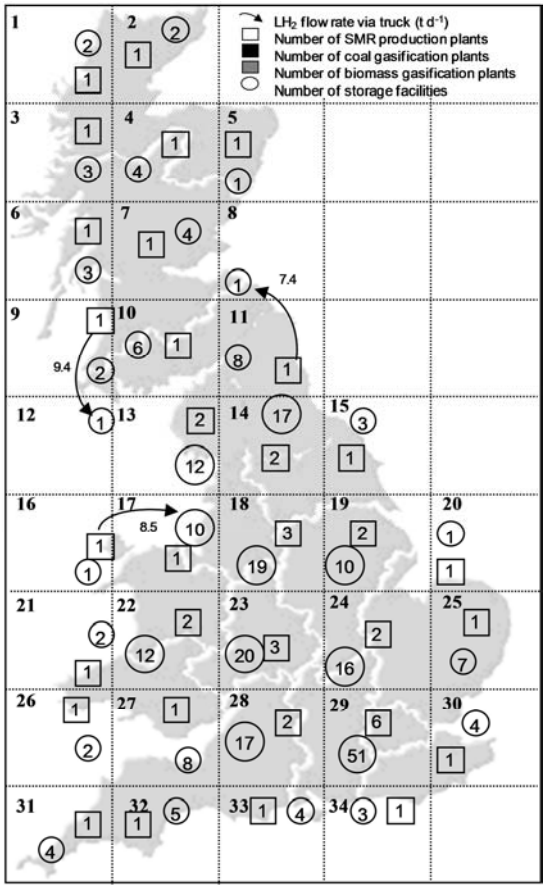


Figure 4.5 Network structure of liquid hydrogen produced via medium-to-large SMR plants, stored in medium-to-large storage facilities, and distributed via tanker trucks for the case 3 (risk optimisation).

The kind of technology plays a key role in the CO_2 emissions: biomass gasification technology decreases GWP but represents also a higher investment affecting the total daily cost of the HSC which is more than two times higher compare to the *case 1*. Guillén et al. (Guillén Gosálbez et al., 2010) also found that the most promising alternative to achieve significant environmental savings consisted in replacing SMR by biomass gasification. In Figure 4.4, it can be highlighted that only three transportation links are established (from grids 9 to 12, 11 to 8 and from 16 to 17). As mentioned in Guillén et al. (Guillén Gosálbez et al., 2010), *case 2* HSC design results in a decentralised network where almost all the grids are autonomous in LH_2 production.

4.10.1.3 Case 3 (minimal relative risk)

Case 3 minimises the total relative risk. The optimal configuration is shown in Figure 4.5. Figures 4.4 and 4.5 show similarity in the degree of decentralisation with only three distribution links and three tanker trucks assigned for the whole supply chain. Less links and transport units are assigned and are related to a higher number of installed production facilities, which is consistent with the results of *cases 1* and *2*. Specific features for *case 3* can be highlighted for production units with a total of 47 facilities located in all the grids except in grid 8 and 12; even though (Kim et al., 2011) found that the installation of plants changed in those grids with less population density, this was not found here (i.e. grid 29 involves a total of 6 production units). The main difference between *case 2* and *3* is the production technology which results in 100% of installed SMR plants when risk is minimised.

The total relative risk for this case is of 5970 units and is basically influenced by the storage risk (86%) since storage is scattered in each grid to cover a volume equivalent to 10 days of demand of LH_2 per grid. Yet, from the results of this case study, it cannot be deduced that safety risk will be lower if more small storage units are installed since the different storage sizes were not considered. A variation in the number of storage units was not found. The production risk is the second major risk (13%). The transportation relative risk was reduced to find a more safety configuration considering at the same time the links and distance to be run. It must be pointed out that the number of tanker trucks was dramatically reduced from *case 1* to *cases 2* and *3 (*from 171 to 3 units); in the second case this was made to decrease GWP but in this case the transportation risk represented 44% in *case 1* and represents less than 1% for *case 3*. Through analysis of production plants and the transportation modes, (Kim and Moon, 2008) determined that changing the type of plant or mode does not offer additional financial benefits or safety guarantees. Yet, in our case, we find that the production technology mix of *case 3* represents a financial benefit of 44% as compared to the *second case* where 100% of biomass gasification plants were installed.

4.11 Multi-objective optimisation

From the three independent mono-objective cases, each objective function range can be obtained so that, the ε-constraint method can be applied. From the lexicographic optimisation results of Table 4.4(b), the utopia and nadir points of each criterion can be found. The total risk can be divided into three intervals to make the interpretation easier: *low risk*=5970 corresponding to the best possible obtained, *medium risk*=8132 (the intermediate value defined by the epsilons ε_n) and *high risk*=10292 units corresponding to the nadir point according the pay-off table. Similarly, 15 epsilon points were defined for GWP. Then, the objective function TDC has to be minimised while Total GWP and total risk are considered as inequality constraints. The solution consists of a Pareto front composed of solutions for supply chain configurations (see Figure 4.6). The cost of both *high* and *medium* risks is similar since these two levels of risks have close impacts of CO_2 emissions, that is because of the degree of centralisation higher in the *high risk* network and also with longer route links and with more

trips per day. This represents a benefice in TDC compared with the *low risk*. In Figure 4.7 lines of *medium* and *high* risks options are very close, according to this result if the decision maker prefers to decrease the safety risk from high to medium, this decision will not represent a high cost affectation compared to the investment cost that would be necessary to change from *high* to *low* risk. The degree of decentralisation in the *low risk* is the main difference and at the same time the impact of the technology type that impacts directly the cost and the GWP (i.e. the capital cost of establishing biomass gasification plant is of M$ 1412 vs. M$ 535 for the SMR technology (Almansoori and Shah, 2006)). Then if the risk level is to be low and to assure to emit less CO_2 a higher investment is necessary.

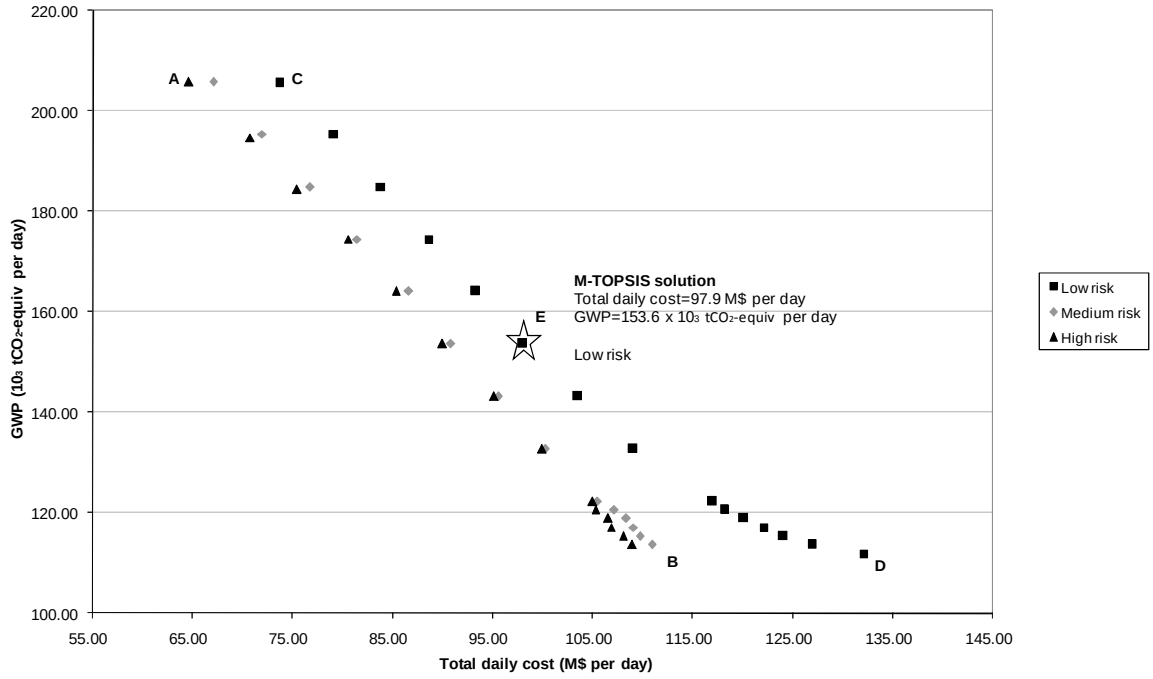


Figure 4.6 Pareto solutions for the multi-objective model

Five points are plotted (*A* to *E)* in the Pareto front (see Figure 4.6) to give an example of the difference in the degree of decentralisation. The point *A* is the most centralised configuration with 36 distribution links and 171 tanker trucks assigned for the whole supply chain. The flow rate for this configuration can be seen in Table C.1. This solution corresponds to a *high risk* with low cost with a maximum of CO_2 emissions. At the same time, the point *B* is connected by 26 links and 115 tanker trucks, similar results are found for the other solutions of *medium risk*. Finally, a low degree of centralisation is found for solutions with *low risk*, points *C-E* require only 3 transport units to distribute less than 1% of the total daily demand of hydrogen, the remaining part is produced on-site. The 43 possible set solutions in the Pareto front were evaluated via TOPSIS and M- TOPSIS analysis (Ren et al., 2007)(Morales Mendoza et al., 2011) carried out with the same weighting factor for the cost, safety and environmental factors (see Appendix A.2.3).

4.11.1 Multi-objective optimisation results

Based on the data and assumptions, the optimal configuration of the future HSC involves 47 production plants as a mix of production technologies (i.e. 66% for SMR and 34% for biomass gasification) located in a decentralised configuration. This network uses tanker trucks to deliver liquid LH_2 to storage facilities. This option involves a TDC of 97.97 M$ per day, a GWPTot of 153.63 10^3 tons CO_2 per day and a low safety risk.

The results concerning the decision variables for the multi-objective optimisation problems are displayed in Table 4.6 and Figure 4.7 shows the corresponding configuration. The analysis of the network is quite different from the mono-objective configuration of Figure 4.2. In the *base case*, it can be observed that long transportation links are installed between grids because such an option is cheaper than building a new production facility. It must be emphasized that the degree of decentralisation increases in the multicriteria solution and is similar in cases *2 and 3*.

The change from a centralised to a decentralised supply chain is the main difference observed when the safety risk and the CO_2 emissions are taken into account in the optimisation phase. The production plants work with less efficiency because they have a maximum capacity of 480 tons per day and in some cases they are producing only 10 tons per day. Different plant sizes could be studied in a future approach.

Table 4.7 shows that the best value obtained for TDC in the multi-objective approach *(case 1)* is higher (an increase by 34% is observed) than for mono-objective case (*case 4*). Moreover, the CO_2 emissions and the risk are improved in *case 4* reducing GWP by 34% and the total risk by 72%. The total GWP decreases by 27% in *case 2* as compared with *case 4* while the reduction in CO_2 emissions implies a higher cost (35%) while not affecting the risk. Finally, the minimal risk was found in cases 3 and *4* (best results are shown in Table 4 for the lexicographic optimisation) but the other two criteria are different. The TDC increases by 25% in *case 4* but the CO_2 emissions are decreased by 34% as compared with *case 3*.

Finally, the unitary cost of hydrogen per case is presented in Figure 4.8. It must be highlighted that no refuelling station is included in this optimisation of the HSC, even though these results could give us an idea about the competitiveness of H_2 with fossil fuels. One kilogram of hydrogen is approximately equivalent to one gallon of gasoline based on its lower heating value energy content (Bartels et al., 2010). Any hydrogen source that has a hydrogen cost below the current cost of gasoline has an economic advantage over gasoline. Gasoline prices in 2012 are 3.5-4.0 $/gallon (retail price range ("U.S. Gasoline and Diesel Retail Prices".)).

Case 4	
Number of production facilities	47
Number of storage facilities	265
Number of transport units	3
Capital cost	
Plants and storage facilities (M$)	71,507
Transportation modes (M$)	1.5
Total daily capital cost (M$ per day)	65.30
Operating cost	
Plants and storage facilities (M$ per day)	32.67
Transportation modes (M$ per day)	0.001
Total operating cost (M$ per day)	32.67
Total cost	
Total network cost (M$ per day)	***97.97***
Production facilities (10^3 t CO_2-equiv per day)	83.30
Storage facilities (10^3 t CO_2-equiv per day)	70.33
Transportation modes (10^3 t CO_2-equiv per day)	0.002
Total GWP (10^3 t CO_2-equiv per day)	***153.63***
Transportation modes risk	40
Production facilities risk	775
Storage facilities risk	5155
Total Risk (Units-level)	***5970***

Table 4.6 Multi-objective optimisation results of the hydrogen supply chain.

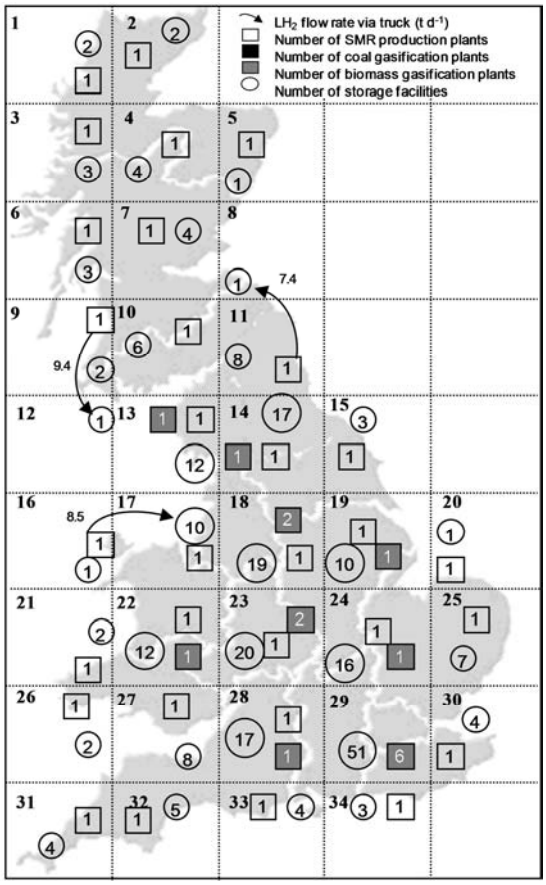


Figure 4.7 Network structure of liquid hydrogen produced via medium-to-large SMR and biomass gasification plants, stored in medium-to-large storage facilities, and distributed via tanker trucks for the case 4 (multi-objective optimisation).

According to (Ball and Wietschel, 2008), the specific hydrogen supply costs are estimated at around 4–4.6 $/kg for being representative for both the European Union and North America in the early phase. They are mainly due to the required overcapacity of the supply and refuelling infrastructure as well as to the higher initial costs for new technologies because of the early phase of technology learning. Around 2030, hydrogen costs range from 3.6–5.3 $/kg in the abovementioned regions, mainly depending on the feedstock. In the long term until 2050, hydrogen supply costs will stabilize around this level, but with an upward trend due to the assumed increase in energy prices and CO_2 certificate prices. The average H_2 delivered cost found in (Hugo et al., 2005) varies from 4.5 - 6.8 $/kg (prices in 2008). According to these references, it can be concluded that the cost of the HSC defined in this problem is still high for the problem that was considered and it will not be competitive to the current fossil fuel system unless some parameters (e.g. the capital change factor-payback period) are modified.

Table 4.7 Comparison of results among treated cases.

	Total daily cost (M$ d^{-1})	Total GWP (10^3 t CO_2-equiv d^{-1})	Total risk (units)
Multi-objective optimisation (Case 4)	97.97	153.6	5970
Minimal TDC (Case 1)	64.57	205.86	10,292
Difference between Case 4 vs Case 1	34%	-34%	-72%
Minimal GWP (Case 2)	132.05	111.85	5970
Difference between Case 4 vs Case 2	-35%	27%	0%
Minimal risk (Case 3)	73.65	205.6	5970
Difference between Case 4 vs Case 3	25%	-34%	0%

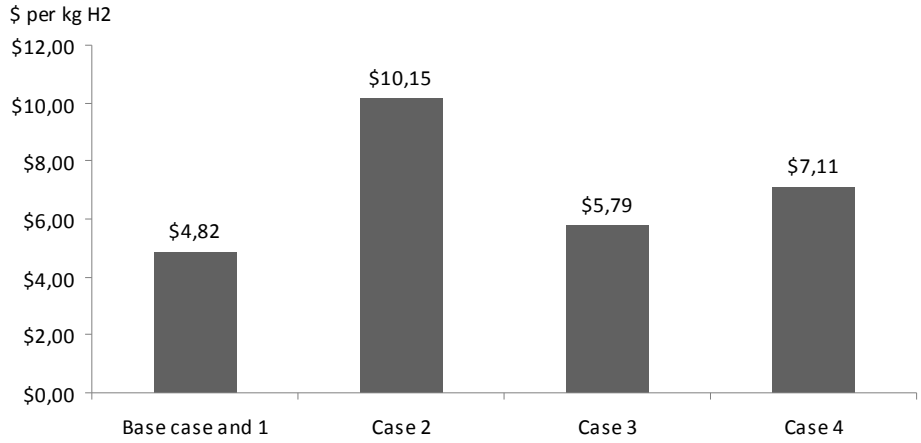


Figure 4.8 Hydrogen cost ($ per kg).

4.12 Conclusions and comments

This chapter has presented a general methodology for the design of a HSC using multi-objective optimisation. The model developed is an extension of the approach developed in (Almansoori and Shah, 2006). In this work, while total daily cost is minimised, investment strategies have been found for designing a sustainable hydrogen economy based on careful analysis that takes into account other critical issues such as safety and environmental impact. The solution strategy is based on the ε-constraint method as a multi-objective optimisation technique for considering three objectives to be minimised simultaneously, involving economic, environmental and safety indicators. From the case study analysis, it must be highlighted that the model can identify the optimal HSC including the number, location, capacity, and type of production, transport and storage facilities, production rate of plants and average inventory in storage facilities, hydrogen flow rate and type of transportation links to be established. The main differences found between the two approaches are related to the degree of the production decentralisation that starts to increase as the risk and CO_2 emissions are taken into account. This means that the demand of hydrogen will be supplied by a number of production facilities scattered throughout GB and the number of transport units will decrease under the assumptions made considering no intra grid transport. Production plants resulted only in SMR type for the base case but when multi-objective optimisation is performed, a mix of technologies is involved, i.e. SMR and biomass gasification. Some further works are proposed in order to improve the model within this

scope: demand variation in different time periods needs to be considered; the energy sources and the fuelling stations nodes to the hydrogen supply chain must be included in the model; a geographic division based on states or regions instead of grid squares would be more realistic to facilitate data collection; the model must be extended to treat a panel of renewable energy sources, these point are treated in the next chapter.

Chapter 5

HYDROGEN SUPPLY CHAIN OPTIMISATION FOR THE DEPLOYMENT SCENARIOS IN THE MIDI-PYRÉNÉES REGION

Résumé

Ce chapitre est consacré à la modélisation et l'optimisation de la chaîne d'approvisionnement d'hydrogène pour la région Midi-Pyrénées à travers le projet « H_2 vert carburant » initié par PHyRENEES, Midi-Pyrénées Innovation et le LGC. Le modèle mathématique présenté dans le chapitre 4 est adapté aux caractéristiques spécifiques de la région et de ses sources d'énergie. Un problème mono/multi-objectif est traité. Des scénarios d'optimisation sont effectués d'abord pour le cas mono-objectif, considérant de façon séparée les trois fonctions objectifs (coût, CO_2 et risque), puis le cas multi-objectif est résolu. Comme cela a déjà été observé sur l'exemple du chapitre précédent, les résultats montrent des différences significatives, concernant principalement le degré de centralisation et le type de technologie ainsi que la taille des nouvelles installations. Le système d'information ArcGIS® est ensuite utilisé pour valider les solutions obtenues par optimisation multi-objectif. Cette technologie permet d'associer une période de temps aux configurations de la chaîne logistique hydrogène et d'analyser plus finement les résultats de la conception du réseau H_2.

Abstract

This chapter is dedicated to the modelling and optimisation of the hydrogen supply chain in the Midi-Pyrénées region through the "Green H_2 fuel" project initiated by PHyRENEES, Midi-Pyrénées Innovation and the LGC. The mathematical model presented in Chapter 4 is adapted to the specific features of the region and its energy sources. A mono/multi period problem is treated. Optimisation scenarios are performed first through mono-objective cases considering the three objective functions (cost, CO_2 and risk) and then the multi-objective case is tackled. The obtained results exhibit significant differences in the optimised networks concerning mainly the centralisation degree and the technology type as well as the size of the new facilities. A geographic information system (GIS) is introduced in the last section of this chapter. This technology provides a better insight in the design of the hydrogen supply chain.

Abbreviations

AFHYPAC	French Association for Hydrogen and Fuel Cells
BEV	Battery Electric Vehicle
CCS	Carbon Capture and Storage
CH_2	Compressed Gaseous Hydrogen
FCEV	Fuel Cell Electric Vehicles
GHG	Greenhouse gas
H_2	Hydrogen
HSC	Hydrogen Supply Chain
ICE	Internal Combustion Engine
LGC	Laboratoire de Génie Chimique (Chemical Engineering Laboratory)
LH_2	Liquid hydrogen
MILP	Mixed Integer Linear Programming
MPI	Midi-Pyrénées Innovation (Regional Innovation Agency)
PHEV	Plug-in Hybrid Electric Vehicle
RES	Renewable Energy Sources
WtW	Well-to-Wheel

Nomenclature and units

Indices

g: grid squares and g': grid squares such that g' ≠ g
e: energy source
p: plant type with different production technologies
i: product physical form
s: storage facility type with different storage technologies
l: type of transportation modes
j: size of the production facilities
t: time periods of the planning horizon

Parameters and variables

α	Network operating period (days per year)
γ_{epj}	Rate of utilization of primary energy source *e* by plant type *p* and size *j* (unit resource/unit product)
$A0_{egt}$	Initial average availability of primary energy source *e* in grid *g* during time period *t* (units per day)
CCF	Capital change factor -payback period of capital investment (years)
DT_{igt}	Total demand for product form *i* in grid *g* during time period *t* (kg per day)
ESC_t	Primary energy source cost during time period *t* (US$ per day)
$Fcap_i$	Capacity of fuelling station for product form *i* (kg per day)
FCC_t	Facility capital cost during time period *t* (US$)
FOC_t	Facility operating cost during time period *t* (US$ per day)
GW^{Prod}_{ep}	Production global warming potential by plant type *p* (*g* CO_2-equiv per kg of H_2)
IP_{pijgt}	Investment of plants of type *p* and size *j* producing product form *i* in grid *g* during time period *t*
$IPES_{egt}$	Import of primary energy source *e* to grid *g* from overseas during time period *t* (units per day)
IS_{sijgt}	Investment of storage facilities of type *s* and size *j* storing product form *i* in grid *g* during time period *t*
LR_t	Learning rate - cost reductions as technology manufacturers accumulate experience during time period *t* (%)
NFS_t	Number of fuelling stations dispensing product form *i* in grid *g* during time period *t* (units)
NP_{pijgt}	Number of plants of type *p* and size *j* producing product form *i* in grid *g* during time period *t*
$NP0_{pjig}$	Initial number of plants of type *p* and size *j* producing product form *i* in grid *g* (units)

NS_{sijgt}	Number of storage facilities of type *s* and size *j* for product form *i* in grid *g* during time period *t*
$NS0_{sjig}$	Initial number of storage facilities of type *s* and size *j* storing product form *i* in grid *g* (units)
$NTU_{ilgg't}$	Number of transport units between g and *g*' during time period *t*
PCC_{pji}	Capital cost of establishing plant type *p* size *j* producing product form *i* (US$)
PR_{pijgt}	Production rate of product form *i* produced by plant type *p* size *j* in grid *g* during time period *t* (kg per day)
RP_{pj}	Risk level of the production facility *p* size *j* (units)
SCC_{sij}	Capital cost of establishing storage type *s* size *j* storing product form *i* (US$)
SSF	Safety stock factor of primary energy sources within a grid (%)
TCC_t	Transportation capital cost during time period *t* (US$)
TDC	Total daily cost of the network (US$ per day)
TOC_t	Transportation operating cost during time period *t* (US$ per day)
UDC_e	Unit cost of distributing primary energy source e between grids (US$ per unit / km)
UFC_i	Unit fuelling cost of product form *i* ($ per kg)
UIC_e	Unit import cost of energy source ($ per unit)
UPC_{pij}	Unit production cost for product form *i* produced by plant type *p* and size *j* (US$ per kg)

5.1 Introduction

Chapter 4 of this manuscript was devoted to the HSC design with multi-objective. The solution strategy was validated for a mono-period case with lexicographic and ε-constraint methods. This chapter tackles the HSC design for the case study of the Midi-Pyrénées region: a multi-period problem is considered (2020-2050) and a geographic division based on districts instead of grid squares which is more consistent with administrative data thus facilitating data collection is used.

Midi-Pyrénées, the largest region of mainland France (similar to the surface of Denmark), is located in the South West corner of the country, next to Spain. The Midi-Pyrénées region counts with a large number of stakeholders and has great potential for producing hydrogen based on renewable sources which represented over than 25% in the region and 14% of national production in 2008 (Le Schéma Régional Climat Air Energie, 2012). In this context, the Climate Plan has as targets to divide by 4-5 the French GHG emissions by 2050 (Patay, 2008). This policy of "Factor 4" then requires a 75% reduction in GHG emissions by 2050 compared to current levels (Bento, 2010): these objectives enhance the region to study new scenarios related to the transportation system.

The "Green H_2 fuel" project (*Hydrogène vert carburant)* was initiated by the PHyRENEES[32] association, the Regional Innovation Agency (Midi-Pyrénées Innovation-MPI)[33] and the Chemical Engineering Laboratory (Laboratoire de Génie Chimique-LGC) on February 2012. This study emerged as an initiative to evaluate the hydrogen economy in the Midi-Pyrénées region to enhance renewable energies and at the same time to evaluate the potential CO_2 reductions. More specifically, the objectives of the project are based on the following items:

- identification of the key stakeholders in Midi-Pyrénées.
- scenarios definition.
- data collection and assumptions.
- model adaptation and validation.
- results analysis.

Three main themes were identified during project development. The first item concerned the *technical issue*: the methodological framework presented in the previous chapter served as a basis. The adaptation of the multi-objective optimisation tool developed in chapter 4 requires the definition of energy transition planning in agreement with the renewable energy potential of Midi-Pyrénées. It required field visits, interviews, data collection and analysis/ synthesis of information. The second axis

[32] PHyRENEES Association was established on October 2007 around several partners (Ecole des Mines, Trifyl, N-GHY, Airbus, GDF INPT, ARAMIP and the General Council of the Tarn ...).

[33] MPI was created in 2006 at the initiative of the Regional Council to improve the visibility of the institutional landscape and guide companies in their innovation projects.

was related to *human resources*: a multidisciplinary team supported the management of the project for planning activities among all the stakeholders associated with the project. The steering committee was composed of regional organisations and industrials (PHyRENEES, MPI, WH_2[34], ENSIACET and Mobilelec[35]). This committee validated the assumptions. The third axis consisted in the *monitoring of the project* (meetings with the steering committee, reports, etc.): the project management implemented for this hydrogen study was presented in detail in (Dupin-Janson, 2012) and will not be developed here. The results of the project were selected to be presented in the National Debate for the Energy Transition ("Débat national sur la transition énergétique," 2013) the last 3rd June 2013 in Toulouse organised by MPI. This work led to two publications (De-León Almaraz et al., 2013b) and (De-Léon Almaraz et al., 2014).

The methodological framework of the study is proposed in Figure 5.1. The *input* block corresponds to all the databases, hypothesis and scenarios chosen by the steering committee. The integration of the mathematical model and the multi-objective optimisation approach constitute the core of the approach. The snapshots and the results concerning the decision variables and objective functions are the main *outputs*.

The remainder of this chapter is organised as follows: in the next section, the methodology and the problem definition are explained. The parameters and typical features of the Midi-Pyrénées case are described in section 5.3. It must be highlighted that current information available related to hydrogen activities were obtained from part of the main stakeholders in the hydrogen field. As the HSC is still in the study phase, not all data is available, the missing data to build the model was obtained through bibliographic sources. In section 5.4, the extended version of the mathematical model presented in chapter 4 is proposed. Section 5.5 is dedicated to the solution strategy. Due to the multi-period problem involving four time periods, three approaches are used to solve the problem: first, three mono-objective optimisations (referred as case A) are carried out in section 5.6; the methodology is then applied for multi-criteria approaches (cases B1 and B2). The case B1 treats the multi-objective problem in section 5.7 as a multi-period one (the four-time periods are integrated) and the solution is based on the so-called Ɛ-constraint methodology. The case B2 solves four mono-period problems with the lexicographic optimisation and then applies the Ɛ-constraint methodology and TOPSIS to each time period in section 5.8. The optimisation results and subsequent discussion for all cases are given in section 5.9. Moreover, in section 5.10 the ArcGIS® tool is introduced to allow a more precise spatial analysis. Finally, some highlights conclude this chapter.

[34] WH_2: start-up 2011, green H_2 energy broker in France.

[35] Mobilelec: Company placed in Toulouse. They are placed in the electronic engineering for mobility (study, design and development of electrical and electronic architectures (embedded or otherwise) for vehicles (trucks, cars, bicycles, scooters, motorcycles).

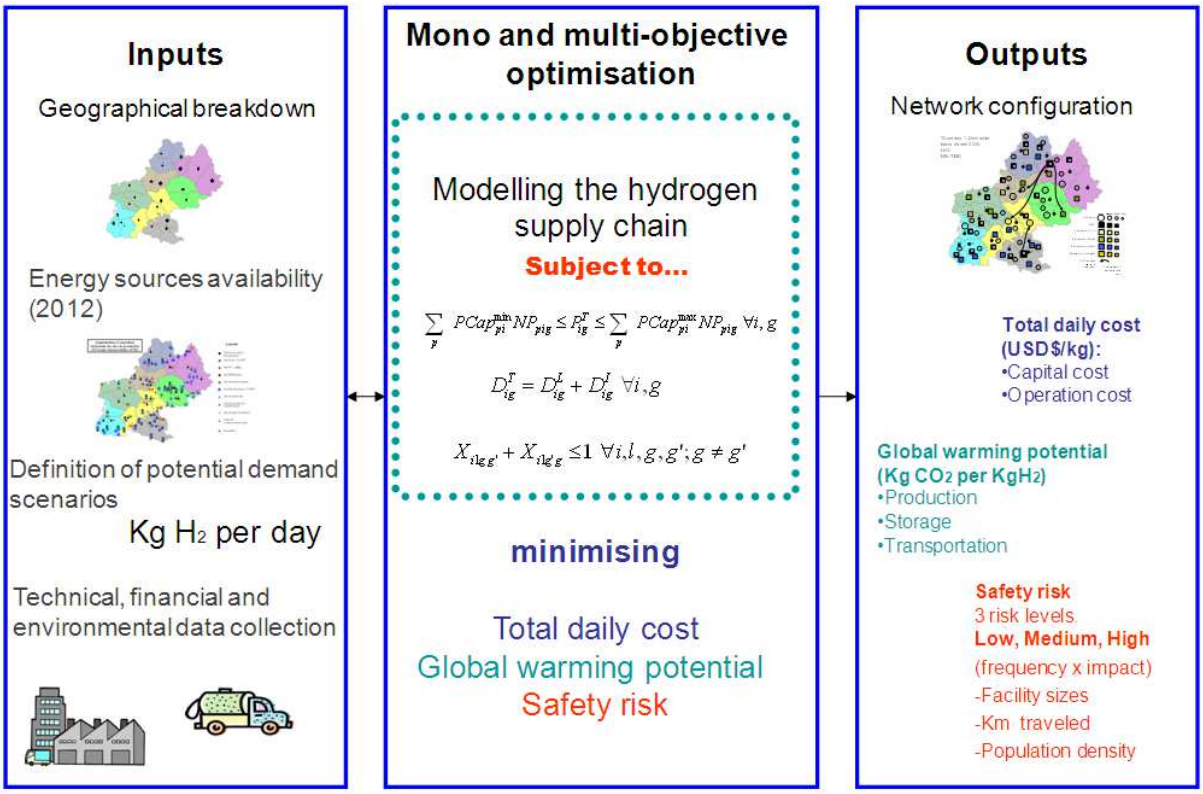


Figure 5.1 Methodology framework for the "Green H_2 fuel" project (Midi-Pyrénées).

5.2 Methodology

5.2.1 Problem definition

The optimisation approach of HSC proposed by (De-León Almaraz et al., 2013a, 2012) and presented in Chapter 4 has been adapted to the Midi-Pyrénées region to answer the following questions:

- what is the best option for production and storage of hydrogen in Midi-Pyrénées?
- is centralised production or decentralised production (small-scale production at local fuelling) more cost effective?
- what are the most cost effective transportation modes and pathways to connect hydrogen demand with its supply?
- is it possible to find competitive targets for a region?
- does the WtW of the HSC result in less CO_2 emission than those related to gasoline and diesel?
- what is the safest configuration of the HSC in Midi-Pyrénées?

5.2.2 Objective

This work focuses on the design of a HSC for the Midi-Pyrénées region in five levels: energy sources, production, storage, transport and market (Figure 5.2). There are three objectives to be minimised: the cost, the environment impact expressed in terms of GWP (CO_2 emissions) and the safety risk.

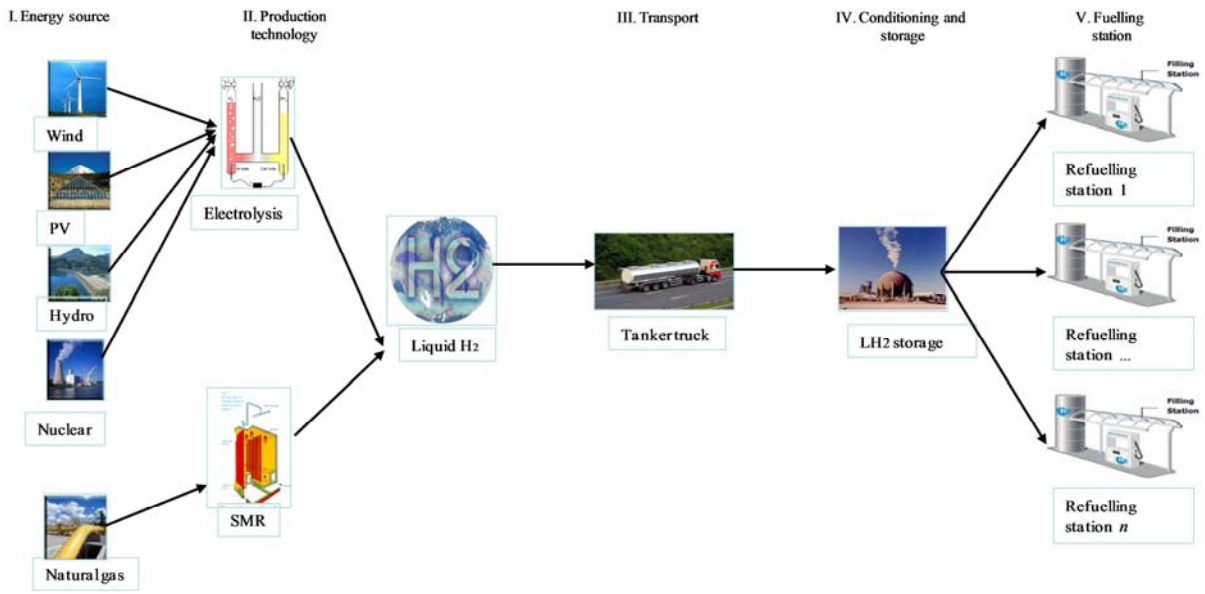


Figure 5.2 The HSC studied for Midi-Pyrénées

5.3 Data collection

As abovementioned, the division of the territory into districts is adopted and a deterministic demand is assumed. The data set includes information relating to the hydrogen demand, technical, environmental, economic and risk data associated with each component of the HSC. Some values have been collected from recent publications (ADEME, INSEE, CNRS, etc.), visits to sites, and interviews with professionals in the energy region and professors (sociologists and researchers specialized in the field energy). In this approach, the demand for hydrogen is assumed fixed. The problem is defined as multi-period and the time horizon considered is 2020-2050 with a time step of 10 years.

5.3.1 Techno-economic data

A large amount of input data is required to solve the problem. All the techno-economic parameters (i.e., minimum and maximum production and storage capacities, average delivery distance between grids and capacity of each transportation mode, etc.) are defined in Appendix B1. In this section we present only the main specific issues linked to the Midi-Pyrénées region.

5.3.2 The geographic division

According to its geographic and administrative segmentation, Midi-Pyrénées is divided into prefectures and sub-prefectures: this represents 22 zones (see Figure 5.3). This division has been used to obtain a realistic path between districts with the existence of major roads and to estimate the potential demand from regional statistics INSEE 2012.

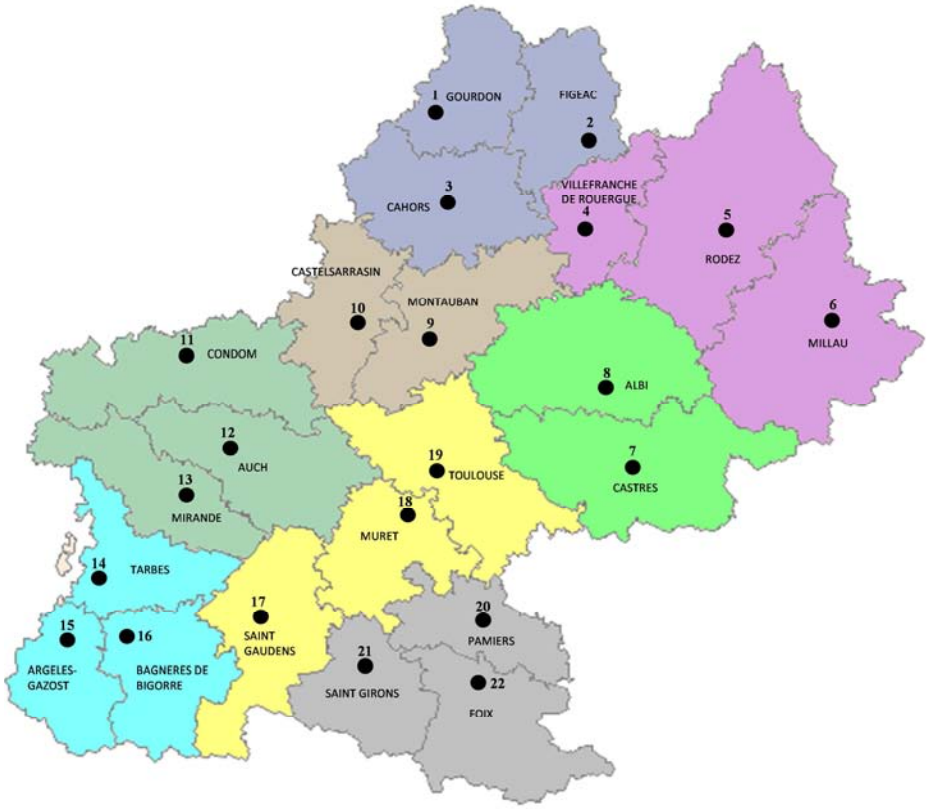


Figure 5.3 Geographic division of the Midi-Pyrénées region

5.3.3 Energy sources and production facilities.

The availability of renewable energy sources used for this study was gathered from the investigation carried out by (Salingue, 2012). Figure 5.4 takes into account the large RES sites for wind power with a capacity higher than 0.5 MW, for PV more than 1 MWp and hydropower of more than 0.5 MW. The data was in agreement with the study of the Regional Climate Air Energy forecasting for Midi-Pyrénées (Le Schéma Régional Climat Air Energie, 2012) approved in June 2012 by the region. This report presents the strategic objectives for the development of renewable energy in 2020.

The zones with potential development of RES are presented in Figure 5.5. Based on this study and considering the current energy situation, the initial average availability of primary energy source *e* in grid *g* during time period *t* (kWh per day) from 2020 to 2050 is presented in the Appendix B.1.11. For hydropower, only facilities "run-of-river" are considered (based on data collection from EDF), which represent 28.6% of the total hydropower in the region against 71.4% for the "pumped-storage hydroelectricity" facilities. Because of the potential of renewable energy (wind, solar and hydro) in the region, production of hydrogen by electrolysis of water was selected. The potential use of nuclear electricity is also considered. However, the commercial production technology used today is mainly based on steam methane reforming: the comparison of this method with those using renewable sources appears relevant.

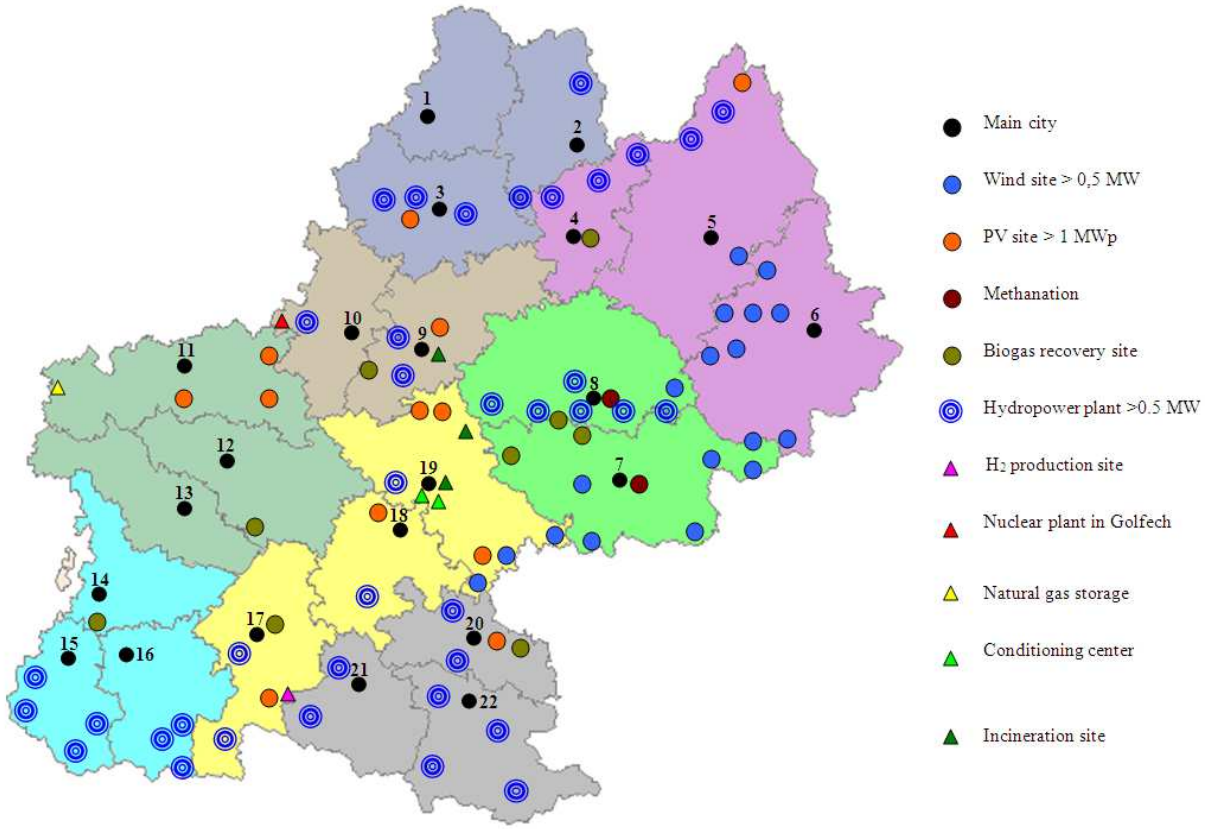


Figure 5.4 Segmentation and geographic distribution of production sites Renewable Energy

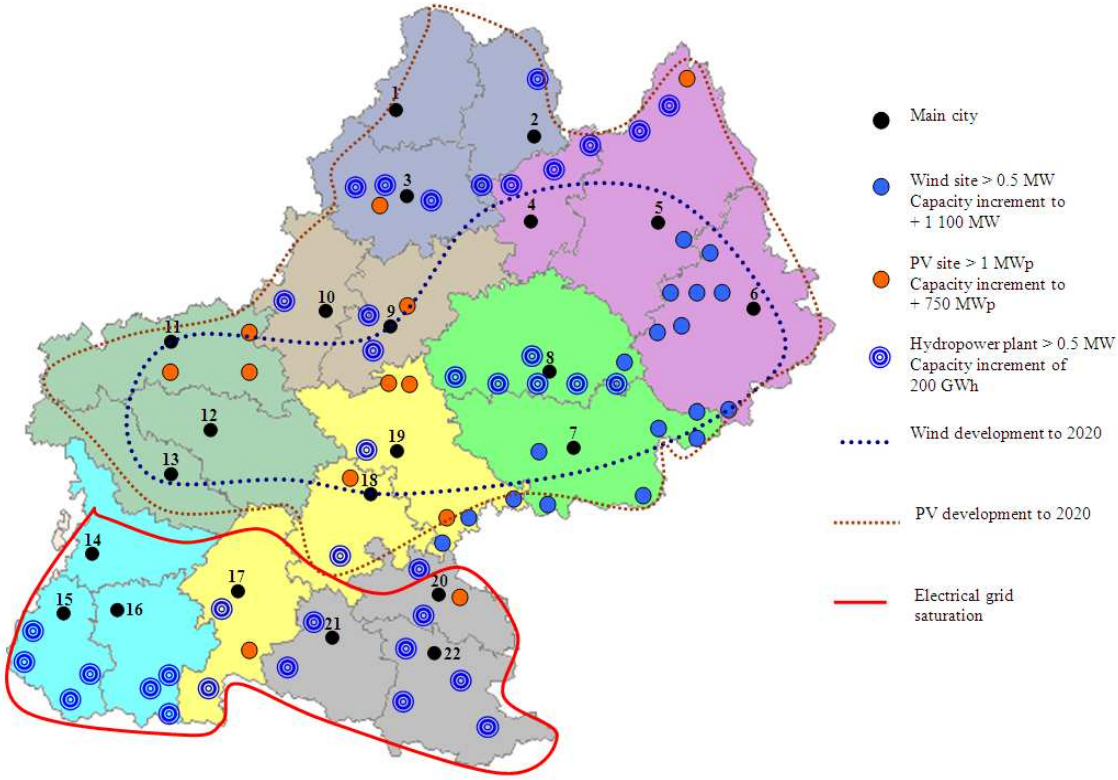


Figure 5.5 Projection of renewable energy production capacity in 2020 in Midi-Pyrénées.

The RES evolution in the region is shown in Figure 5.6 from 2012 to 2050. A big difference in the proportion of energy sources is highlighted in 2012, 2020 and 2030 (e.g. hydro ratio is 78% in 2012, 48% in 2020 and 39% in 2030); this change is due to the projections of the Regional Climate Air Energy forecasting for Midi-Pyrénées. For 2040-50 no projections were found and we made the hypothesis of 2% of augmentation in the total production capacity but the percentage per type of RES remains the same.

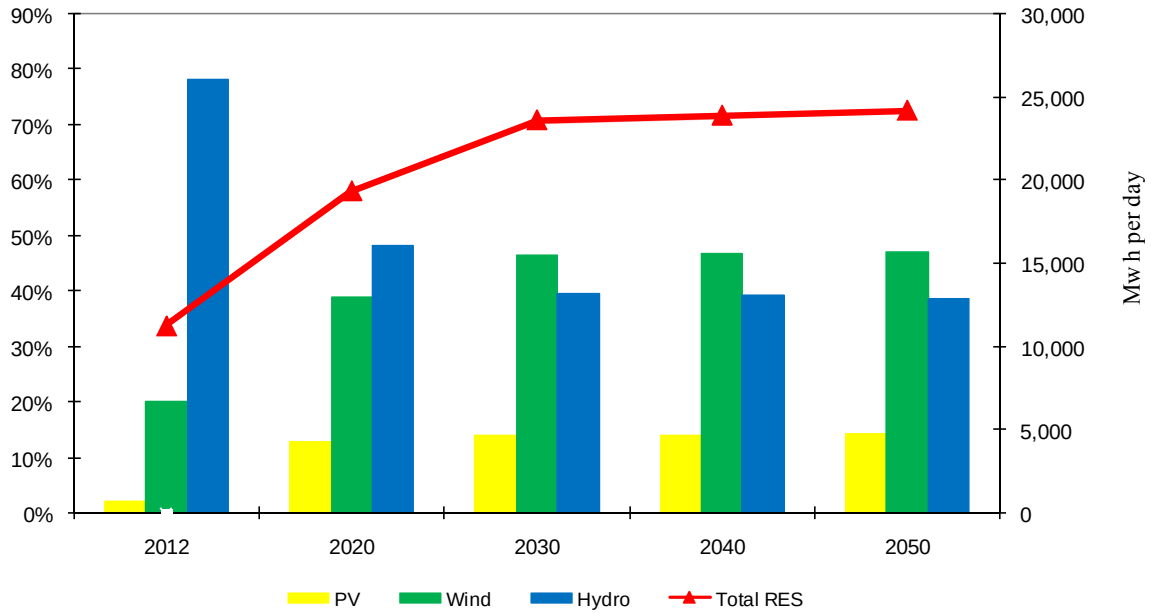


Figure 5.6 Evolution of selected RES 2012-2050

5.3.4 Conditioning, storage and transportation

This study focuses only on the conditioning, storage and distribution of liquid hydrogen (LH_2) that is considered instead of compressed gaseous hydrogen (CH_2) because it has several advantages over gas. LH_2 has a very high energy density, it is easier to handle, transport and store (Almansoori and Shah, 2009). From the economic point of view, transportation of LH_2 is cheaper than from a gas network, as highlighted by (Almansoori and Shah, 2006). Storage could be performed in liquid phase with stainless steel tanks (cryostats) by the Claude cycle which lowers the temperature to -253°C (liquefaction temperature) (Agator et al., 2008) with a density of 70.85 kg/m^3 vs. 0.0899 kg/m^3 for the CH_2.

5.3.5 Refuelling stations

The final step is the refuelling station for the vehicles supply. The model only computes the number of fuelling stations to be installed. (McKinsey & Company, 2010) considered 3 types of refuelling stations where H_2 is considered as liquid at 30 bar pressure or gaseous at 250 or 450 bar. Then, H_2 is compressed to 350 or 700 bar; for this case, only one size of refuelling station with 10 dispensers to provide maximum 2.5 t H_2 per day is considered.

5.3.6 Demand estimation

A deterministic demand of hydrogen for FCEV is considered, including fleets such as buses, private and light-good-vehicles and forklifts at 2010 levels. Market demand scenarios selected for this project were based on two main studies: (i)- a prospective study conducted by (McKinsey & Company, 2010) entitled «A portfolio of power-trains for Europe» and (ii)- Bento's thesis manuscript (Bento, 2010). From these studies and the involved assumptions, two scenarios concerning two levels of demand for fuel cell electric vehicles penetration were developed (see Figure 5.7 and Table 5.1). The scenario S1 refers to a low demand scenario and the S2 is an optimistic one.

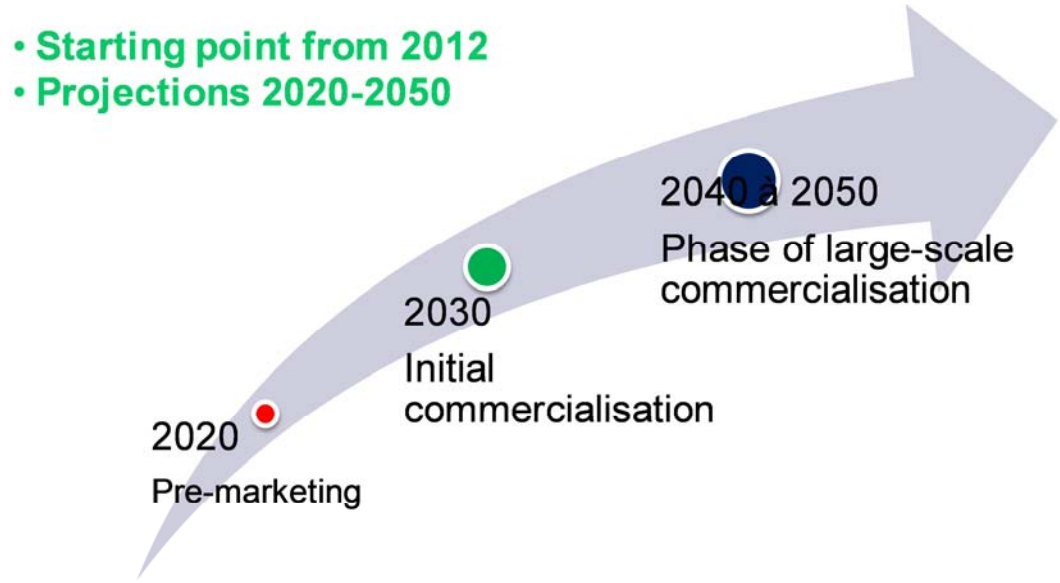


Figure 5.7 Development phases of the hydrogen economy in Midi-Pyrénées based on (Bento, 2010)

Table 5.1 Demand scenarios of fuel cell electric vehicles penetration by period

Scenario/year	2020	2030	2040	2050
S1: Scenario 1 (buses, private and light-good-vehicles)	1%	7.50%	17.50%	25%
S2: Scenario 2 (buses, private and light-good-vehicles)	2%	15%	35%	50%
S1/S2: Scenarios 1 and 2 (forklifts)	4%	30%	70%	100%
Total S1 (t H_2 per day)	7.9	59.4	138.7	198.1
Total S2 (t H_2 per day)	15.5	116.9	272.8	389.8

The demand potential for hydrogen in these two scenarios is computed according to Eq. 5.1 as in the works of (Almansoori and Shah, 2006) and (Murthy Konda et al., 2011b).

$$D_{ig}^{T} = FE.d.Qc_{g} \quad \textbf{5.1}$$

where the total demand in each district (D^{T}_{ig}) results from the product of the fuel economy of the vehicle (FE) (Table 5.2), the average total distance travelled (d) and the total number of vehicles in each district (Qc_g) (see Appendix B.1.1). The demand of LH_2 for each scenario and type of vehicle can be found in (Salingue, 2012).

Table 5.2 H_2 fuel economy of different types of FCEV and the average total distance travelled for gasoline and diesel cars

Type of vehicles	*FCEV Kg H_2/100 km*	*Gasoline vehicle (km/year)*	*Diesel vehicle (km/year)*
Private vehicles[36]	0.98	8 730	15 799
Bus[6]	11.7	-	35 879
Light-good-vehicles (GVWR[37]< 1,5 T)[2]	1.00	7 000	11 400
Light-good-vehicles (1,5 T > GVWR < 2,5 T)[2]	1.14	8 700	17 600
Light-good-vehicles (GVWR< 3,5 T)[38]	1.56	9 100	17 500
Forklifts[2] 1.44 kg per day			

5.3.7 Assumptions

The study is based on the following assumptions:

- a capital change factor of 12 years is introduced;
- several sizes and types of production units and storage facilities are considered;
- a minimum capacity of production and storage equal to 50 kg of H_2 per day is taken into account;
- renewable energy is directly used on-site because of grid saturation. This allows to allocate the CO_2 impact to each source;
- inter-district transport is allowed;
- the maximum capacity of transportation is fixed at 3500 kg liquid-H_2 (Dagdougui et al., 2012);
- a 10-days LH_2 safety stock is considered;
- the risk index is calculated by the methodology proposed by (Kim and Moon, 2008) (Kim et al., 2011);
- a RES increase of 2% in each period from 2030 to 2050;
- the number of plants is initialized at a null value: the H_2 plants that exist are supposed to provide exclusively the demand for chemical industry requirements (i.e., Linde in Boussens);
- the cost of migrating a current refuelling station to H_2 fuel is not considered;
- the learning rate cost reductions due the accumulated experience is considered as 2% per period (McKinsey & Company, 2010);
- the scenario 1 (low demand) is solved.

[36] (Almansoori and Shah, 2006)

[37] GVWR: Gross vehicle weight rating

[38] (Salingue, 2012, pp,29-30)

5.4 Mathematical model

The elements of a HSC are shown in Table 5.2. In the proposed formulation, the hydrogen can be produced from an energy source *e*, delivered in a specific physical form *i*, such as liquid or gaseous, produced in a factory type involving different production technologies *p*, stored in a reservoir unit *s* and distributed by a transportation mode *l* from one district or grid *g* to another *g'* (with $g' \neq g$).

To model the HSC for the region, constraints used are similar to that of the previous chapter and (Almansoori and Shah, 2009). The model remains as mixed integer linear programming (MILP). However, for the Midi-Pyrénées case study, a multi-period optimisation approach was carried out with the objective of minimising the criteria on the entire time horizon *t*. Another specific feature for this case is the integration of renewable energy constraints. The indices *t* (time period) and *j* (facility size) are added to all the constraints of the model presented in chapter 4, in this section only the new constraints are presented.

5.4.1 Energy source constraint

The average availability of primary energy sources *e* in a grid *g* during time period *t* is given as a sum of three terms. These are the initial average availability of primary energy sources, the import of primary energy sources and the rate of consumption of these sources. γ_{epj} is the rate of utilisation of primary energy source *e* by plant type *p* and size *j* and is multiplied by the safety stock factor (SSF = 5%) for storing a small inventory of primary energy sources. The terms are expressed respectively by the following constraint:

$$A_{egt} = A0_{egt} + IPES_{egt} - SSF \sum_{pji} \gamma_{epj} PR_{pijgt} \forall e,t,g; g \neq g' \quad \textbf{5.2}$$

5.4.2 Production facilities constraints

The number of production facilities type *p* and size *j* installed in *g* in the first time period NP_{pijgt1} is determined by the sum of the total initial number of production facilities ($N0_{pjig}$), and the number of new plants of type *p* producing product form *i* in grid *g* in the period one (IP_{pijg1}):

$$NP_{pijgt_1} = NP0_{pjig} + IP_{pjigt_1} \quad \forall p,i,j,g,t = 1 \quad \textbf{5.3}$$

For all the other periods, the definition of the number of new production facilities takes into account the production plants established in the previous time period.

$$NP_{pijgt} = NP_{pjigt-1} + IP_{pjigt} \quad \forall p,i,j,g,t \neq 1 \quad \textbf{5.4}$$

In the case of new electrolysis plants that use renewable energy ($IP_{electrolysis\text{-}RES,i,j,g,t}$) they can be established only when renewable energy *e* is available in the grid *g*. For the Midi-Pyrénées region, exportation of renewable energy between grids *g* to *g'* is not considered due to network saturation,

then, if the initial availability of renewable energy source $A0_{egt}$ in *g* is zero, non-electrolysis plants can be installed in this district *g*.

$$IP_{electrolysis(RES)ijgt} = 0 \quad if \quad A0_{e(RES)gt} = 0 \forall g \qquad \textbf{5.5}$$

The number of storage (NS_{sijgt}) is determined by the sum of the total initial number of storage facilities of type *s* and size *j* storing product form *i* in grid *g* established in the previous time period *t-1*($NS0_{sjig}$ or NS_{sigt-1}) and the number of new storage units of type *s* producing product form *i* in grid *g* during the time period *t* (IS_{sigt}):

$$NS_{sijgt_1} = NS0_{sjig} + IS_{sijgt_1} \quad \forall s,i,j,g,t:1 \qquad \textbf{5.6}$$

$$NS_{sijgt} = NS_{sjigt-1} + IS_{sijgt} \quad \forall s,i,j,g,t \neq 1 \qquad \textbf{5.7}$$

5.4.3 *Refuelling stations*

The number of refuelling stations within a grid *g* dispensing a product form *i* depends on the total equivalent demand and the installed capacity of the fuelling stations, as follows:

$$NFS_t = \sum_{i,g} \frac{D_{igt}^T}{FCap_i} \forall t \qquad \textbf{5.8}$$

5.4.4 Objective function: total daily cost

5.4.4.1 Facility capital cost

Constraint 4.23 from chapter 4 should be replaced by the constraint 5.9. The facility capital cost is calculated by multiplying the number of new plants and new storage facilities by their capital cost and the learning rate as the cost reductions when technology manufacturers accumulate experience during time period *t*.

$$FCC_t = \sum_{i,g} \frac{1}{LR_t} \left(\sum_{p,j} PCC_{pij} IP_{pjigt} + \sum_{s,j} SCC_{sij} IS_{sijgt} \forall t \right) \qquad \textbf{5.9}$$

5.4.4.2 Primary energy sources transportation cost

The cost of transportation of primary energy sources for all scenarios during the entire planning horizon is equal to:

$$ESC_t = \sum_{e,g} UIC_e IPES_{egt} \forall t \qquad \textbf{5.10}$$

5.4.4.3 *Economic objective function*

Constraint 4.34 from chapter 4 should be replaced by the constraint 5.11. By combining the cost terms derived earlier presented in section 4.5 (chapter 4) and the new element introduced in constraint 5.10, we obtain the total daily cost (TDC) of the hydrogen supply chain:

$$TDC = \sum_t \frac{FCC_t + TCC_t}{\alpha CCF} + FOC_t + TOC_t + ESC_t \qquad \textbf{5.11}$$

The first term of the right-hand-side of this objective function (facility and transportation capital costs, FCC_t and TCC_t in the time period *t*) is divided by the network operating period (α) and the annual capital charge factor (CCF) to find the cost per day in US dollars. This result is added to the facility and transportation operating (FOC_t, TOC_t) costs and to the cost of transportation of the energy source ESC_t.

5.5 Solution strategy

This problem is treated in GAMS 23.9 and solved by CPLEX 12. Two main cases are analysed here: case A for mono-objective optimisation and B for multi-objective approaches (see Figure 5.8).

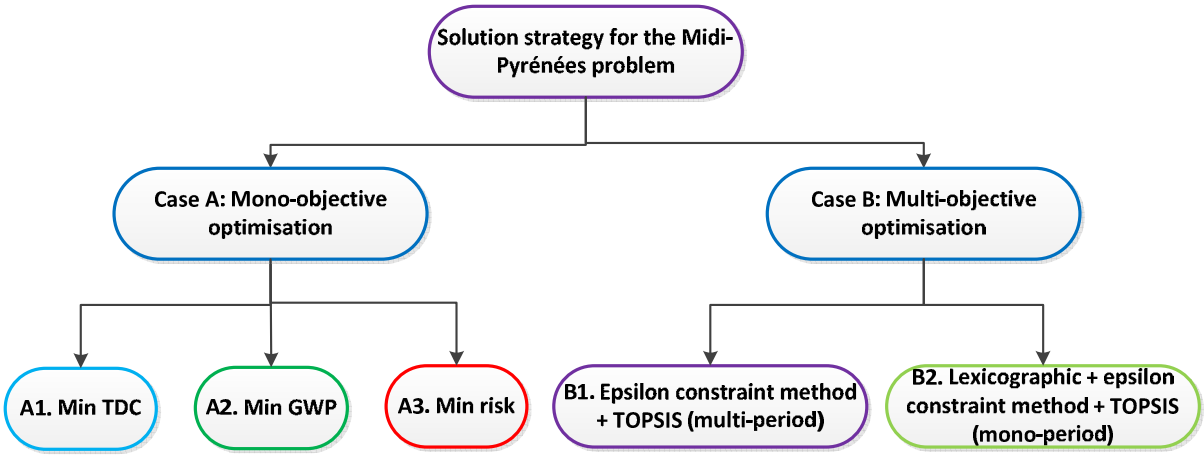


Figure 5.8 Optimisation approaches for the Midi-Pyrénées region.

5.5.1 *Case A. Mono-objective approach.*

Each mono-objective problem is optimised for the entire time horizon (multi-period). The geographic Midi-Pyrénées region is selected and divided in districts. The possible configurations of the HSC to be located in the region are defined (such as product physical form, viable production processes, transportation type, etc…).

5.5.2 *Case B1. Multi-objective optimisation through ε-constraint method.*

In this case, the nadir and utopia points resulted from the pay-off table in the case A are considered. The problem is treated as a multi-period one. The tri-objective optimisation problem is solved by implementing the ε-constraint method. Once the epsilon points are defined, the objective function

TDC has to be minimised. The GWP and risk objective functions are transformed into inequalities constraints.

5.5.3 Case B2. Multi-objective optimisation based on lexicographic and ε-constraint methods.

The hybrid strategy coupling lexicographic and ε-constraint method was also used in the previous chapter for a mono-period problem. At the beginning we made some efforts to solve the Midi-Pyrénées case as multi-period to construct the pay-off table through lexicographic optimisation but the multi-period problem turns out to be a difficult problem due to the problem size and the use of binary variables so that a feasible solution was not obtained. In order to overcome this limitation, the problem is treated here as four mono-period problems. We optimise the time period *t1* for the 3 objectives through lexicographic optimisation, the pay-off allows the application of the ε-constraint method; a TOPSIS analysis is then carried out for each Pareto front with the same weighting factor for cost, safety and environmental criteria. The optimised network configuration then serves as initialising existing network for the period *t+1* and the same procedure is applied until the four time periods are solved.

5.6 Mono-objective optimisation results (case A)

The first results for scenario 1 "low demand" are presented in this section. The single-objective optimisation was performed and considered as a preliminary step to the multi-objective stage. In each case, the calculation of other criteria was done without be optimised. There results were presented in the XIV congress organised by SFGP, 2013 in Lyon, France (De-León Almaraz et al., 2013b).

5.6.1 Case A1. Minimising the total daily cost

Figure 5.9 shows the evolution of the supply chain for a period of 10 years by optimising the cost of hydrogen. Specifically, Figure 5.9 (year 2020) shows a distributed configuration with a mix of productions plants with different energy sources such as wind, solar, hydro and gas. It may be noted that the transport is not considered due to weak demand in LH_2. The minimal cost in this period is \$16.2/kg H2 with 6.9 kg CO_2-equiv/kg H_2 and a risk of 35 units (see Table 5.3). The capital investment in 2020 is very high due in this transition phase each district with regard to both production units and storage facilities needed to develop the network.

The total daily cost decreases strongly in the period 2030-2050, due to a decrease in capital costs, reaching \$3.7/kg H_2 in 2050. In this period, a centralised network is found operating with steam methane reforming as the major production technology.

The increase in demand in 2050 (198 t vs. 7.9 t in 2020) promotes the use of transportation units. A total of twenty-two tanker trucks are necessary to supply LH_2 to different districts from the grids 4 and

22 where the plants have a sufficient installed capacity to export hydrogen. Eighty six percent of the total LH_2 demand is imported from these two districts and 14% of the request is provided on-site by the electrolysis production units. The configuration of the chain in 2050 increased the risk (263 units) related to transportation, the size of the storage units and the district where they are located. The results lead to 44% risk related to the transport and 50% to the storage. Finally, in Figure 5.9 for the year 2050, there are 43 plants of small and medium sizes (43% of these plants using steam reforming process). SMR produces 99% of the regional total demand of hydrogen, which leads to relatively high emissions of CO_2 (10.9 kg CO_2-equiv/kg H_2 for the year 2050).

Table 5.3 Cost optimisation results of the hydrogen supply chain (case A1)

Year	2020	2030	2040	2050
Demand (t per day)	7.9	59.4	138.8	198.2
Number of total production facilities	25	43	43	43
Number of new production facilities installed in this period	25	18	0	0
Number of total storage facilities	22	41	71	116
Number of new storage facilities installed in this period	22	19	30	45
Number of transport units	-	5	14	22
Capital cost				
Plants and storage facilities (10^3 $)	338 554	1 081 476	171 154	127 793
Transportation modes (10^3 $)	0	2 500	7 000	11 000
Total daily capital cost (10^3 $ per day)	77	247	41	32
Operating cost				
Plants and storage facilities (10^3 $ per day)	50	245	496	676
Transportation modes (10^3 $ per day)	0	2	7	11
Total operating cost (10^3 $ per day)	50	247	503	686
Cost of transportation of energy source (10^3 $ per day)	0	3	6	8
Total network cost (10^3 $ per day)	*127.67*	*496.63*	*549.28*	*726.58*
Cost per kg H_2 ($)	**16.17**	**8.36**	**3.96**	**3.67**
Production facilities (t CO_2-equiv per day)	48.8	584.2	1 393.0	1 992.8
Storage facilities (t CO_2-equiv per day)	5.6	41.8	97.7	139.5
Transportation modes (t CO_2-equiv per day)		4.0	14.2	22.8
Total GWP (t CO_2-equiv per day)	54.4	630.1	1 504.9	2 155.1
Kg CO_2-equiv per kg H_2	**6.9**	**10.6**	**10.8**	**10.9**
Production facilities	6	12	12	12
Storage facilities	29	67	99	134
Transportation modes		34	75	116
Total Risk (Units-level)	**35**	**113**	**186**	**263**

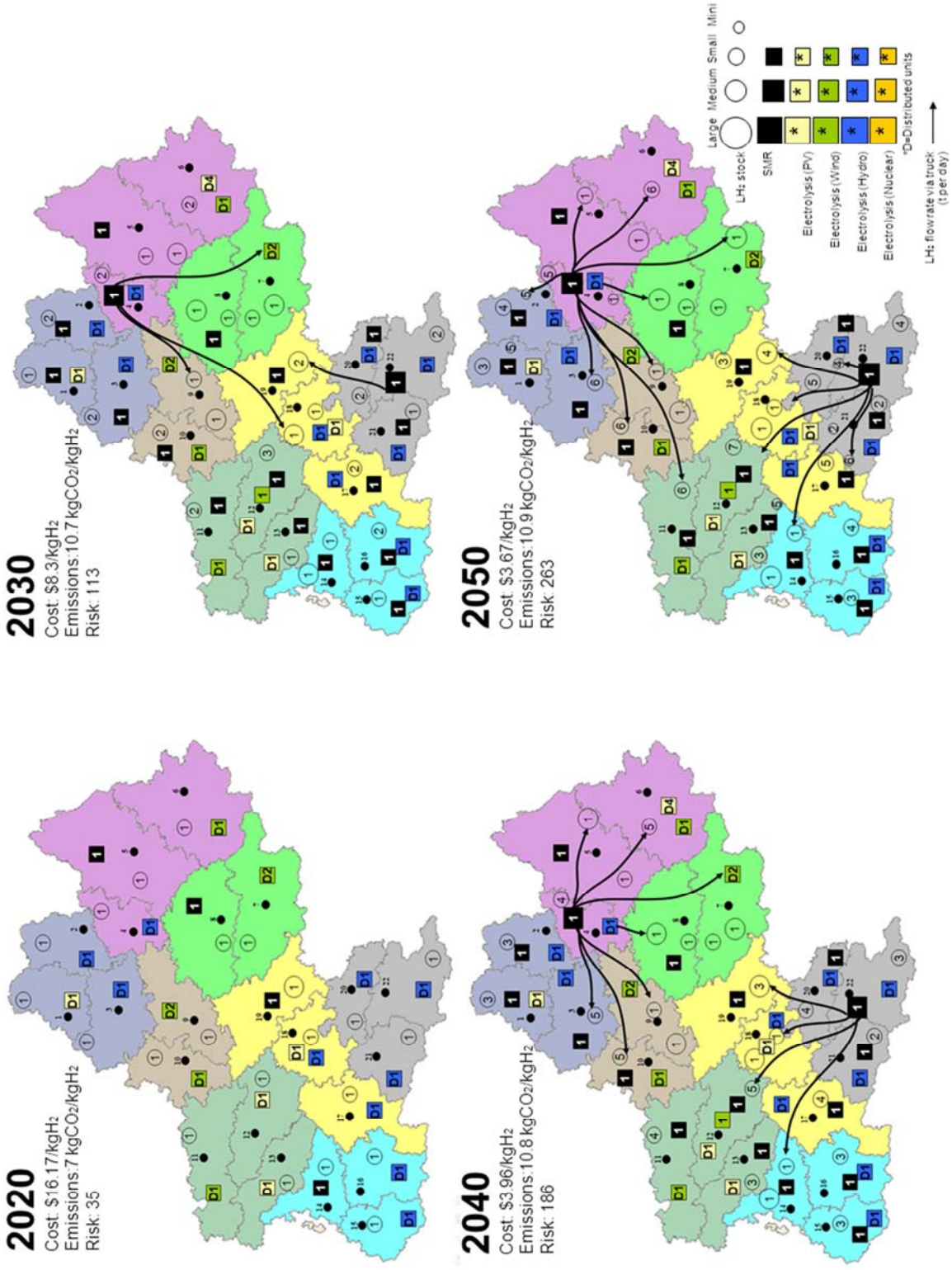


Figure 5.9 Network structure of liquid hydrogen distributed via tanker trucks. Case A1: Cost minimisation in a low demand scenario in the Midi-Pyrénées region.

5.6.2 Case A2. Minimising the global warming potential

Figure 5.10 shows the possible configurations of the infrastructure for the Midi-Pyrénées region where CO_2 emissions are minimised. For the 2020 period, a fully decentralised configuration with wind as primary energy source is obtained (see Table 5.4) GWP is 2.1 kg CO_2-equiv per kg H_2, which represents 30% of CO_2 that would be issued for the same period in the scenario of cost minimisation. Conversely, the price is \$24 per kg H_2 in 2020 (see all results in Table 5.5), this represents an increase of 52% compared to the minimal cost. The cost is logically higher in the first period mainly due to weak demand, which limits production capacity with electrolysis technology without transportation links. The existence of 24 storage units also contributes to a higher risk. The year 2030 requires the installation of several production and storage units with similar CO_2 emissions, but the total daily cost decreases to \$14 per kg H_2, the risk takes a relatively average value over this period and the years to come.

Table 5.4 Distribution Use ratio of energy sources for hydrogen production by electrolysis for the scenario 1 minimising CO_2 emissions.

Energy source/Period	2020	2030	2040	2050
Wind	70%	76%	83%	90%
Hydraulic	22%	16%	13%	7%
Nuclear	8%	8%	3%	3%

Table 5.5 GWP optimisation results of the hydrogen supply chain (case A2)

Year	2020	2030	2040	2050
Demand (t per day)	7.9	59.4	138.8	198.2
Number of total production facilities	23	42	43	48
Number of new production facilities installed in this period	23	19	1	5
Number of total storage facilities	24	40	46	46
Number of new storage facilities installed in this period	24	16	6	0
Number of transport units		1	3	6
Capital cost				
Plants and storage facilities (10^3 \$)	610 449	2 020 692	913 462	2 559 434
Transportation modes (10^3 \$)	0	500	1 500	3 000
Total daily capital cost (10^3 \$ per day)	139	461	209	585
Operating cost				
Plants and storage facilities (10^3 \$ per day)	54	369	856	1 216
Transportation modes (10^3 \$ per day)	0	0	1	2
Total operating cost (10^3 \$ per day)	54	370	857	1 218
Cost of transportation of energy source (10^3 \$ per day)	0	2	10	19
Total network cost (10^3 \$ per day)	*193.25*	*832.66*	*1 075.85*	*1 821.45*
Cost per kg H_2 (\$)	**24.47**	**14.01**	**7.75**	**9.19**
Production facilities (t CO_2-equiv per day)	11.3	81.3	172.0	231.9
Storage facilities (t CO_2-equiv per day)	5.6	41.8	97.7	139.5
Transportation modes (t CO_2-equiv per day)		0.1	1.3	3.1
Total GWP (t CO_2-equiv per day)	16.9	123.2	271.0	374.4
Kg CO_2-equiv per kg H_2	**2.1**	**2.1**	**2.0**	**1.9**
Production facilities	6	13	14	19
Storage facilities	36	78	98	98
Transportation modes		7	13	24
Total Risk (Units-level)	**42**	**98**	**124**	**141**

In 2040 and 2050, the cost is significantly lower, \$7.8 and \$9.2 per kg H_2 respectively, so that the cost increases in the period 2050 with the installation of five new plants for providing LH_2. CO_2 emissions are minimal in 2050: 1.9 kg CO_2 per kg H_2 and the final configuration leads to 97% of electrolysis production using renewable energy (see Table 5.4). The allocation of emissions is as follows: 62% for production, 37% for liquefaction and only 1% for transportation.

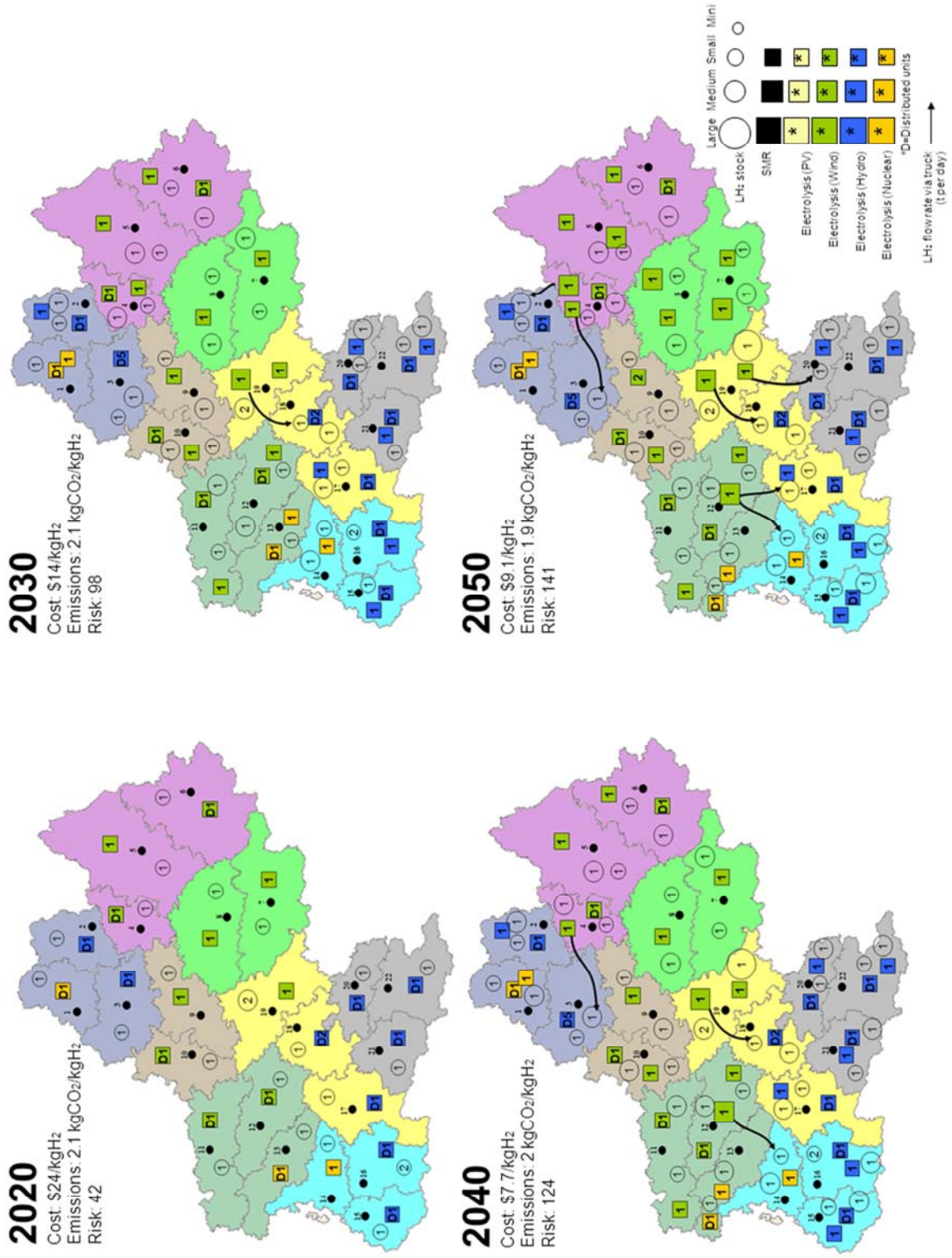


Figure 5.10 Network structure of liquid hydrogen distributed via tanker trucks. Case A2: CO_2 minimisation in a low demand scenario in the Midi-Pyrénées region.

5.6.3 Case A3. Minimising the total relative risk.

Figure 5.11 shows the possible configurations obtained by minimising the risk with a mix of production technologies (SMR and electrolysis) that includes all the available energy sources in the region. The main production technology involves steam reforming of natural gas (99%) and only 1% electrolysis using electricity from nuclear sources, solar, wind and hydro. For this mono-objective optimisation, the network is 100% decentralised. The four storage sizes are used in the four considered periods.

Table 5.6 Risk optimisation results of the hydrogen supply chain (case A3)

Year	2020	2030	2040	2050
Demand (t per day)	7.9	59.4	138.8	198.2
Number of total production facilities	22	38	38	44
Number of new production facilities	22	16	0	6
Number of total storage facilities	22	40	48	52
Number of new storage facilities	22	18	8	4
Number of transport units	-	-	-	-
Capital cost				
Plants and storage facilities (10^3 $)	401395.8	1603921.6	204807.7	156247.5
Transportation modes (10^3 $)				
Total daily capital cost (10^3 $ per day)	91.6	366.2	46.8	35.7
Operating cost				
Plants and storage facilities (10^3 $ per day)	45.8	303.3	730.2	1043.9
Transportation modes (10^3 $ per day)	0.0	0.0	0.0	0.0
Total operating cost (10^3 $ per day)	45.8	303.3	730.2	1043.9
Cost of transportation of energy source (10^3 $ per day)	0.7	5.4	16.9	24.4
Total network cost (10^3 $ per day)	*138.2*	*674.8*	*793.9*	*1104.0*
Cost per kg H_2 ($)	**17.5**	**11.4**	**5.7**	**5.6**
Production facilities (t CO_2-equiv per day)	64.0	525.7	1092.5	1553.8
Storage facilities (t CO_2-equiv per day)	5.6	41.8	97.7	139.5
Transportation modes (t CO_2-equiv per day)				
Total GWP (t CO_2-equiv per day)	69.6	567.6	1190.2	1693.3
Kg CO_2-equiv per kg H_2	**8.8**	**9.6**	**8.6**	**8.5**
Production facilities	6	12	12	15
Storage facilities	29	77	95	97
Transportation modes				
Total Risk (Units-level)	**35**	**89**	**107**	**112**

The minimal risk of the HSC in 2020 is 35 units (Table 5.6), with cumulative risks for production units and storage: the obtained values of the risk index are equal to 89, 107 and 112 units for 2030, 2040 and 2050, respectively. The risk scale was calculated with the lowest value obtained from the minimisation of this objective for all periods. The calculations for the Midi-Pyrénées case are shown in Appendix B.2. The total daily cost of LH_2 for this scenario is lower than in the environmental scenario but logically higher than the economic scenario for all periods. In 2050 (see Figure 5.11) the cost is \$5.6 per kg H_2 and emissions of 8.5 kg CO_2 per kg H_2. The main risks in this configuration are mainly due to storage 85% and production 15%.

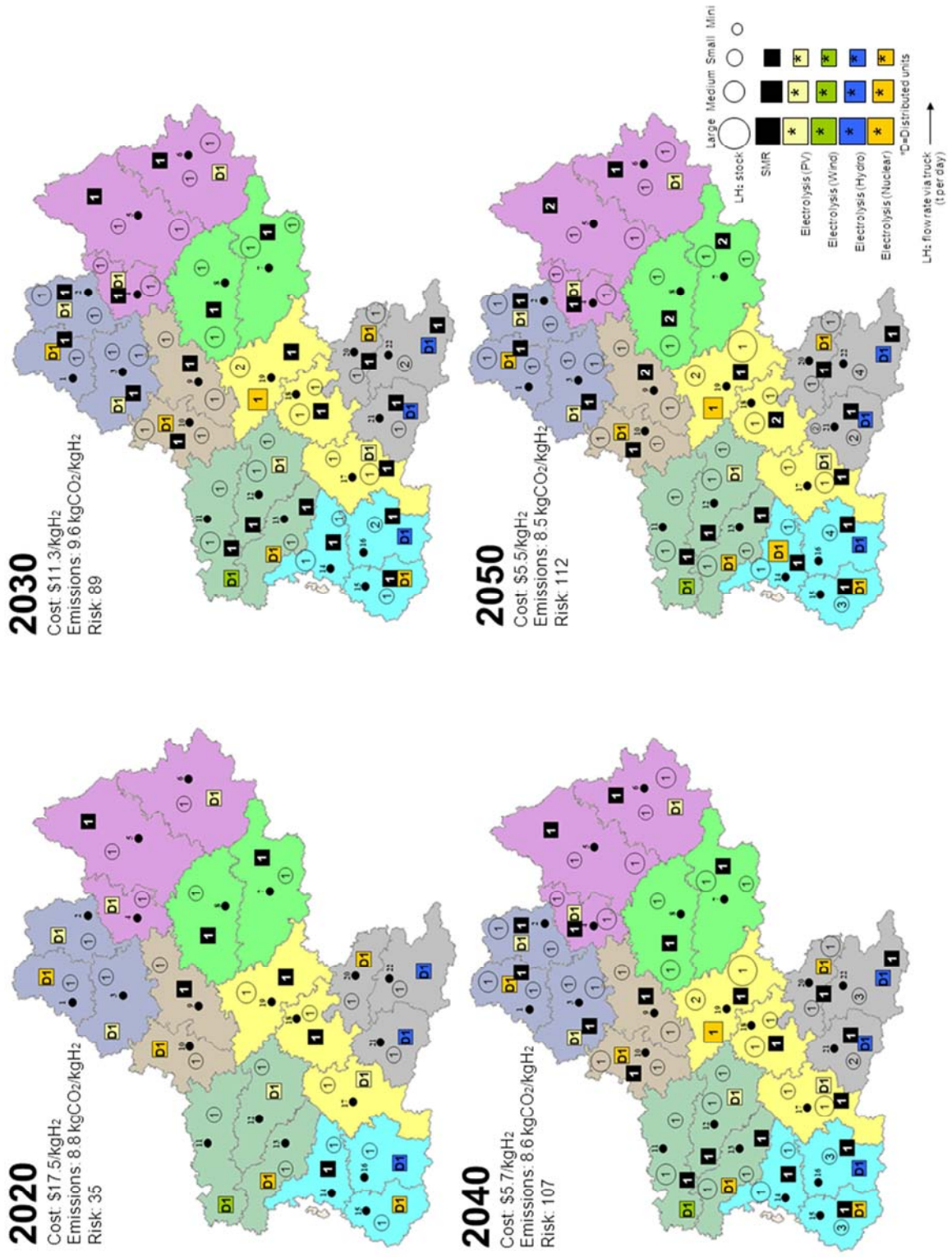


Figure 5.11 Network structure of liquid hydrogen distributed via tanker trucks. Case A3: risk minimisation in a low demand scenario in the Midi-Pyrénées region.

5.6.4 Conclusions for the mono-objective optimisation

Table 5.7 displays the main differences among the three mono-objective cases. This first approach gives a reference for the various criteria considered separately over several periods. The cost criterion in the first time period is prohibitive. The multi-objective optimisation seems to be an alternative to address these antagonist objectives and to find a better compromise based on lexicographic and ε-constraint methods.

Table 5.7 Summary of each mono-objective optimisation case.

Minimising	TDC	GWP	Risk
Centralisation degree	Centralised production network supplied by tanker trucks	Decentralised production	100% decentralised production
Cost	Significant cost declining until 2040 and 2050	High investment capital cost in 2020, lower over next time periods but double than the scenario of cost minimisation in 2040	Digressive cost over the time, $5.7 per kg H_2 in 2040
Energy sources	Natural gas is the main energy source with a small share of RES	Choice of RES for the production of H_2	Choice of fossil energy sources
Risk	Very significant risks associated with the intensification of transport	Moderate risk and lower than the cost scenario	Low risk (mainly due to the lack of transportation)
Emissions	Significant environmental impact and especially strong increases over time until 2040.	Use of hydrogen as an energy carrier (storage) to optimise the performance of renewable energy, which focuses on the H_2-RES coupling.	High environmental impact

5.7 Multi-objective optimisation through Ɛ-constraint method (case B1)

The best and worst values for each criterion obtained from the results of case A lead to the nadir and utopia points for the whole time horizon: 25 ε-points were defined (combining intervals as shown in Figure 5.12); the lower and upper bounds for the GWP correspond to the total GWP divided by the total demand resulted in 1.94 (case A2) and 10.7 kg CO_2-equiv per kg H_2 (case A1). Similarly, lower risk limit is related to the case A3 and higher bound to the case A1. The ε-constraint methodology was applied adding inequality constraints related to the GWP and the risk values in the mathematical model and then optimising the TDC. The multi-period approach was applied.

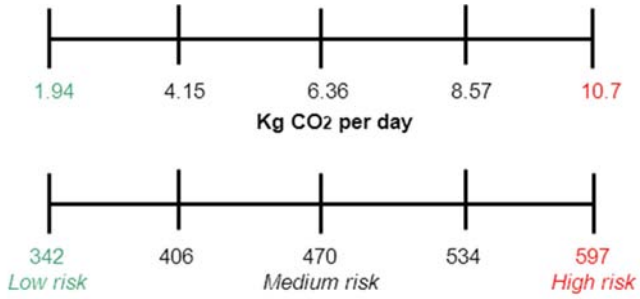


Figure 5.12 Epsilons definition for the multi-period problem with the average values 2020-2050

The solution consists of a Pareto front composed of 22 feasible solutions for supply chain configurations (Figure 5.13). The top solution (see Appendix B.3.1) corresponds to the option with the average cost of \$7.81 per kg H_2, GWP of 1.94 kg CO_2 per kg H_2 (average values are obtained dividing the TDC and the total GWP by the total demand for the 4 time periods) and a total risk of 406 units. The detailed configurations in each time period are presented in Figure 5.14 and decision/operating variables are displayed in Table 5.8.

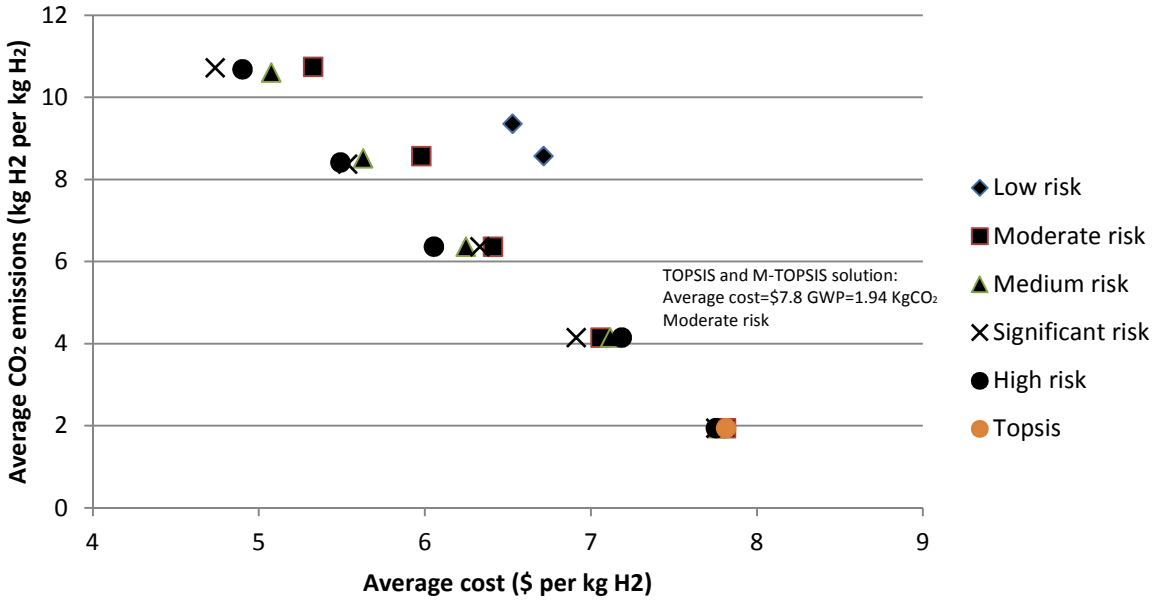


Figure 5.13 Pareto solutions for the multi-objective model for the case B1

Renewable energy is used to produce hydrogen from 2020. The cost is yet extremely high (\$23.4 per kg H_2) with a huge benefice in environmental impact. The risk of this configuration remains low for all the time periods because of the low level of transportation. Electrolysis is the main production technology using mainly wind power especially from 2030 to 2050. Once again, the change from a centralised to a decentralised supply chain is the main difference observed when the three criteria are taken into account in the optimisation phase compared to the cost minimal network. The production and storage sizes are mainly small-distributed units. Exported demand represents 6% in 2030 and 20% in 2050. Hydrogen is transported from districts 4, 12 and 19. The cost of the multi-objective approach is close to the targets set by the HyWays roadmap (European Commission, 2008) by 2050 in the range \$4.74-\$7.11 per kg H_2. In the optimisation, the obtained costs per kg H_2 are \$7.2 and 6.7 for 2040 and 2050 respectively. Not surprisingly, Table 5.9 shows that the best value obtained for cost in the multi-objective approach (case B1) is higher than for mono-objective case minimising TDC (an increase by 80% is observed by 2040-50). Besides, the unitary cost in 2020 is higher by 44%, which is a non-competitive cost of \$23.4 per kg H_2. The associated risk for this network is 42% lower by 2050. Besides, it was found that the GWP decreases by 70-80% comparing multi-objective vs. cases A1 and A3 because of the production mix.

Table 5.8 Multi-objective optimisation results of the hydrogen supply chain for the case B1

Year	2020	2030	2040	2050
Demand (kg per day)	7898	59430	138790	198170
Number of production facilities	23	44	56	70
Number of storage facilities	22	40	55	75
Number of transport units		1	3	6
Capital cost				
Plants and storage facilities (10^3 $)	*5724485*	*1161990.3*	*512401.5*	*335000.9*
Transportation modes (10^3 $)	*0*	*500*	*1500*	*3000*
Operating cost				
Plants and storage facilities (10^3 $ per day)	53.7	375.9	867.9	1239.6
Transportation modes (10^3 $ per day)	0	0.1	0.7	1.6
Total operating cost (10^3 $ per day)	53.7	376.0	868.6	1241.1
Total cost				
Total network cost (10^3 $ per day)	184.6	643.0	995.3	1333.7
Cost per kg H_2 ($)	***23.4***	***10.8***	***7.2***	***6.7***
Production facilities (10^3 t CO_2-equiv per day)	11.3	81.3	172.0	231.9
Storage facilities (10^3 t CO_2-equiv per day)	5.6	41.8	97.7	139.5
Transportation modes (10^3 t CO_2-equiv per day)	0	0.1	1.3	3.1
Total GWP (10^3 t CO_2-equiv per day)	16.9	123.2	271.0	374.4
Kg CO_2-equiv per kg H_2	***2.1***	***2.1***	***2.0***	***1.9***
Production facilities risk	6	12	17	25
Storage facilities risk	29	73	95	105
Transportation modes risk	0	7	13	24
Total Risk (Units-level)	***35***	***92***	***125***	***154***

Table 5.9 Comparison of results among mono-objective cases and multi-objective results through Ɛ-constraint methodology

		Mono-objective			Multi-objective			
Solution strategy		Case A: Pay-off table obtained by mono-objective optimisation (multi-period)			Case B1, ε-constraint + TOPSIS (multi-period)	Difference between B1 and A1	Difference between B1 and A2	Difference between B1 and A3
Year	Case	A1	A2	A3	All criteria			
2020	Cost per kg H_2 ($)	**16.2**	24.5	17.5	23.4	44%	-4%	34%
	Kg CO_2 per Kg H_2	6.9	**2.1**	8.8	2.1	-70%	0%	-76%
	Total Risk (Units)	35	42	**35**	35	1%	-17%	1%
2030	Cost per kg H_2 ($)	**8.4**	14	11.4	10.8	29%	-23%	-5%
	Kg CO_2 per Kg H_2	10.6	**2.1**	9.6	2.1	-80%	0%	-78%
	Total Risk (Units)	113	98	**89**	92	-19%	-6%	4%
2040	Cost per kg H_2 ($)	**3.9**	7.8	5.7	7.2	80%	-8%	26%
	Kg CO_2 per Kg H_2	10.8	**2.0**	8.6	2	-81%	0%	-77%
	Total Risk (Units)	187	125	**107**	125	-33%	0%	17%
2050	Cost per kg H_2 ($)	**3.7**	9.2	5.6	6.7	81%	-27%	20%
	Kg CO_2 per Kg H_2	10.9	**1.9**	8.5	1.9	-83%	0%	-78%
	Total Risk (Units)	263	141	**112**	152	-42%	8%	36%

It must be highlighted that similar trends are observed for GWP between cases A2 and B1 but a benefice in cost resulted in B1 being hydrogen cheaper in 2030 (23%) and 2050 (27%). The use of

renewable energy has a ratio of 92% in 2020, wind power is the predominant energy source followed by hydropower. Nuclear energy starts with a rate of 8% in 2020 but decreases to 3% by 2050. A moderate risk can be observed due to the lack of transportation.

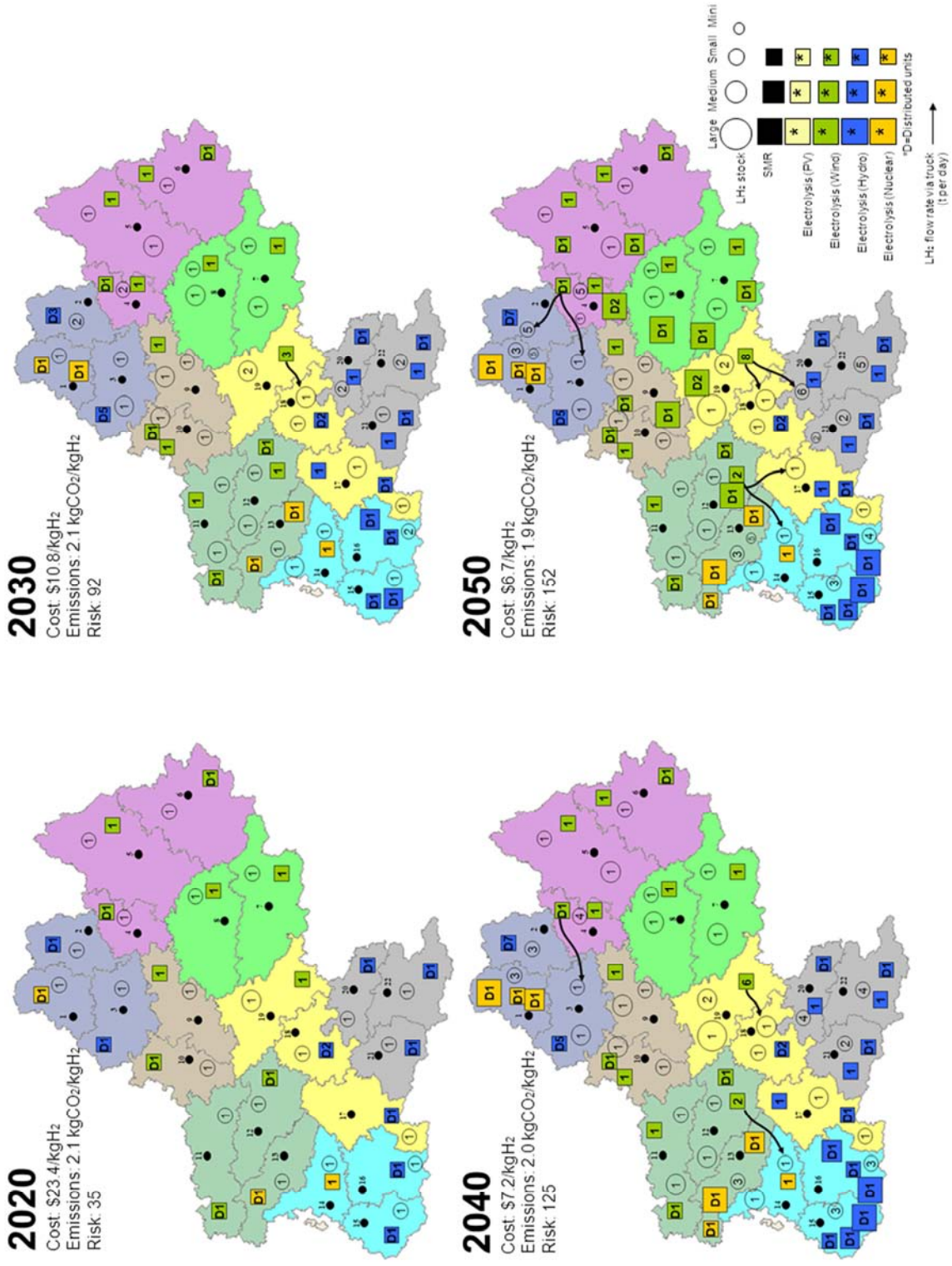


Figure 5.14 Network structure of liquid hydrogen distributed via tanker trucks. Case B1: Multi-objective optimisation through Epsilon constraint in a low demand scenario in the Midi-Pyrénées region.

The main problem that can be found in this approach is that the integration of the four time periods leads to a high cost value in 2020 that may be viewed as prohibitive and thus may hinder the development of hydrogen deployment in the region. For this reason, another strategy was adopted assessing the whole problem as a mono-period problem in order to find if more competitive results can be reached.

5.8 Multi-objective optimisation through lexicographic and Ɛ-constraint methods (case B2)

An alternative to solve the multi-objective problem involves the lexicographic optimisation to build the pay-off table (see Table 5.10) of only non-dominated solutions minimising one objective function but also to find the best values for the two other criteria.

We tried to apply the lexicographic optimisation for the multi-period problem but the large problem size involving especially a high number of binary variables was computationally prohibitive and no feasible solution was obtained after 48 hours with GAMS version 23.9. Then, we changed the multi-period approach for the mono-period one.

Table 5.10 Pay-off table obtained by the lexicographic optimisation

	2020			2030			2040			2050		
Minimise	TDC	GWP	RISK	TDC	GWP	RISK	TDC	GWP	RISK	TDC	GWP	RISK
Cost per kg H_2 ($)	13.4	15.6	14.7	7.8	10.1	8.4	5.7	9.1	8.4	5.0	8.0	6.7
Kg CO_2-equiv per kg H_2	5.1	**2.1**	**5.6**	8.7	**2.1**	**9.5**	**9.4**	**2.0**	6.5	**9.1**	**2.0**	5.8
Total Risk (Units-level)	**42**	34	**34**	**117**	92	**91**	**258**	177	**167**	**372**	259	**246**

In the lexicographic optimisation, the first time period (2020) was treated for the three objective functions. The pay-off table was built and Ɛ-constraint method was applied with 3 risk levels and 10 GWP points (see intervals in Figure 5.15). The Pareto fronts are proposed in Figure 5.15 for the 2020-2050 periods. The TOPSIS analysis was then carried out and the top option selected (see Appendix B.3.2). The decision variables are inserted as the initial number of production/storage facilities of type *s* and size *j* storing product form *i* in grid *g* in period *t*. Then, it is possible to optimise the next period time and so on until 2050.

Table 5.10 displays that the cost of \$13.9 per kg H_2 in 2020 in the lexicographic optimisation is lower than the value obtained from mono-objective and B1 optimisation approaches. A significant cost reduction is obtained for B2 compared to B1, i.e., 41% (see Table 5.12): this is the main advantage of the case B2 because this cost reduction in the introduction phase of the H_2 fuel can be viewed as a limiting factor.

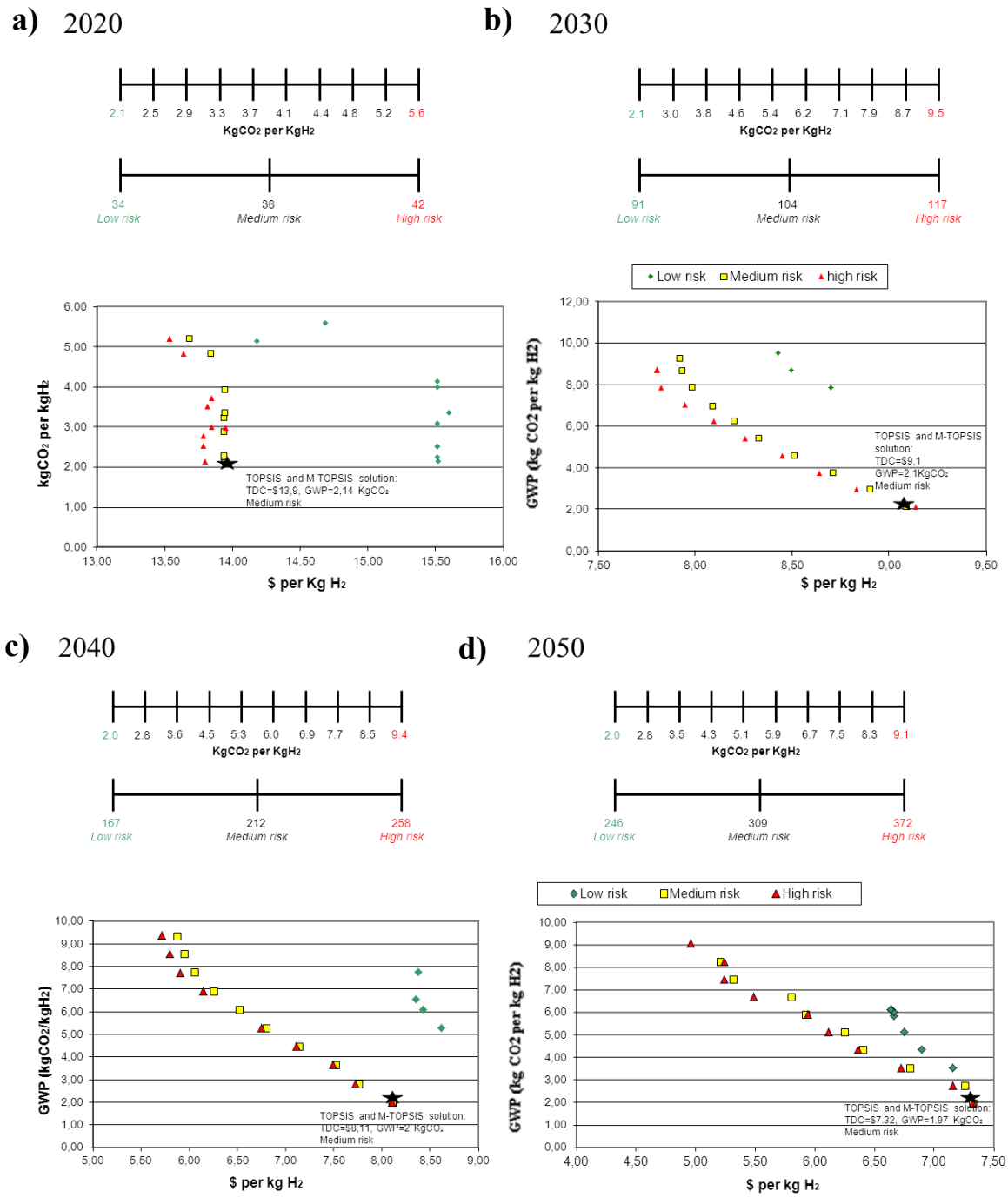


Figure 5.15 Pareto solutions for the multi-objective model for the case B2

The cost is gradually reduced in the case of the lexicographic optimisation and in 2050 exhibit a similar value to case B2 but it is twice the cost of the TDC minimisation in the same year. The list of the decision variables is presented in Table 5.11 and the network structure of liquid hydrogen distributed via tanker trucks for this case B2 in Figure 5.16. Electrolysis is the production technology, in 2050, 82% of H_2 is produced from wind, 15% from hydro and 3% from nuclear power. In the same year, 12% of the total demand is exported (district 18 is the main importer).

Table 5.11 Multi-objective optimisation results of the hydrogen supply chain (case B2)

Year	2020	2030	2040	2050
Demand (kg per day)	7898	59430	138790	198170
Number of production facilities	24	59	89	120
Number of storage facilities	44	90	159	213
Number of transport units	-	-	2	3
Capital cost				
Plants and storage facilities 10^3 $)	*235231.9*	*632143.9*	*963670.4*	*671306.4*
Transportation modes (10^3 $)	*0*	*0*	*100*	*1500*
Operating cost				
Plants and storage facilities (10^3 $ per day)	56.2	395.1	896.3	1282
Transportation modes (10^3 $ per day)	0	0	0.5	0.9
Total operating cost (10^3 $ per day)	56.2	395.1	896.8	1282.9
Total cost				
Total network cost (10^3 $ per day)	110.1	540.1	1125.7	1450.8
Cost per kg H_2 ($)	***13.9***	***9.1***	***8.1***	***7.3***
Production facilities (10^3 t CO_2-equiv per day)	11.3	85.2	179.1	249.8
Storage facilities (10^3 t CO_2-equiv per day)	5.6	41.8	97.7	139.5
Transportation modes (10^3 t CO_2-equiv per day)	0	0	0.9	1.6
Total GWP (10^3 t CO_2-equiv per day)	16.9	127	277.6	390.9
Kg CO_2-equiv per Kg H_2	***2.1***	***2.1***	***2.0***	***2.0***
Production facilities risk	6	16	29	40
Storage facilities risk	32	86	167	223
Transportation modes risk	0	0	10	13
Total Risk (Units-level)	***38***	***102***	***206***	***277***

Similar values for GWP are found for CO_2 minimisation and for cases B1 and B2, this represents a benefit in cost compared to cases A. Higher values for the relative risk index are obtained in the approach B2 because more production and storage units are established; the functions of relative risk are directly related to the number of these units. The partial vision regarding the demand only for one period promotes the design of small units only to be used in the defined time period instead of designing larger production plants to cover demand increments.

Yet, the flexibility of this method is that each period can be analysed in detail and that some parameters can be changed to reflect the preferences of the decision maker. Finally, the necessity to run each optimisation separately and to capture the decision variables (NP, NS and NTU) to optimise the next period could represent a risk in data capture and processing.

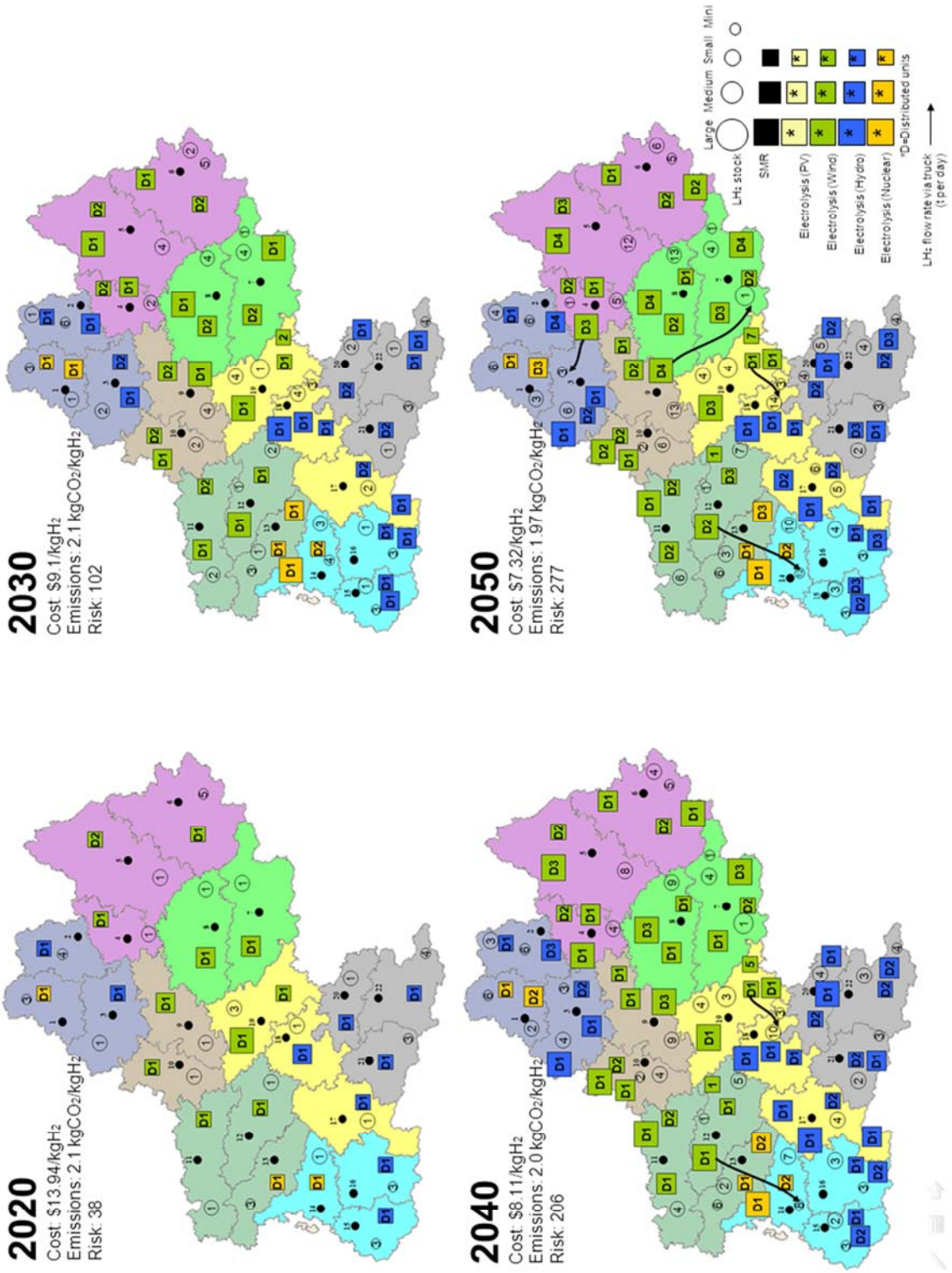


Figure 5.16 Network structure of liquid hydrogen distributed via tanker trucks. Case B2: Multi-objective optimisation through Lexicographic+ Ɛ-constraint in a low demand scenario in the Midi-Pyrénées region.

5.9 Results comparison

The best option for the 2020 period is given by the case B2 which exhibits very good results for all criteria. Yet a cost of \$13.9 per kg H_2 may still be viewed as prohibitive. In 2050, three scenarios are under the maximal target of the HyWays roadmap concerning cost: the cost and risk minimisation cases and the multi-objective approach B1, however case B2 is very close to the limit (see Figure 5.17).

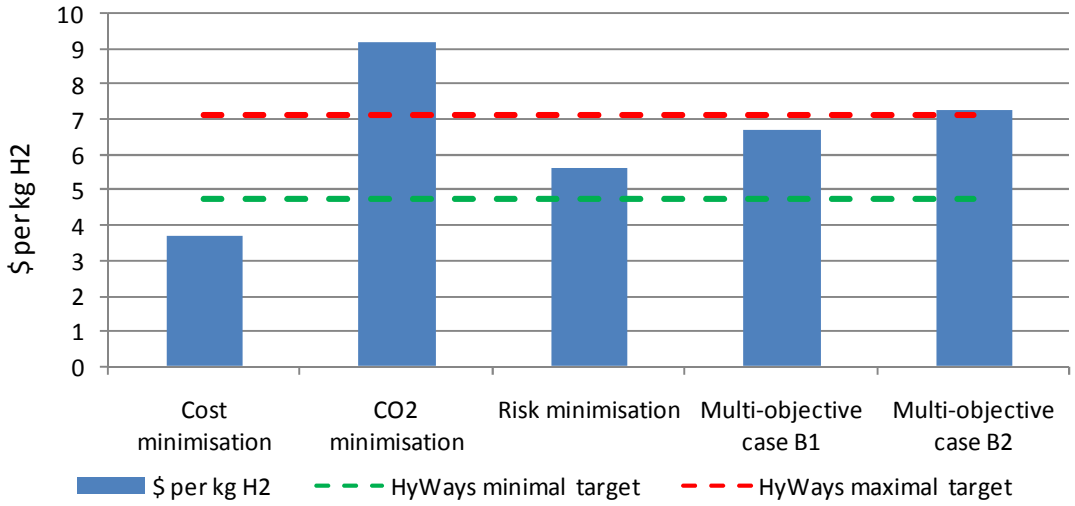


Figure 5.17 Cost per case in 2050 ($ per kg H_2).

The results show that considering all the time periods, hydrogen remains expensive compared to the targets. A different geographic division could be treated in order to study other possibilities. Moreover, the potential in RES promotes its use in the region. M-TOPSIS ranking leads to a significant decrease in CO_2 emission, for example, the gain is of a factor 5 on CO_2 in 2050 with a cost of \$7.3 per kg H_2 with respect to the cheapest option (around \$5 per kg H_2), (see Figure 5.15d)). Let us remember in this context that the French government adopted a Climate Plan to divide by 4-5 the French GHG emissions by 2050.

In Figure 5.18, the emissions related to HSC are compared to those of gasoline and diesel fuels. Only well-to-tank emissions need to be considered for FCEV. The average emissions of vehicles in France from gasoline and diesel cars are taken from (ADEME, 2010). The hydrogen would fulfil with the planned EU regulation being under 113 g CO_2 per km but an important contribution would result from the configuration from the GWP minimisation as well as the multi-objective cases B1 and B2 with emissions of 19 g CO_2 per km for H_2 fuel against 220 g CO_2 per km for the diesel cycle, implying a reduction of 91%. For the case of cost minimisation, emissions are under the target: let us remember that the CCS has not being considered in the input configuration and this could constitute an option to be explored to reduce the environmental impact.

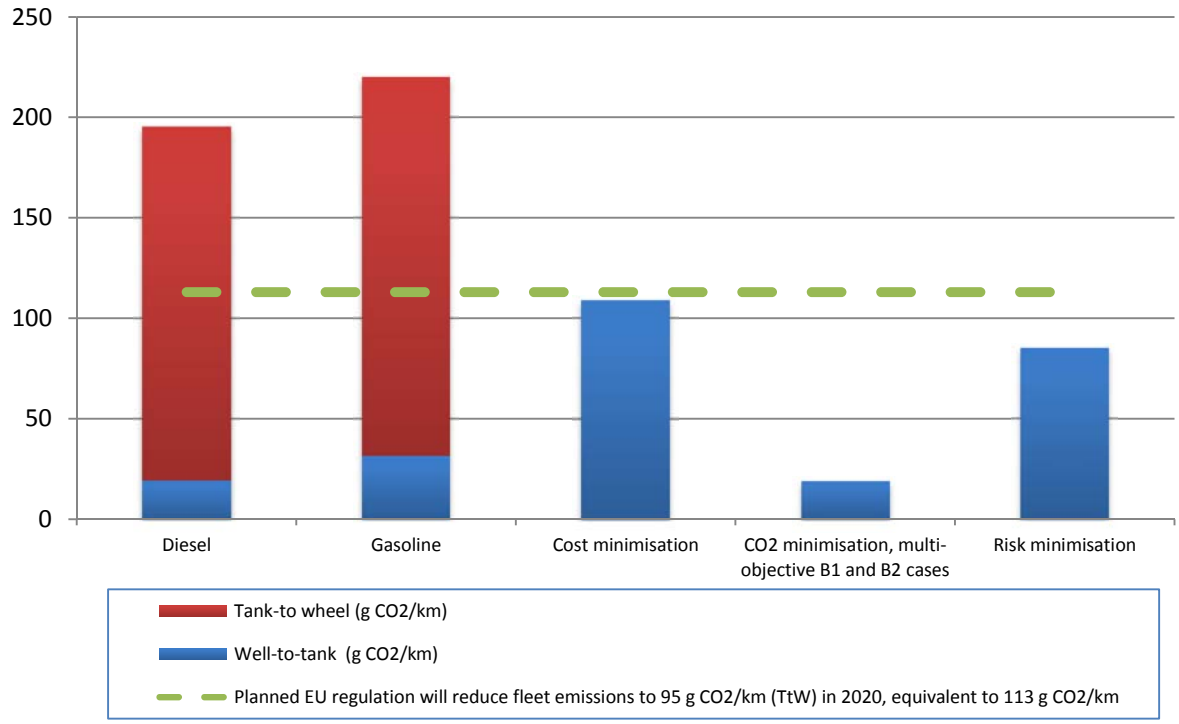


Figure 5.18 Comparison of emissions by sector in 2050 (Data from gasoline and diesel: (ADEME, 2010))

In Table 5.12 all results between mono- and multi-objective cases are listed. The bold characters in table are relative to the value of the optimised criterion for the mono-objective optimisation and in the case of the lexicographic optimisation are related to the first optimised objective (higher priority).

Table 5.12 Comparison of results among mono-objective cases and multi-objective results for approaches B1 and B2

	Solution strategy	**Case A**: Pay-off table obtained by mono-objective optimisation. (multi-period)			**Case B1.** All criteria (multi-period)	**Case B2**. Pay-off table obtained by the lexicographic optimisation (mono-period)			**Case B2.** (mono-period)	Difference between B2 and B1
2020	Cost per kg H_2 ($)	**16.2**	24.5	17.5	23.4	**13.4**	15.6	14.7	13.9	-41%
	Kg CO_2 per Kg H_2	6.9	**2.1**	8.8	2.1	5.1	**2.1**	5.6	2.1	0%
	Total Risk (Units)	35	42	**35**	35	42	35	**35**	37.5	7%
2030	Cost per kg H_2 ($)	**8.4**	14.0	11.4	10.8	**7.9**	9.6	8.1	9.1	-16%
	Kg CO_2 per Kg H_2	10.6	**2.1**	9.6	2.1	8.9	**2.1**	9.7	2.1	0%
	Total Risk (Units)	113	98	**89**	93	123	84	**83**	102	11%
2040	Cost per kg H_2 ($)	**4.0**	7.8	5.7	7.2	**5.2**	8.3	6.9	8.1	13%
	Kg CO_2 per Kg H_2	10.8	**2.0**	8.6	2	10.1	**2.0**	8.5	2	0%
	Total Risk (Units)	187	125	**107**	125	283	133	**117**	206	65%
2050	Cost per kg H_2 ($)	**3.7**	9.2	5.6	6.7	**4.3**	7.6	5.8	7.3	9%
	Kg CO_2 per Kg H_2	10.9	**1.9**	8.5	1.9	10.3	**2.0**	8.5	1.9	4%
	Total Risk (Units)	263	141	**112**	152	360	163	**146**	277	82%

If cases B1 and B2 are now compared, option B2 is better in 2020 and 2030 with a cost reduction of 41% and 16% respectively, while no variation in CO_2 is observed but the associated risk increases due to the presence of more production and storage units that are installed in the region. The highest impact for the risk lies in 2040 and 2050.

In Figure 5.19a, the discrepancies are more marked in 2020 and 2030 with costs ranging from \$13 per kg H_2 to more than \$23 per kg H_2. By 2050, the cost lies between \$3.7-9.2 per kg H_2. Figure 5.19 b shows that multi-objective optimisation (both cases: B1 and B2) presents similar results than the case A2 (CO_2 minimisation). Finally, 5.19c attributes the high level of risk to transportation.

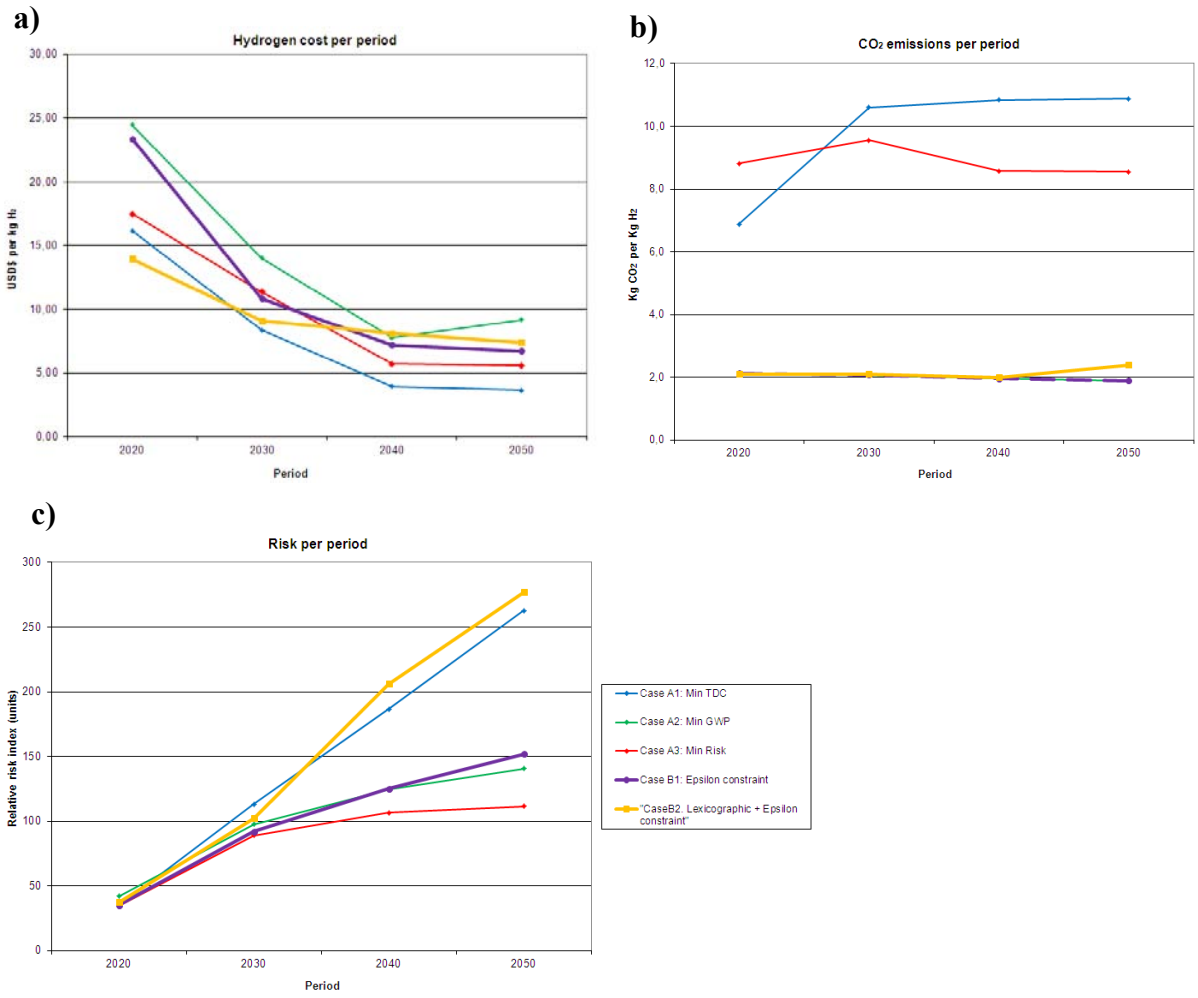


Figure 5.19 Results comparison between mono-objective cases and multi-objective results for approaches B1 and B2.

The multi-objective problem dimension treated in the case B1 was compared with the case B2 considered in our work (see Table 5.13). The criterion of computational time is not sufficient to select a method: the computational effort is also required for the creation of the pay-off tables. For the case B1, three mono-objective optimisation needed around 13 hours (mainly due to the TDC minimisation), then the Ɛ-constraint method with five epsilons for the GWP and five for the risk took around 3 hours for calculation. The Pareto front and TOPSIS analysis finally took around 1 hour. Globally, we needed

around 18 hours for obtaining results in case B1. For the case B2, three optimisations for each criterion to create the pay-off table through lexicographic optimisation were executed (36 calculations). The application of the Ɛ-constraint method took several hours to solve the four mono-period problems. Globally, around 3 days are necessary for obtaining results in case B2.

Table 5.13 Statistics for multi-objective approaches (Mono- and multi-period).

Case	B1	B2
Number of constraints	205057	50564
Number of continuous variables	31255	7816
Number of integer variables	11088	2772
Computational time (hour)	18	72

Figures 5.9-11, 5.14, and 5.16 show the HSC configurations in an approximated way locating the NP, NS and flow rate via tanker truck in the corresponding grid but not in the precise place. If a more detailed study would be needed, a spatial-based approach could be used and with this tool, a more realistic snapshot can be built. In addition, new constraints concerning the geographic features might help the decision making. This issue will be treated in the next section where the maps are confronted with those constructed with ArcGIS® that contains all the geographic and demographic data of the region. To illustrate the use of the geographic information system, the case B2 has been chosen because of the low environmental impact, the more competitive cost in 2020 and de decentralisation degree.

5.10 Spatial-based approach of the HSC in the Midi-Pyrénées region, France

The aim of this section is to use a Geographic Information System (GIS) as a new tool for multi-criteria decision making after the optimisation step. The ArcGIS® software (developed by ESRI, Environmental Systems Research Institute) is a GIS used to organise, analyse and map spatial data. A typical GIS project contains an extensive database of geographic information, graphical capabilities of displaying maps with overlays pertaining to the company's supply chain activities (Shapiro, 2001). Literature review shown in chapter 3 reveals that few researchers have used the spatial dimensions to build the infrastructure of HSC. Some examples of geographic approaches include the studies (Ball et al., 2006; Dagdougui, 2011a; Johnson et al., 2008).

It must be highlighted that by contrast to the mathematical optimisation approaches, a spatial or GIS-based study cannot be considered as a general methodology for the design of the optimal HSC. In order to analyse some optimised configurations, the spatial-based approach is applied to represent the network structure in the Midi-Pyrénées region resulted from the case B2 and previously displayed in Figure 5.16. In this figure, refuelling stations are not considered and renewable sources are not connected to their production facility. Before optimisation, the distances between each district were defined with Mappy® by considering all types of routes. However, it must be highlighted that for

heavy transportation (e.g. tanker truck), only highways must be taken into account. The post-optimisation step by ArcGIS® allows analysing the feasible and the best solutions considering geographic criteria. All these geographic constraints motivate the utilization of a specific tool as ArcGIS®.

5.10.1 Spatial analysis with ArcGIS®

The main question to be answered is: where is the best place for new hydrogen production plants and storage units? Then, some layers of data are needed. The first step is to map the energy source units (Salingue, 2012) the main roads (IGN) and the refuelling stations according to the databases. The region remains divided into 22 districts. The spatial analysis leads to localize very precisely the different components of the HSC. The refuelling stations and renewable energy production sites are positioned with the GPS coordinates of the main existing stations of each district. Only main roads are represented so that the transportation by heavy truck is allowed. The projection Lambert93 is the official projection for maps in metropolitan France since December 2000; it is related to RGF93 datum. This is the projection used to geo-reference all our layers in this work (De-Léon Almaraz et al., 2014) .

5.10.2 Midi-Pyrénées snapshot HSC with ArcGIS®

Resulted snapshot is presented in Figures 5.20 and 5.21. Renewable energy sites were located by importing the GPS coordinates (Salingue, 2012) for each point which represents one photovoltaic plant, one wind farm or one hydroelectric power plant. The Golfech nuclear power plant was also located. The road network connects all the districts of the region, but the distances between the districts could vary from this approach where only motorways are considered and the distances obtained by Mappy where mainly roads for particular vehicles are displayed.

The new production facilities are placed near the energy source and in the case of exporters, the production unit should be placed next to the main roads. For electrolysis plants using renewable energy, the facility must be close to the energy source and to the main road. For electrolysis plant using nuclear energy, the main constraint is related to the refuelling station to assure the on-site production. Storage centers (small, medium and large) are near to production plants, to the main road and refuelling stations.

Refuelling stations close to the motorways and national roads and/or in a city are shown. The coordinates of current refuelling station are presented by (Esso, 2013) and (Total, 2013). For the Midi-Pyrénées case, at least 1 station is considered per district. This analysis tool reveals the need to consider real field constraints in the implementation of the optimal solution.

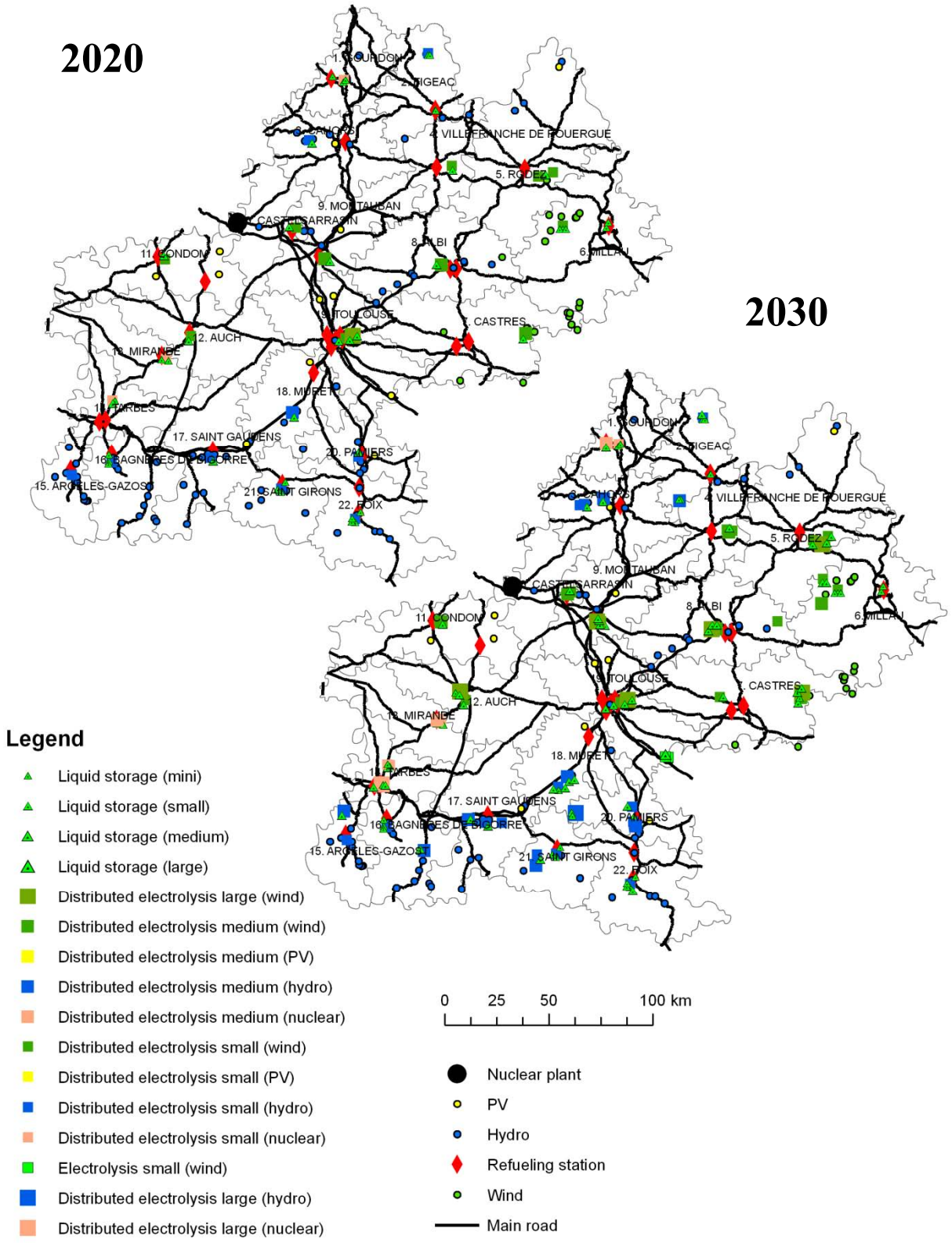


Figure 5.20 Detailed map of the HSC in Midi-Pyrénées region in 2020 and 2030 after the spatial analysis.

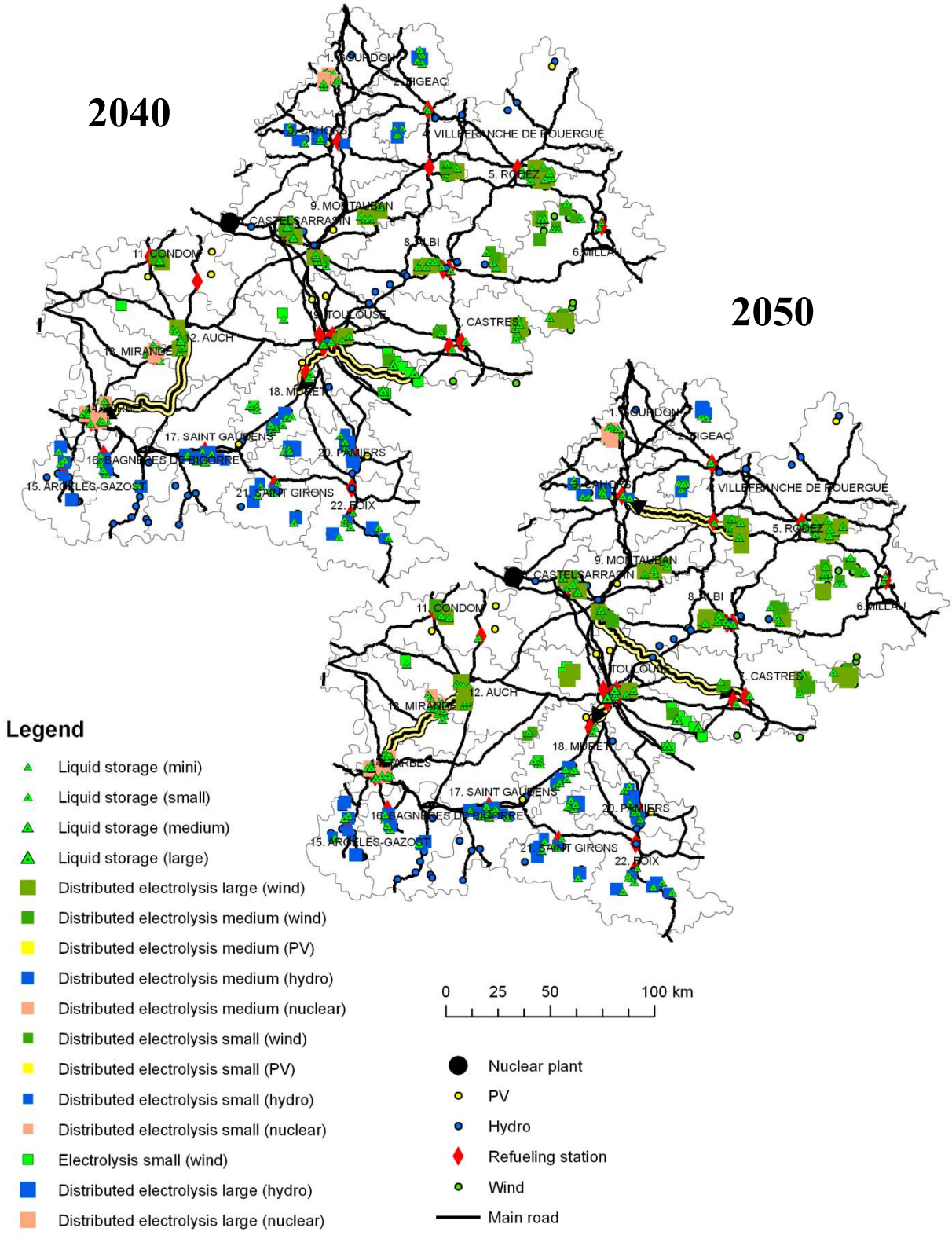


Figure 5.21 Detailed map of the HSC in Midi-Pyrénées region in 2040 and 2050 after the spatial analysis.

5.11 Conclusions

In this chapter, the HSC was designed for the Midi-Pyrénées region through the "Green H_2 fuel" project to evaluate the potential of H_2 to be used in FCEV in the time horizon from 2020 to 2050. The mathematical model presented in Chapter 4 was adapted to the region and considered for energy sources and refuelling stations. Two approaches were taken into account involving mono- and multi-objective optimisation. For the latter one, case B1 (ε-constraint method in a multi-period problem) and case B2 (lexicographic+ ε-constraint method in four mono-period problems) were compared when three objectives (cost, CO_2 and risk) were optimised.

In the mono-period phase, a centralised production network supplied by tanker trucks was obtained for TDC minimisation, producing H_2 from natural gas via SMR with a significant environmental impact. From the given data it was observed that if all the RES would be available to produce H_2, 89% of them would be necessary in 2050 to cover H_2 fuel demand. This could represent an electric demand affectation, then some previsions should be taken and the political strategy would require more RES investment or the use of other type of energy to cover the electrical grid need. This topic was also treated in the National Debate of the Energetic Transition. For GWP and risk optimisations, decentralised configurations resulted. In the first one, the use of RES had a good impact in the environmental criterion but cost is very high. In the case of risk, that lack of transportation decreases the risk, but the use of fossil sources has a high environmental impact.

For case B1, cost in the first time period is prohibitive. One of the main problems found in this approach is that the integration of the four time periods does not allow treating a specific time period. A better option for the 2020 period is given by the case B2 having good results for GWP and risk but the cost is still high ($13.9 per kg H_2). In case B2, the TOPSIS chose seems to give preference to the GWP criterion but results are logical because of the reduction of CO_2 emission (the gain is of a factor 5 on CO_2) with a low impact in the cost. It can be concluded that the risk is affected mainly to transportation.

A spatial-based approach was used to have a more realistic snapshot. ArcGIS® allowed the integration of geographic and demographic data of the region: the results show that the production centers (small, medium and large) and the refuelling stations are near as possible from the main road. This post-optimisation step allows analysing the feasible and the best solutions considering geographic criteria. One interesting perspective could be to optimise again the solution obtained with ArcGIS® by considering the real distances between each plant in order to evaluate a more realistic value of the optimal cost of the H_2. Another perspective is to evaluate different region/district sizes to know if more competitive cost could be reached. These two perspectives will be treated in the next chapter.

Chapter 6

EXTENDING THE FRONTIERS: DESIGN OF A HYDROGEN SUPPLY CHAIN IN FRANCE

Résumé

Dans ce chapitre, l'optimisation de la chaîne d'approvisionnement « hydrogène » est appliquée au cas de la France. L'objectif est double : d'une part, tester la robustesse de la méthode à une échelle géographique différente et, d'autre part, examiner si les résultats obtenus au niveau régional sont cohérents avec ceux de l'échelle nationale. Une nouvelle phase de collecte de données est effectuée et des scénarios de prédiction de la demande adaptés au cas de la France sont utilisés en se basant sur l'analyse des feuilles de route. Le même modèle que celui appliqué à la région Midi-Pyrénées est utilisé avec des différences mineures qui sont exposées. Dans cette étude de cas, l'outil spatial ArcGIS® est utilisé avant optimisation pour identifier les éléments géographiques. Dans un premier temps, la stratégie d'optimisation mono-objectif pour les trois critères indépendants (coût, empreinte environnementale et risque) est menée (cas A). Dans un deuxième temps, l'approche multicritère (cas B1, voir chapitre 5) mettant en œuvre la méthode ε-contrainte est analysée et discutée. Enfin, un nouveau scénario prenant en compte un cycle économique (cas B2) est traité. Ce chapitre se termine par une brève comparaison entre les résultats obtenus avec les trois approches.

Abstract

In this chapter, the optimisation of the hydrogen supply chain is applied to the case of France. The objective is twofold: first, to test the robustness of the method at a different geographic scale and, second, to examine whether the results at regional level are consistent with those at national scale. A new phase of data collection and demand scenarios are performed to be adapted to the French case based on the analysis of roadmaps. The same model applied to the Midi-Pyrénées region was used here with minor differences. In this case study, the Arc-GIS® spatial tool was used to consider the geographic constraints before optimisation. Then, three case studies are analysed. First, the mono-objective optimisation for three criteria is presented (case A). Then, the multi-optimisation approach (as presented in case B1 in chapter 5) by ε-constraint method is analysed and discussed. Finally, a new scenario which considers the decision-maker preferences is described following the economic cycle of case B2. This chapter ends with a brief comparison between the results of these three approaches.

Abbreviations

CH_2	Compressed hydrogen
FCEV	Fuel cell electric vehicle
GB	Great Britain
GHG	Greenhouse gas
GWP	Global warming potential
HSC	Hydrogen supply chain
LH_2	Liquid hydrogen
MILP	Mixed Integer Linear Programming
NSU	Number of storage units
NTU	Number of transportation units
SMR	Steam methane reforming

6.1 Introduction and context

One of the main questions arising from the Midi-Pyrénées case is whether or not the geographic segmentation that was adopted, i.e., the regional scale is consistent to ensure a competitive cost. From an economic viewpoint, an average cost of hydrogen of US$ 4.74 per kg H_2 (3.6 €/kg) could be considered as acceptable by 2050 if not subject to excessive taxes (Patay, 2008), which exhibits a similar order of magnitude to the value reported in HyWays roadmap (European Commission, 2008).

Even if in some countries such as the United States, California has noticeably taken a key role as a pilot state, the future of the hydrogen supply chain (HSC) obviously depends on the interconnection between big cities and countries. Intercontinental analysis seems here premature but a national study similar to that treated in Chapter 4 for Great Britain (GB) can be considered with real constraints and data. As reported in the H_2 Mobility roadmap, Germany and GB have already introduced the use of fuel cell electric vehicle (FCEV) (Williamson, 2010) while H_2 mobility initiatives have now started in France, in 2013. A new geographic scale is thus considered in this chapter in order to study the feasibility of large-scale hydrogen production in France.

France is the largest country in Western Europe and the European Union, and the third-largest in Europe as a whole with a total population of around 65.5 million (Insee, 2010). Transportation is a major contributor to greenhouse gas (GHG) emissions in France. In 2009, the final energy consumption due to transportation was 49.8 Mtoe and the associated GHG emissions resulted in 132 Mt CO_2-equiv. In general terms, the total emissions in France decreased (mainly due to electricity mix based on very low carbon emission technologies as nuclear and hydropower) between 1990 and 2009 but those associated to the transport sector increased in the same period (*Direction générale de la compétitivité, de l'industrie et des services,* 2011).

The French government adopted a Climate Plan ("*Plan climat"*) in 2004 presenting a strategy for technological research to divide by 4-5 the French GHG emissions by 2050. The Factor 4 target then requires a 75% reduction in GHG emissions by 2050 compared to current levels. Hydrogen is considered as a potential fuel in France to decrease pollution but also to fall the fossil fuel dependency.

If H_2 is able to gain an important market share, its availability must be guaranteed at an intercontinental supply chain. France has a strategic location because Spain, Andorra, Italy, Switzerland, Germany, Luxemburg and Belgium are all neighbouring countries. French hydrogen production was of 7 billion Nm^3 in 2007 and there are 10 production sites already installed throughout the territory (PHyRENEES, 2009). The most of hydrogen is produced onsite for captive uses for the chemical industry by steam methane reforming (SMR). Besides, a significant portion of H_2 is produced today as a by-product in the chemical industry (e.g. chloralkali electrolysis) but, since there is no specific purpose, this is sometimes wasted, flared or treated by gas industries. France has the second

ranking place in chlorine production just after Germany; the main producers are Arkema, Solvay and Chloralp.

Recently, regional, national and international, private and public stakeholders were brought together by the French Association for Hydrogen and Fuel Cells ("AFHyPaC") and supported by the Ministry of Ecology, Sustainable Development and Energy, to share their knowledge and expertise in order to develop coordinated deployment scenarios for hydrogen vehicles and refuelling stations, and to identify the strengths and costs of this transition. The results of the report are currently unavailable.

Several regions aim at developing hydrogen energy roadmaps for electromobility: some examples are Midi Pyrénées (PHyRENEES and Midi-Pyrénées Innovation), Nord-Pas-de Calais (Roadmap 2014-2020), Lorraine (Nancy project and Livre blanc Alphea), Pays de Loire (Navy-bus project), Bretagne, Provence-Alpes-Côte d'Azur, Franche-Comté, Rhône Alpes, Corse (Myrthe project), Nord Pas de Calais and Haute-Normandie (AFHYPAC et al., 2013). In this chapter, an overall approach integrating all the French regions has been considered.

The remainder of this chapter is organised as follows: section 6.2 is devoted to the methodology aspects and formulation of the HSC problem followed in this work. The objectives are presented and the solution strategy is briefly explained including the Arc-GIS approach. The definition of the case study is presented in section 6.3 with explanation of new parameters such as: demand, energy sources, initial production plants and storage units, refuelling stations and roads. The results of the mono- and multi-objective optimisations are analysed and discussed in section 6.4 following for the multi-objective problem to solving strategies: B1 (Ɛ-constraint in multi-period approach) and B2 (economic cycle in mono-period approach). This chapter ends with conclusions and perspectives.

6.2 Methodology and formulation of the HSC problem

In this chapter, the guidelines of the methodology proposed in Chapters 4 and 5 are used. For brevity, only the problem statement, assumptions and objectives that were adopted are presented. The considered items of the HSC are mentioned to establish the general structure of the network. Finally, the solution strategy phase is also developed.

6.2.1 Problem definition

The optimisation approach for HSC design proposed in chapter 5 has been adapted to the case study France in order to address the following questions:

- what is the best option for production and storage of hydrogen in France?
- what are the main product flow rate and transportation modes to supply the hydrogen demand?
- is it possible to find competitive targets for a national case compared to a regional study?

6.2.2 Objective

This work is focused on the design of a five-echelon HSC (energy, source, production, storage, transportation and fuelling station), taken into account cost, environmental impact and risk consideration. The model that was previously developed in chapter 5 is adapted to French case studies and results for mono-objective optimisations are compared with the multi-objective solution.

6.2.3 Given data

Several data sets are necessary to design the HSC including demand volume, availability of energy sources, initial number of production plants and storage facilities, techno-economic, environmental and risk data of the components in the HSC. A group of students of the Eco-energy Master NTE in the ENSIACET University carried out data collection and analysis during an internship from February to May 2013. The set of parameters is presented in Appendix B.1 and C.2.

6.2.4 Design decisions

Design decisions are based on the number, type, capacity, and location of production and storage facilities. More precisely, they involve the number and type of transport units required as well as the flow rate of hydrogen between locations as well as the number of refuelling station. Cities or regions are also considered.

6.2.5 Operational decisions

Operational decisions concern the total production rate of hydrogen in each region, the total average inventory in each region, the demand covered by imported hydrogen and the H_2 demand covered by local production.

6.2.6 Assumptions

- a deterministic demand of hydrogen for the transportation system (particular-light cars and buses) is considered;
- the computed risk associated with production plant, storage facilities and transportation modes are assumed to be independent of the considered demand scenario.
- the model is assumed to be demand driven.

6.2.7 General structure of the HSC

In this formulation, hydrogen can be delivered in specific physical form *i*, such as liquid, produced in a plant type with different production technologies *p* (i.e. SMR, gasification and electrolysis); using energy source e (i.e. natural gas, biomass, nuclear, solar, wind and hydro powers) distributed by a specific type of transportation modes *l* (tanker truck) going from the location *g* to *g'* referred as

regions; such that *g'* is different than *g*; for storage facility type *s*, different storage sizes *j* (mini, small, medium and large) are involved (see Figure 6.1). Once more, the administrative segmentation has been taken into account, so that the granularity level that is considered is the regional one (the 21 French regions are involved).

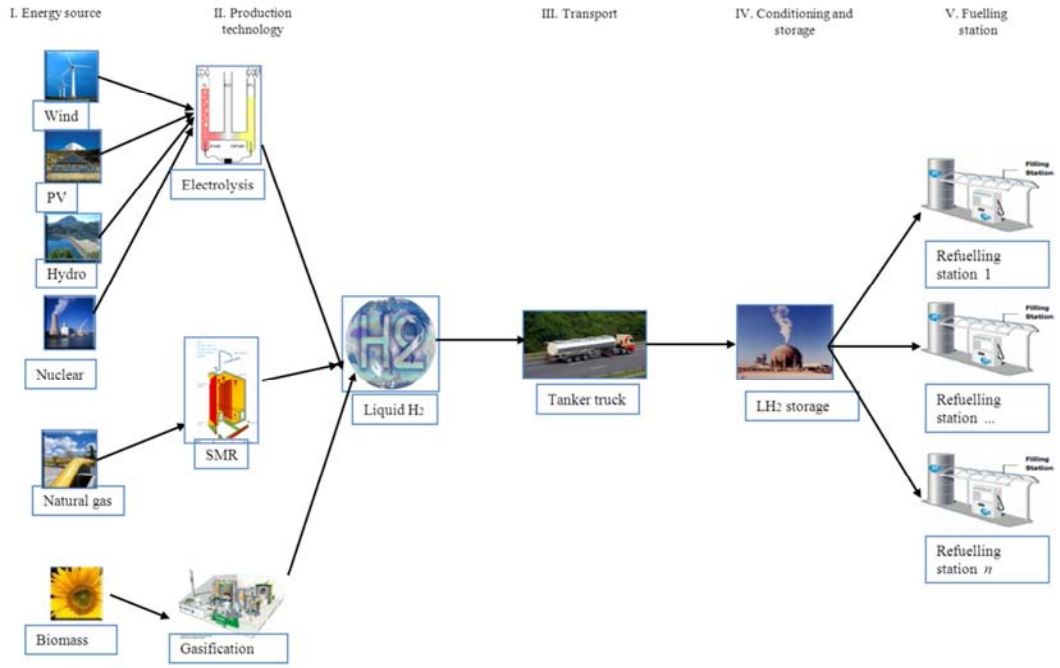


Figure 6.1 The HSC studied for France

6.2.8 *Mathematical model*

The model presented in Chapter 5 is used here for the national case study. As previously, the problem is then captured in a mixed-integer linear programming (MILP) framework. All continuous and integer variables must be non-negative. No major changes are required. It must be mentioned that new electrolysis plants that use renewable energy are allowed to be implemented when renewable energy *e* is available in the region *g*. Then, as for Midi-Pyrénées, the exportation of renewable energy between regions *g* to *g'* is not considered for France. These two items are introduced as constraints in the problem formulation.

6.2.9 *Optimisation solution strategy*

The problem is treated by three different approaches using the mathematical model developed in this work and formulated within the GAMS version 24 (Brooke et al., 1988) and solved using CPLEX. The solution strategy is similar to that presented in Figure 5.8 in Chapter 5 (section 5.5). It yet embeds some minor changes in the case B2 due to the typical features of the French case study.

6.2.9.1 *Case A. Mono-objective approach*

Case A corresponds to the mono-objective optimisation. Each objective function is optimised separately in a multi-period treatment corresponding to the optimisation cases A1 (cost), A2 (GWP)

and A3 (risk). The multi-period problem is addressed. Case B is related to multi-objective optimisation. Two sub-cases are studied here.

6.2.9.2 Case B.1. Multi-objective optimisation through ε–constraint method

Case B1 refers the treatment of a multi-period problem through ε–constraint method as previously explained in chapter 5 (section 5.5.2). Once the Pareto front is built, the TOPSIS method is applied. The model dimension for B1 involves 175,667 constraints and 31,943 variables (among them, 11,088 are integer).

6.2.9.3 Case B2. Multi-objective optimisation through lexicographic+ Ɛ-constraint methods.

For case B2, the HSC is evaluated following an economic cycle logic for decision making instead of applying an M-TOPSIS analysis. For this purpose, four mono-period problems are considered:

- in 2020, a lexicographic optimisation prioritising cost is carried out. The resulting configuration is then integrated for the following periods.
- in 2030, a lexicographic optimisation prioritising GWP is carried out.
- in 2040 and 2050, the cost and GWP are respectively optimised.
-

The risk is not considered here assuming that the decision maker has not preference for this criterion. The robustness of the model is studied using different input configurations in each time period considering the decision maker preferences. The model dimension for B2 involves 43,226 constraints and 7,988 variables (among them, 2772 are integer).

6.2.10 Spatial-based approach through ArcGIS®

A spatial-based approach was used to allow the integration of geographic and demographic data of the country. Figure 5.2 shows the integration of the ArcGIS® database to the optimisation approach and the hydrogen supply chain design. As a first step, ArcGIS® is used to locate: initial conditioning centers, initial hydrogen production plants, by-product plants, refuelling stations, roads, hydro sites, biomass centers and nuclear centrals. All these elements are displayed in Table 6.1. In the case of PV sites and wind farms, the precise GPS coordinates were not collected, but the most important regions in terms of availability of these sources were detected according (Rte, 2013). The optimisation step is then carried out for different scenarios.

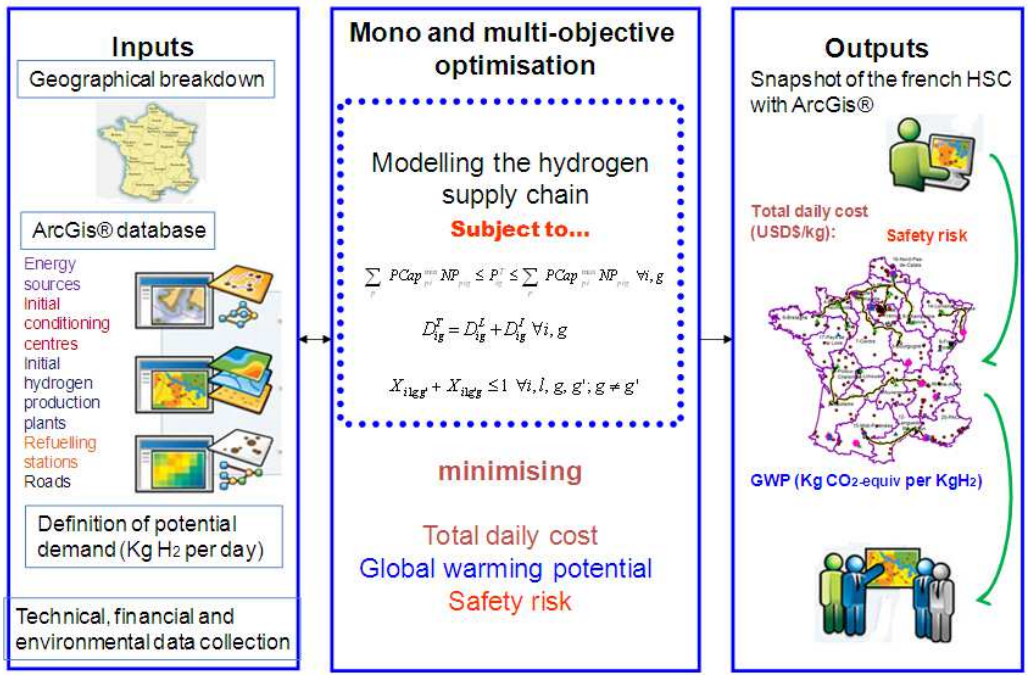


Figure 6.2 Methodology framework for the French case study

Table 6.1 ArcGIS® database layers

Pre-optimisation data treatment		
Layer	*Layer description*	*Source*
Regional limit	21 regions	(IGN, 2013)
Initial conditioning centers	Current Air-Liquide and LINDE and PRAXAIR sites.	(PHyRENEES, 2009)
Initial production plants	Current Air-Liquide and LINDE plants.	(PHyRENEES, 2009)
Refuelling stations	Minimum distance between refuelling stations = 300 km	(ESSO, 2013)
By product plants	Chloralkali electrolysis (Arkema, Solvay and Chloralp)	(Arkema, 2013; UIC, 2013)
Roads	Only motorways and national roads are considered	(IGN, 2013)
Hydro sites	Approximate location for small sites	(EDF, 2011)
Biomass	Biomass installed capacity in 2012, two centers sizes (small and big)	(Observ'ER, 2012)
Nuclear centrals	Classified in 3 sizes (less than 2000 MW, from 2000 to 4000 MW or more than 4000 MW)	(EDF, 2013)
Wind sites	Precise GPS coordinates were not collected	(Rte, 2013, see Figure 6.3)
PV Sites	Precise GPS coordinates were not collected	(Rte, 2013, see Figure 6.3)
Post-optimisation data treatment		
New layers	*Constraints*	
New conditioning centers	To locate the conditioning centers close to the production plants or the refuelling stations.	
New SMR plants	The production unit should be placed next to the main roads	
New electrolysis plants	To place production sites near the energy source and in the case of exporters, next to the main roads. Small decentralised units, PV and wind electrolysers (from which not precise GPS coordinates were collected), are placed near to the refuelling stations and main roads.	
New gasification plants	To place production sites near the biomass centers and the main roads.	
Transportation links	Using main roads	

Finally, the last step is to locate the decision variables in the map. As previously explained in chapter 3, section 3.7, the ArcGIS® database design and an analysis plan involves breaking the problem into logical parts, identifying what layers of data will be needed. This may involve digitizing existing maps, obtaining and translating electronic data from a variety of sources and formats. These layers are listed in Table 6.1 in the pre-optimising data treatment. When optimisation results are obtained, the decision variables are located following defined constraints that are listed in the same table in the post-optimisation data treatment section.

6.3 Case study (France)

France is divided into 21 regions (metropolitan France) without the territorial region of Corsica (see Figure 6.3). Three different production processes are evaluated: SMR, electrolysis and biomass gasification (not considered in the Midi-Pyrénées case). Hydrogen has to be liquefied before being stored or distributed. Liquid hydrogen (LH_2) is stored in super-insulated spherical tanks then delivered via tanker trucks. The whole parameters list is presented in Appendix B.1 and C.2 but the main data collected or calculated for France is explained below.

6.3.1 Demand

The total hydrogen demand in France has been estimated as in Chapter 5 (see Appendix C.2.1). A deterministic demand of hydrogen for FCEV is considered, including fleets such as buses, private and light-good-vehicles at 2012 levels. Following the prospective study conducted by (McKinsey & Company, 2010) and (Bento, 2010), the scenario *S1* is considered: 1% (160 t per day) of market penetration in 2020, 7.5% (1202 t per day) in 2030, 17.5% (2805 t per day) in 2040 and 25% (4007 t per day) in 2050.

6.3.2 Energy sources

Four renewable energy sources are considered:

- the projection of solar and wind energies to 2017 (Rte, 2013)
- the biomass installed capacity in 2012 (Observ'ER, 2012), see Figure 6.3
- hydropower capacity (EDF, 2011) where only facilities "run-of-river" are considered with two ranges for plant sizes: small (50-100 MW) and medium (100-250 MW), see Figure 6.3

The current installed capacity expressed in MWh per day is available from databases for the geographic division in regions, but the information are not as detailed in the Midi-Pyrénées case. The model does not consider the cost of RES capacity extension. From the aforementioned sources, it must be highlighted that some differences regarding the amount of energy sources in the Midi-Pyrénées region exist compared to the dedicated study to Midi-Pyrénées that was conducted in the previous chapter. The order of magnitude leads to less power availability for PV and wind energies (-13.6% and

-37% respectively) and to an increase in hydropower (76%) than observed in the database of the previous chapter. We are aware that this difference could influence the results. No correction was yet performed in order to maintain the same orders of magnitude for all the regions. An average working horizon of 1200h/year is considered for photovoltaic panels and 2500h/year for wind energy (Salingue, 2012). For hydropower plants run of river, a working period of 3500h/year is considered (Observ'ER, 2012) based on the (Le Schéma Régional Climat Air Energie, 2012). The potential use of nuclear electricity is also considered as energy source for the electrolysis process (nuclear sites are displayed in Figure 6.3). However, the commercial production technology used today is the SMR and that is why the comparison of this method with those using renewable appears relevant. Scenarios WWF, SER and Global chance were studied (see Appendix C.1) without any impact in the optimisation results (even if some scenarios are more optimistic) because the big impact of the energy source cost (low impact results from the RES transportation and let us remember that wind, hydro and PV electricity are not allowed to be exported) that is included in the parameter of production cost. If the production cost calculation is more detailed, it is possible to find different HSC configurations for different availability energy sources scenarios.

6.3.3 Production plants and conditioning centers

Ten production plants using mostly SMR are already installed in France (see Figure 6.3), seven plants are Air-Liquide and three of Linde gas according to (PHyRENEES, 2009) and also 15 conditioning centers. These sites are located in Figure 6.3. In the case of the by-product plants, Arkema, Solvay and Chloralp are located but its potential capacities are not considered by the moment because of the lack of information regarding the investment cost necessary to add purification steps for hydrogen in these plants. However, they are located in the territory to see potential sites for future facilities.

6.3.4 Roads and refuelling stations

For roads, only motorways and national roads are considered (IGN, 2013) in Figure 6.3. More than 12000 refuelling stations exist in France. Their location was carried out from (Esso, 2013) data base using the GPS coordinates locating only 300 of these units in ArcGIS® because of graphic readability considering stations close to the main roads, the other stations have been filtered and can be added. The Directive of the European Commission (European Commission, 2013) on the deployment of infrastructure for alternative fuels, recommend a H_2 refuelling station every 300 km.

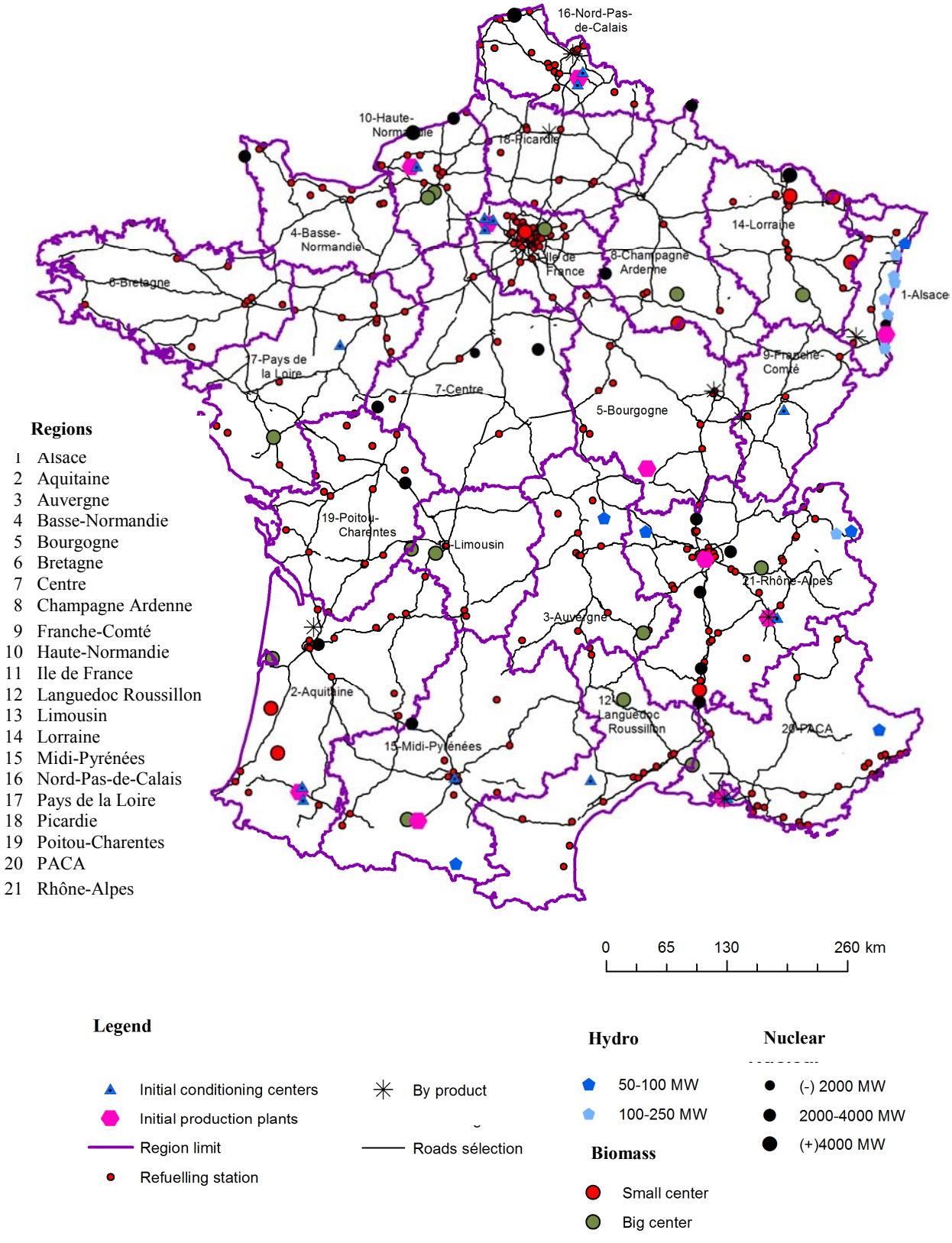


Figure 6.3 Elements of the HSC in France before optimisation in ArcGIS®

6.4 Results and discussion

The optimisation runs were performed for cases A and B with a Pentium (R) Dual-core CPU E6600 @ 3.06 GHz processor machine. All the mono- and multi-objective cases are analysed in this section.

6.4.1 Case A1. Cost optimisation.

The total daily cost optimisation is useful to find the values to build the pay-off table through conventional optimisation. In this case, the solution that minimises the TDC objective function without taking into account the non-dominated solutions can be obtained. The same approach is also valid for the GWP and risk criteria. The configurations that can be obtained are presented in Figure 6.4 and 6.5. They show how the number and types of the facilities as well as the distribution links evolve along the four time periods.

The results obtained in case A1 are in agreement with the centralised configurations obtained in the cost minimisation cases in chapters 4 and 5. A total number of 16 production plants in 2050 is obtained. In this result, only 6 plants are built in the period 2020-30, the other 10 plants are currently in operation with the SMR technology dispersed throughout France territory. In the new production facilities, the SMR plants are installed in regions n° 9, 11, 13, 18, 19 and 21(see the regions numbers in Figure 6.3). The production of LH_2 via SMR turns out to the best production option with cost as an objective function as it was previously observed (Almansoori and Shah, 2006; De-León Almaraz et al., 2013a).

The number of storage units (NSU) in 2020 is 38 (among them, 23 new units). The increase in demand in 2050 (4007 t vs. 160 t in 2020) promotes the use of more transportation units (NTU). Case A1 involves 25 tanker trucks to cover the demand by 2020 between regions and by 2050 transportation increases to 363 trucks (vs. 265 for GB case). Among all the case studies, the highest transportation cost is observed for case A1 as in the previous chapters. Since the number of installed plants is relatively low, more transport units are required to cover all the national demand. This results in a higher transportation operating cost with a centralised HSC network leading to a minimal average hydrogen cost of $3.44 per kg.

A minimal cost in 2020 of $4.7/kg H_2 with 11.1 kg CO_2/kg H_2 and a risk of 285 units is observed in Table 6.2. The cost value obtained in the national approach is 70% lower the value corresponding to the Midi-Pyrénées case in 2020. This result is related to the introduction of 10 production facilities currently in operation in the French territory. This cost could still be improved if the chloralkali electrolysis potential was also considered in the initial configuration (it was not the case because of lack of information related to the purity process). The high value capital investment in 2020 for renewable energy hinders the development of such energy sources with regard to both production units

and storage facilities needed to develop the network. The total daily cost is lower than \$4 per kg H_2 since 2040, due to a reduction in capital costs associated with production plants and technology type, reaching in 2050 (see Table 6.2) \$3.2/kg H_2 while CO_2 emissions do not decrease because only fossil fuels are used to produce H_2. The risk is mainly attributed to the transportation and storage. The highest level of demand in the "Ile de France" region requires the introduction of several storage units and the adaptation of refuelling stations to cover local demand, which implement a large SMR plant in the region.

The regions which export the most of hydrogen are n° 19 (35% of the overall exported demand), 18 (25%), 21 (24%) and 11 (15%) of all of them, only region n° 11 is the most populated region, from region 19 and 21, the transportation occurs mainly from the boundaries to the center. Surprisingly, Midi-Pyrénées (region 15) imports H_2 in all the time periods for two reasons: first, the SMR plant that is installed in the region cannot cover the whole demand and second the RES are not selected when cost is the optimisation criterion so that the region depends of its neighbour suppliers.

Table 6.2 Min TDC. Mono-objective optimisation results of the hydrogen supply chain.

Year	2020	2030	2040	2050
Demand (t per day)	160.30	1202.24	2805.23	4007.47
Number of total production facilities	12	16	16	16
Number of new production facilities	2	4	0	0
Number of total storage facilities	38	94	184	261
Number of new storage facilities	23	56	90	77
Number of transport units	25	117	268	363
Capital cost				
Plants and storage facilities (10^3 \$)	*817000.0*	*5674509.8*	*3540384.6*	*2225865.4*
Transportation modes (10^3 \$)	*12500.0*	*58500.0*	*134000.0*	*181500.0*
Operating cost				
Plants and storage facilities (10^3 \$ per day)	530.1	3549.5	8261.3	11831.7
Transportation modes (10^3 \$ per day)	19.9	108.8	258.3	353.8
Total operating cost (10^3 \$ per day)	550.0	3658.3	8519.6	12185.5
Total network cost (10^3 \$ per day)	746.2	5015.3	9470.5	12895.4
Cost per kg H_2 (\$)	***4.7***	***4.2***	***3.4***	***3.2***
Production facilities (t CO_2-equiv per day)	1618.7	12142.3	28332.4	40475.1
Storage facilities (t CO_2-equiv per day)	112.9	846.4	1974.9	2821.3
Transportation modes (t CO_2-equiv per day)	47.0	253.1	600.6	822.7
Total GWP (t CO_2-equiv per day)	1778.6	13241.7	30907.9	44119.0
Kg CO_2-equiv per kg H_2	***11.1***	***11***	***11***	***11***
Production facilities	18	40	40	40
Storage facilities	108	369	807	1098
Transportation modes	159	745	1714	2298
Total Risk (Units-level)	***285***	***1153***	***2561***	***3436***

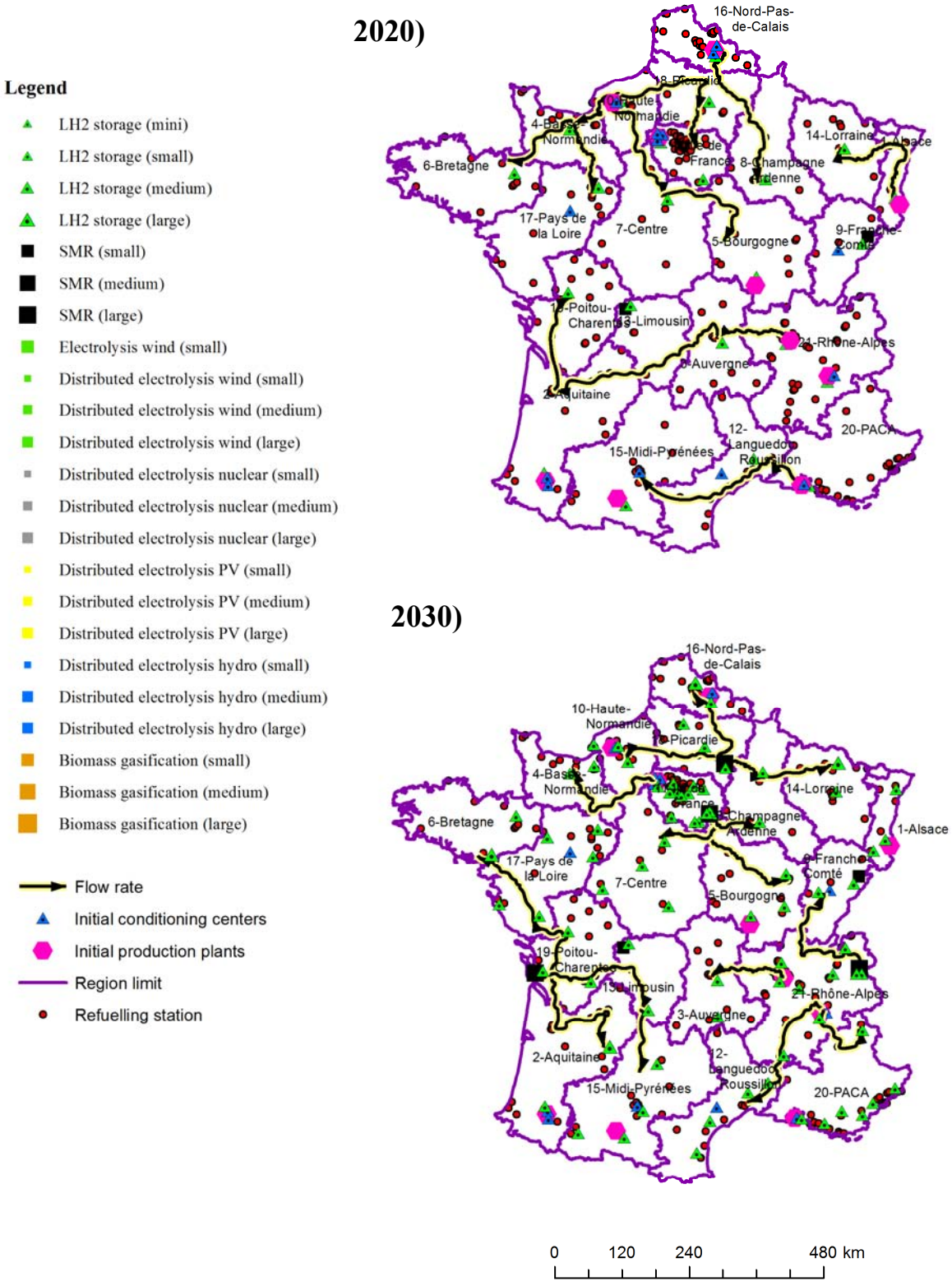


Figure 6.4 Network structure of liquid hydrogen distributed via tanker trucks for the case A1 (cost minimisation) in 2020 and 2030.

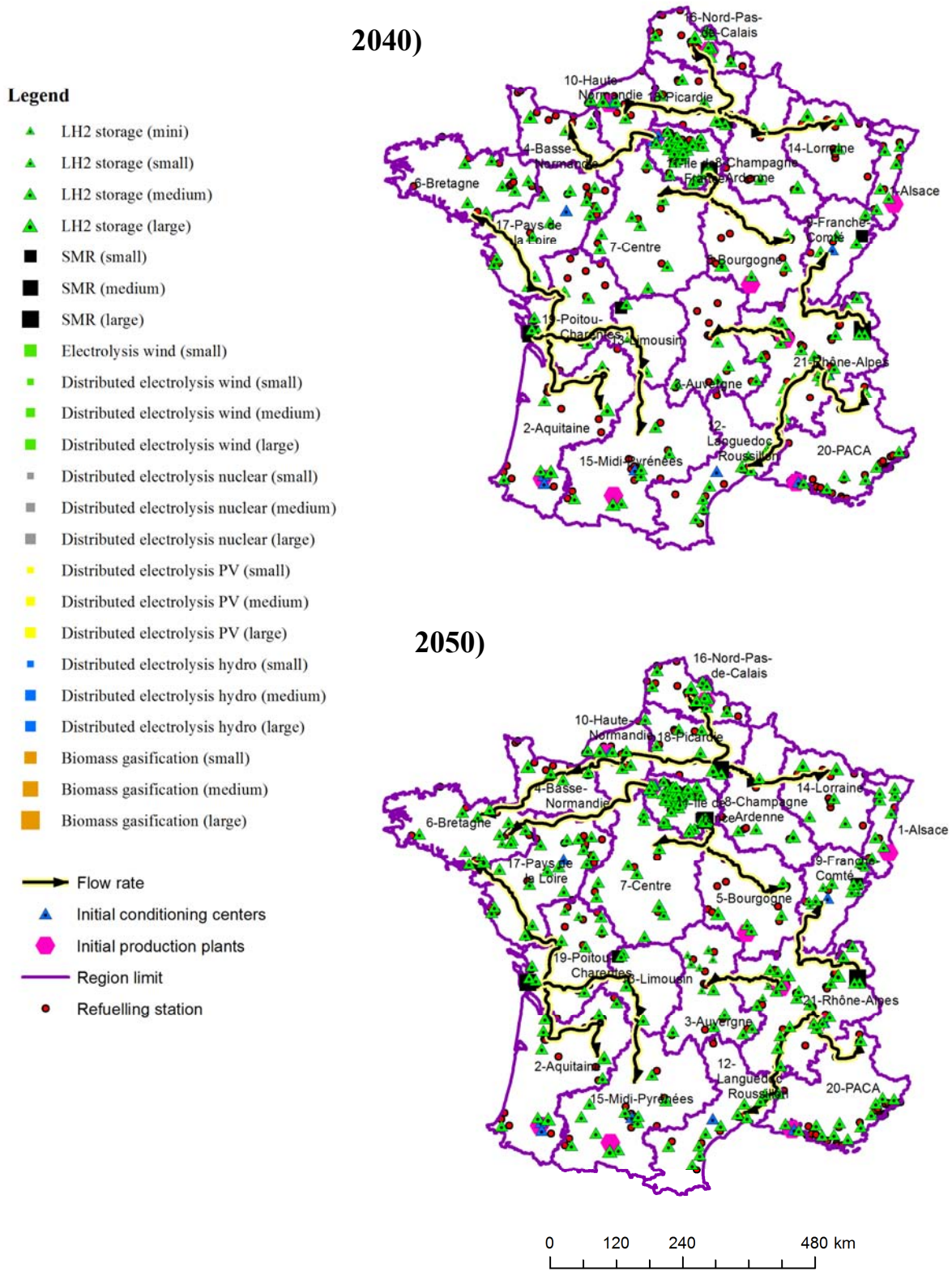


Figure 6.5 Network structure of liquid hydrogen distributed via tanker trucks for the case A1 (cost minimisation) in 2040-50.

6.4.2 Case A2. GWP optimisation.

Case A2 is relative to the minimisation of the global warming potential (GWP). The pay-off table is then implemented by computing the individual optima of the objective functions. Results presented in Table 6.3) represent a dominated solution. In the logic of the mapping task it makes no sense to place such quantity of storage facilities, then, a bi-objective optimisation was executed considering the minimisation of the GWP and risk. The results are presented in Table 6.4. It can be highlighted that the optimal solution obtained through conventional optimisation of GWP (average cost= \$7.7 per kg H_2, average GWP=2.2 kg CO_2 per day and Total risk=14230 units) is a dominated solution in the problem due to alternative optima obtained by the lexicographic optimisation (average cost= \$7.04 per kg H_2, average GWP=2.2 kg CO_2 per day and Total risk=4454 units). The number of production plants is reduced by 2050 in the mono-objective optimisation (in Table 6.3) from 317 to 67 facilities in the bi-criteria optimisation (Table 6.4), as well as the number storage facilities (1748 vs 118 storage units). The production mix remains the same for both solutions with wind-electrolysis as the main producer followed by hydro-electrolysis (see Table 6.5).

Table 6.3 Min GWP. Mono-objective optimisation results of the hydrogen supply chain.

Year	2020	2030	2040	2050
Demand (t per day)	160.30	1202.24	2805.23	4007.47
Number of production facilities	35	64	123	317
Number of new production facilities installed	25	29	59	194
Number of storage facilities	1024	1640	1764	1784
Number of new storage facilities installed	1009	616	124	20
Number of transport units	7	64	154	196
Total network cost (thousand \$ per day)	1957.6	12068.4	20318.1	26519.0
Cost per kg H_2 (\$)	***12.2***	***10.0***	***7.2***	***6.6***
Kg CO_2 per kgH_2	***4.7***	***2.2***	***2.1***	***2.1***
Total Risk (Units-level)	***1221***	***3330***	***4664***	***5014***

The results of the bi-objective optimisation are analysed in what follows. The number of production plants strongly increases (from 16 plants in case A1 to 68 in this case in 2050) and all of them are electrolysis facilities as it can be seen in Figures 6.6 and 6.7. The type of technology plays a key role in the CO_2 emissions: electrolysis technology decreases GWP but also induces a higher investment affecting the average cost of the HSC which is 51% higher than the value obtained in case A1. This minimisation case leads to a large number transportation links; that was not observed for GB and Midi-Pyrénées cases. The main exporters are the regions n°18 (26% of the total H_2 transported), 8 (23%) and 12 (15%). Since some regions have a low potential in wind and hydro energy sources, transportation turns out to be less environmental damaging than installing other production technology types in each region. An important demand in the national case also fits with the capacity of transport units (the capacity of a tanker truck is 3500 kg per trip).

Table 6.4 Min GWP+RISK. Mono-objective optimisation results of the hydrogen supply chain.

Year	2020	2030	2040	2050
Demand (t per day)	160.30	1202.24	2805.23	4007.47
Number of total production facilities	29	46	59	67
Number of new production facilities	19	17	13	8
Number of total storage facilities	37	63	92	118
Number of new storage facilities	22	26	29	26
Number of transport units	7	63	153	195
Capital cost				
Plants and storage facilities (10^3 $)	*3064052.8*	*13454902*	*10831557.9*	*7347739.9*
Transportation modes (10^3 $)	*3500*	*31500*	*76500*	*97500*
Operating cost				
Plants and storage facilities (10^3 $ per day)	841.2	7185.7	16943.4	24265.0
Transportation modes (10^3 $ per day)	4.1	58.0	148.4	187.4
Total operating cost (10^3 $ per day)	845.3	7243.7	17091.8	24452.4
Total network cost (10^3 $ per day)	1547.8	10325.0	19584.4	26154.4
Cost per kg H_2 ($)	***9.7***	***8.6***	***7.0***	***6.5***
Production facilities (t CO_2-equiv per day)	630.0	1707.4	3687.1	5345.2
Storage facilities (t CO_2-equiv per day)	112.9	846.4	1974.9	2821.3
Transportation modes (t CO_2-equiv per day)	9.3	133.8	347.2	435.9
Total GWP (t CO_2-equiv per day)	752.2	2687.6	6009.2	8602.3
Kg CO_2-equiv per kg H_2	***4.7***	***2.2***	***2.1***	***2.1***
Production facilities	31	61	86	102
Storage facilities	105	253	432	581
Transportation modes	39	390	1104	1270
Total Risk (Units-level)	***175***	***703***	***1622***	***1953***

For the 2020 period, a decentralised configuration is obtained importing less than 26% of the total H_2 demand (Figure 6.6-2020) with wind as the major primary energy source (see Table 6.5). GWP is 4.7 kg CO_2 per kg H_2, which represents 70% of CO_2 obtained for the same period in the scenario of cost minimisation. Conversely, the price is \$9.7 per kg H_2 in 2020; this represents a 30% increase compared to the minimal cost. The cost is logically higher in the first period mainly due to the investment in 19 new electrolysis facilities and 22 storage units. The year 2030 (Figure 6.6--2030) requires the installation of several production and storage units with similar CO_2 emissions, but the total daily cost decreases to \$8.6 per kg H_2, with halved CO_2 emissions. The risk is mainly due first to transportation and second to storage. In 2040 (respectively 2050) (Figure 6.7), the cost is lower than \$7.0 per kg H_2 (\$6.5respectively) (see Table 6.4).

Table 6.5 Use ratio of energy sources for hydrogen production by electrolysis min CO_2 emissions.

Energy source/Period	2020	2030	2040	2050
SMR	32%	4%	2%	1%
Wind	68%	96%	87%	81%
Hydro	0%	0%	11%	18%

CO_2 emissions are minimal since 2040, 2.1 kg CO_2 per kg H_2 and the final configuration by 2050 leads to 99% of electrolysis production using renewable energy. The emissions are distributed as follows: 62% for production, 33% for liquefaction and 5% for transportation.

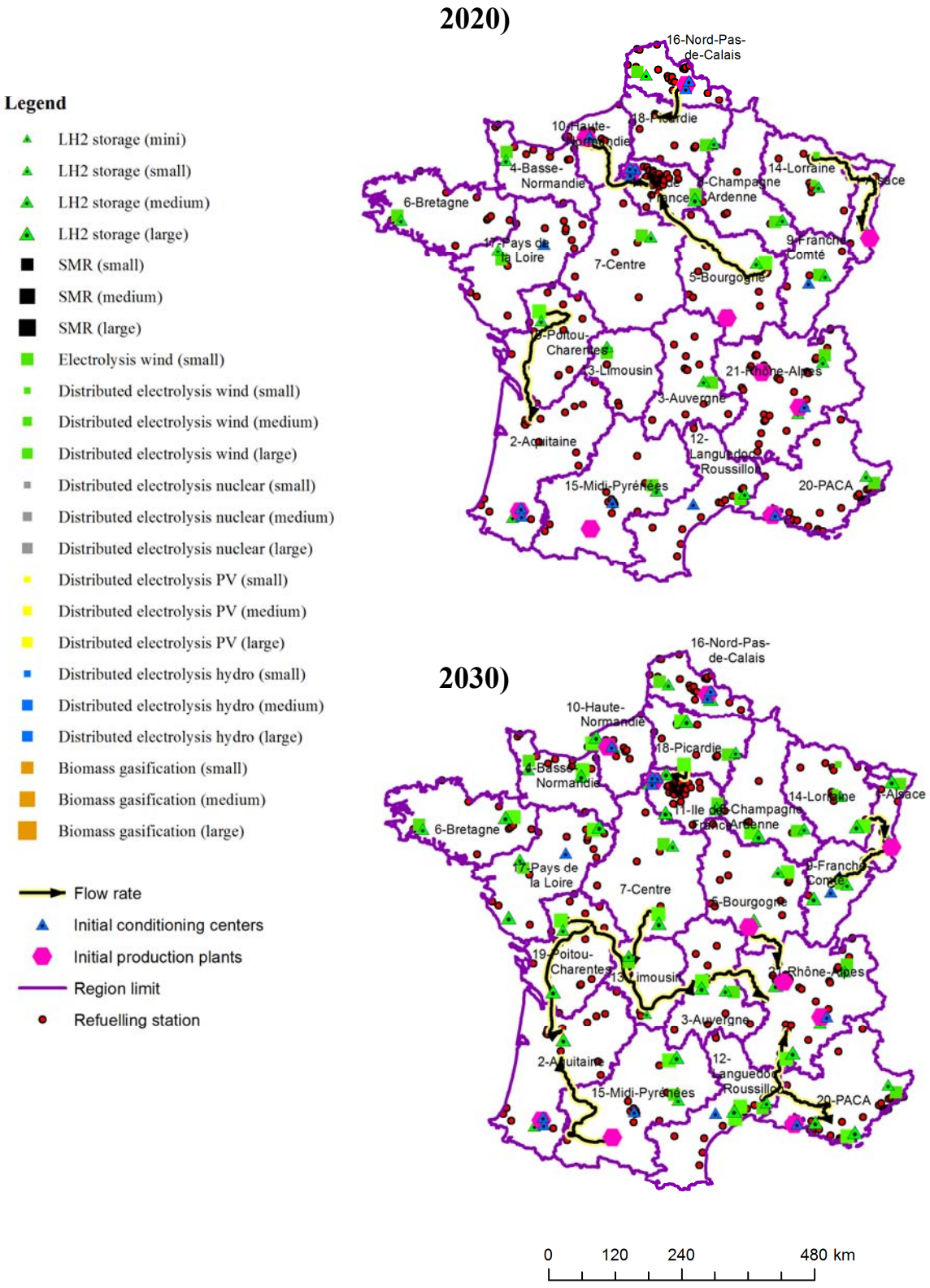


Figure 6.6 Network structure of liquid hydrogen distributed via tanker trucks for the case A2 (GWP minimisation) in 2020-30.

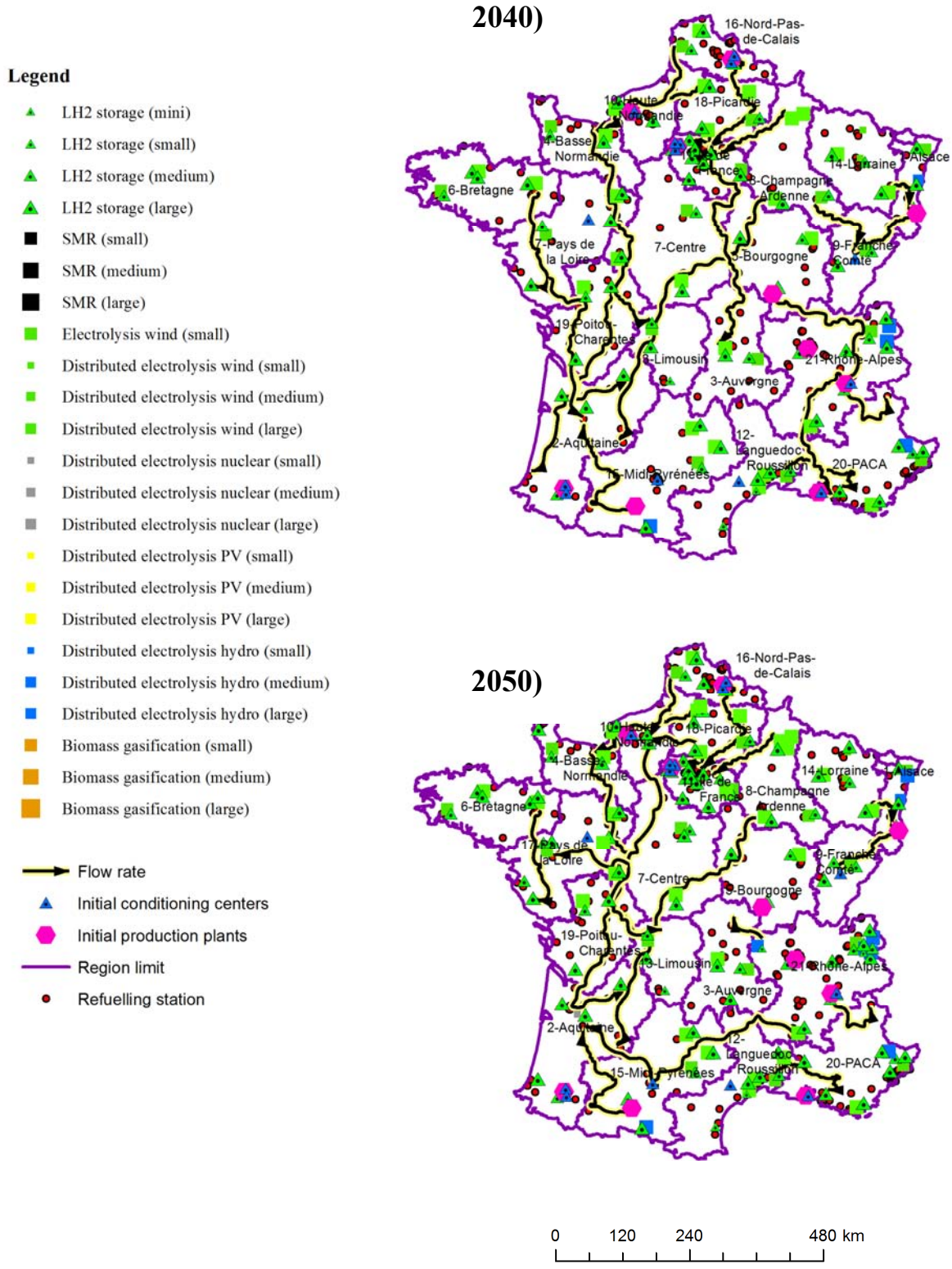


Figure 6.7 Network structure of liquid hydrogen distributed via tanker trucks for the case A2 (GWP minimisation) in 2040-50.

6.4.3 Case A3. Risk optimisation.

Case A3 minimises the total relative risk. The optimal configurations in Figures 6.8 and 6.9 show a high degree of decentralisation with only three distribution links and three tanker trucks assigned for the whole supply chain in 2020. No link and transport unit are assigned from 2030-2050 periods and a high number of installed production facilities is observed, which is consistent with the results from chapters 4 and 5 for the optimisation of the same criterion.

Some specific features for case A3 (see Table 6.6) can be highlighted for production units with a total of 60 facilities located in all the regions in 2050. The main difference between cases A1-A2 and risk minimisation is the degree of decentralisation and the production technology which results in a mix of SMR plants and electrolysis units operating with nuclear electricity when risk is minimised. This can be explained by the inherent risk factor of electrolysis facilities that considers an inherent risk depending the production type and size regardless of the source used.

The total relative risk for this case considering the four periods is of 1598 units and is logically influenced by the storage risk since storage is scattered in each region to cover a volume equivalent to 10 days of LH_2 demand. From the results of this case study where different storage sizes were considered, it must be emphasized that surprisingly a lot of medium and large units of production and storage are presented in the final configuration. Production is the second major risk.

The transportation relative risk was reduced to find a safer configuration considering at the same time the links and distances to be travelled. Yet, production technology mix of case A3 represents a financial benefit of 8% ($6.45 per kg H_2) as compared to case A2 considering the minimisation the average cost ($7.04 per kg H_2) (average values are obtained dividing the TDC and the total GWP by the total demand for the 4 time periods).

In Figures 6.8 and 6.9 the selected production technology mainly involves SMR in 2020 and electricity from nuclear source since 2030. Wind, hydro and solar sources are also used. For this mono-objective optimisation, the network is 100% decentralised. The four storage sizes are used in the four periods.

The minimal risk of the HSC in 2020 amounts to142 units, with cumulative risks for production units and storage: the obtained values of the risk index are equal to 301, 493 and 663 units for the years 2030, 2040 and 2050, respectively. The risk scale is calculated with the lowest value obtained from the minimisation of this objective for all periods. The computations for the French case are presented in detail in Appendix C.2.4-6.

The total daily cost of LH_2 for this scenario is lower than in the environmental scenario but logically higher than the economic scenario for all periods. In 2050 (Table 6.6), the cost is \$6.1 per kg H_2 and emissions of 4.7 kg CO_2 per kg H_2. The main risks in this configuration are mainly due to storage 88% and production 12%.

Table 6.6 Risk optimisation results of the hydrogen supply chain.

Year	2020	2030	2040	2050
Demand (t per day)	160.30	1202.24	2805.23	4007.47
Number of total production facilities	20	36	43	60
Number of new production facilities	10	16	7	17
Number of total storage facilities	37	63	92	118
Number of new storage facilities	22	26	29	26
Number of transport units	3	0	0	0
Capital cost				
Plants and storage facilities (10^3 \$)	*1739000*	*12773529.4*	*5806540.5*	*6397739.9*
Transportation modes (10^3 \$)	*1500*	*0*	*0*	*0*
Operating cost				
Plants and storage facilities (10^3 \$ per day)	715.2	6251.4	15853.1	22519.7
Transportation modes (10^3 \$ per day)	1.5	0	0	0
Total operating cost (10^3 \$ per day)	716.8	6251.4	15853.1	22519.7
Total network cost (10^3 \$ per day)	1127.2	9352.4	17627.5	24596.5
Cost per kg H_2 (\$)	***7.0***	***7.8***	***6.3***	***6.1***
Production facilities (t CO_2-equiv per day)	1450.7	6008.5	10583.1	16058.6
Storage facilities (t CO_2-equiv per day)	112.9	846.4	1974.9	2821.3
Transportation modes (t CO_2-equiv per day)	3.4	0	0	0
Total GWP (t CO_2-equiv per day)	1567.0	6854.9	12558.0	18879.8
Kg CO_2-equiv per kg H_2	***9.8***	***5.7***	***4.5***	***4.7***
Production facilities	24	48	61	82
Storage facilities	105	253	432	581
Transportation modes	13	0	0	0
Total Risk (Units-level)	***142***	***301***	***493***	***663***

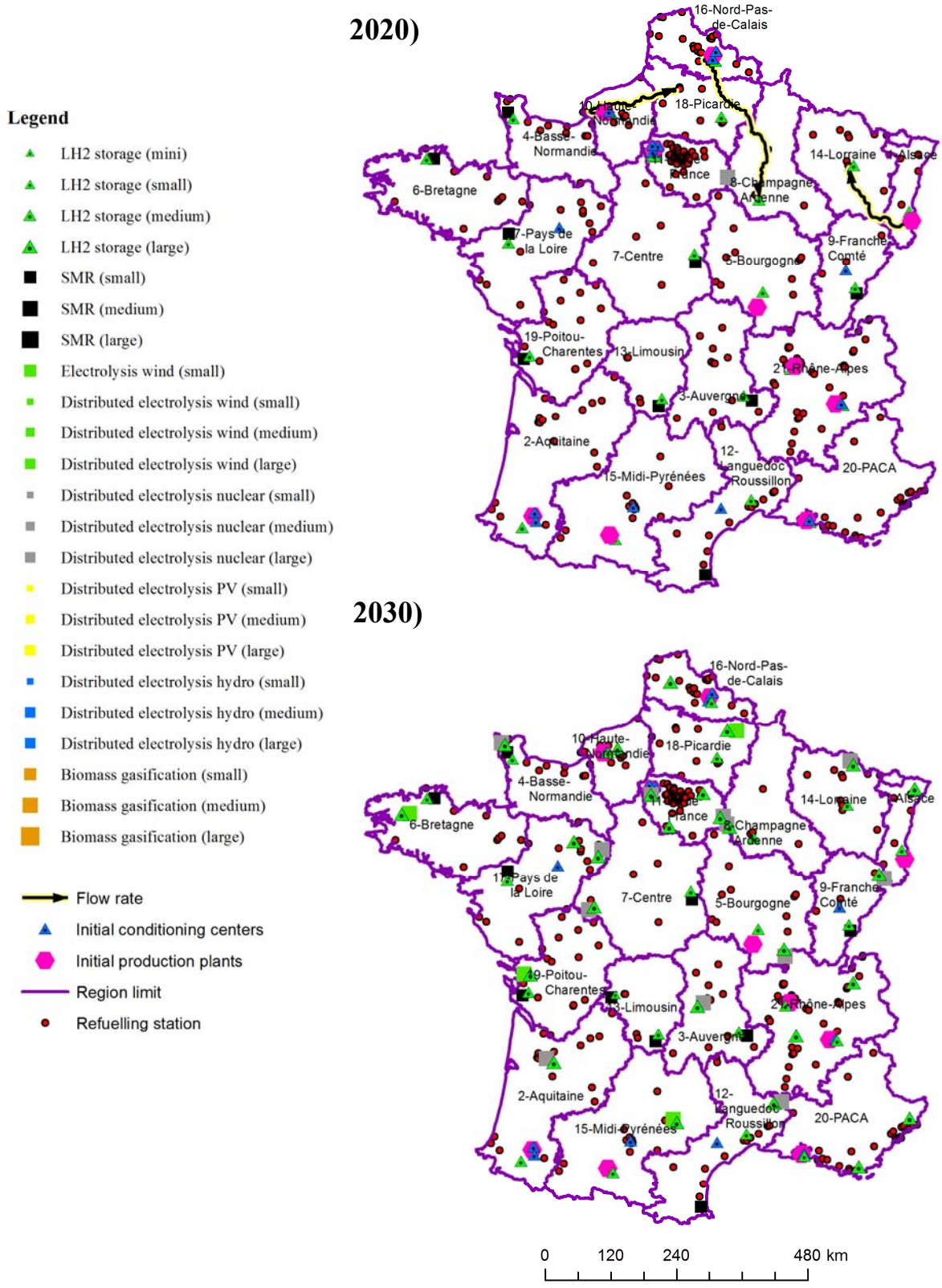


Figure 6.8 Network structure of liquid hydrogen distributed via tanker trucks for the case A3 (risk minimisation) in 2020-30.

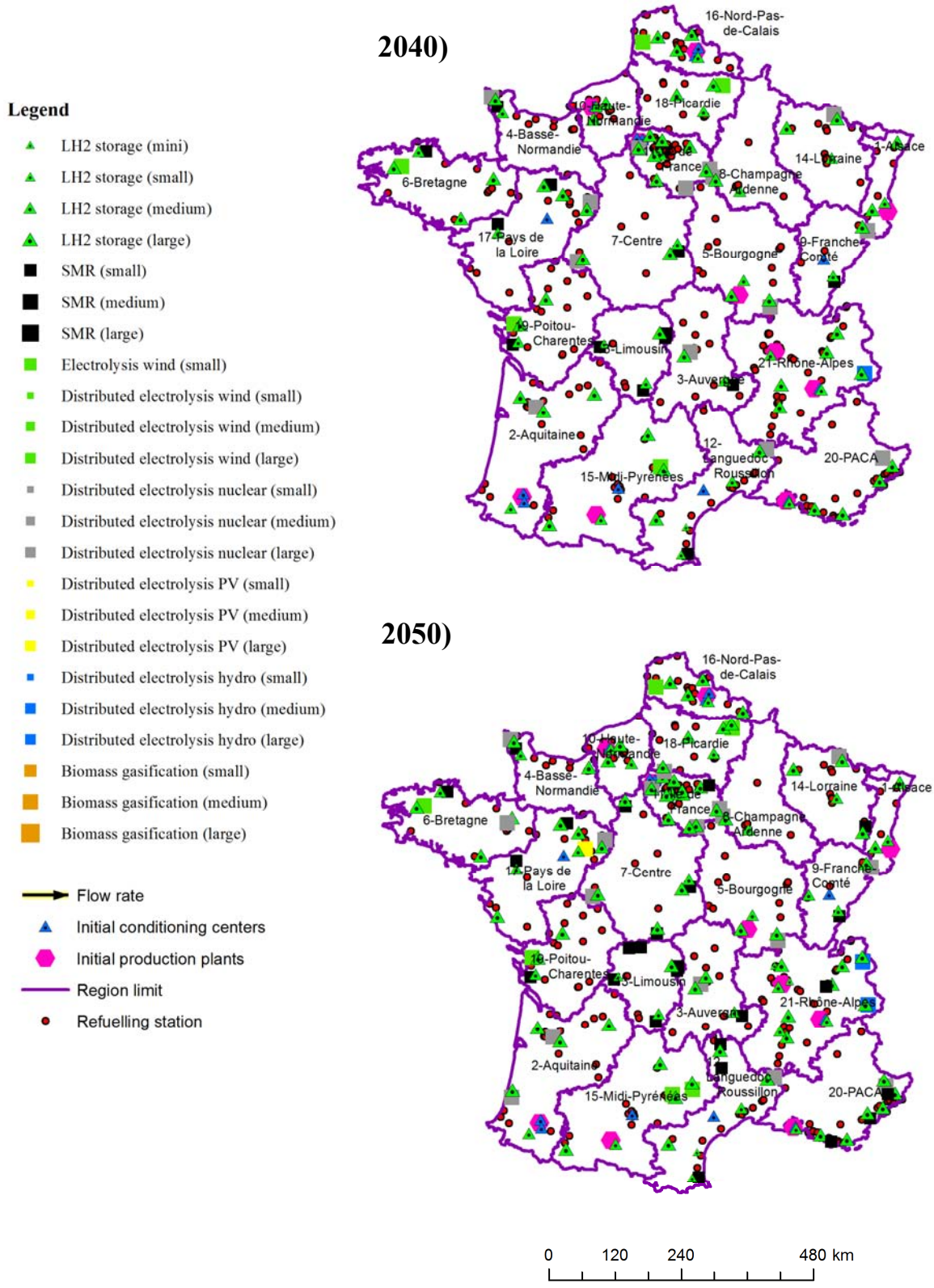


Figure 6.9 Network structure of liquid hydrogen distributed via tanker trucks for the case A3 (risk minimisation) in 2040-50.

6.4.4 Conclusion of the mono-objective stage

This preliminary approach gives a reference for the different criteria over several periods. In the cost minimisation, the SMR process remains as the production process. This optimisation follows the same trends as for Great Britain and Midi-Pyrénées cases. A competitive cost can yet be reached very early due to the consideration of current production plants and conditioning centers. In the case of risk minimisation, no transportation link is observed while at the same time the size of the production plants and storage units has not a significant weight in the final decision. For example in densely populated "Ile de France", the implementation of large size storage units is allowed. The main difference is found when considering GWP optimisation: a decentralised network is obtained with small units scattered throughout all the territory; significant discrepancies exist among the regions since some of them do not have enough installed capacity to supply their own demand; the use of tanker trucks is thus needed and the emissions related to the transportation are found to be less pollutant than the production of hydrogen via another production process for the demand levels of the case study. Table 6.7 summarises the highlights of the three mono-objective cases.

Table 6.7 Summary of each mono-objective optimisation case.

	TDC	GWP	RISK
Centralisation degree	Centralised production network supplied by tanker trucks	Centralised production network supplied by tanker trucks	Decentralised network
Cost	Competitive since 2020	High investment capital cost in 2020, low digressive cost over the time period.	Low digressive cost over the time period
Energy sources	Natural gas	RES for H_2 production	Natural gas and nuclear electricity
Risk	Very significant risks associated with the intensification of transport	Significant risk associated to transportation	Low risk mainly due to the lack of transportation
Emissions	Significant environmental impact due to production via SMR	The major benefit obtained from the high volume produced via wind electrolysis	High environmental impact, due to the use of natural gas

One issue related the methodology is the need to apply bi-or three criteria lexicographic optimisation for the case A2 (GWP minimisation) for the solution of the multi-period problem. As for the Midi-Pyrénées case, the number of variables leads to prohibitive computation time for the application of the bi-criteria lexicographic method for cases A1 and A3.

6.4.5 Case B1. Multi-objective optimisation (ε-constraint)

From the three independent mono-objective cases, each objective function range can be obtained so that the ε-constraint method can be applied (as presented in chapter 5 section 5.7). From the optimisation results of Table 6.8, the utopia and nadir points of each criterion can be found.

Table 6.8 Pay-off table obtained by the mono-objective optimisations for all periods

Case	A1	A2	A3
Decision variables			
Total production plants (installed in 2050)	16	317	60
Total storage units (installed in 2050)	261	1784	118
Number of transport units in 2050	363	196	0
Objectives			
Average cost per kg H_2 ($)	**3.4**	7.4	6.5
Average kg CO_2-equiv per kg H_2	11.0	**2.2**	4.9
Total risk (units)	7435	14229	**1598**

The total risk can be divided into five intervals to make the interpretation easier: low risk is lower than 4600 units, moderate risk lower than 4800, medium risk, 7900, significant risk lower than 11000 and high risk lower than 14200. Similarly, 10 epsilon points are defined for GWP (2.2, 3.1, 4.1, 5.1, 6.1, 7.1, 8, 9, 10 and 11 average kg CO_2 per kg H_2). Then, the objective function TDC has to be minimised while the total GWP and total risk are considered as inequality constraints. The solution consists of a Pareto front composed of solutions for supply chain configurations (see Figure 6.10). The cost of medium, high and medium risks is similar since these two levels of risks have close values for CO_2 emissions. It can be seen in Figure 6.10 that moderate-to-high risk options are very close. The 47 solutions in the Pareto front are evaluated via M-TOPSIS analysis with the same weighting factor for cost, safety and environmental factors (see Appendix C.3.4). The resulting M-TOPSIS solution is shown in Table 6.9 and Figures 6.11- 6.12.

According to these results, the future HSC involves 21 production plants in 2020 (see Figure 6.11-2010) from which 10 are already installed and 11 wind-electrolysis plants are established (38% of the hydrogen is produced via electrolysis in this period). To cover the demand, this network uses 9 tanker trucks to deliver liquid H_2 to medium storage facilities. This option involves a cost of $6.5 per kg H_2, an environmental impact of 7.5 kg CO_2 per kg H_2 and a low risk. It must be emphasized that even if SMR plants are initial installed facilities in this period, the cost remains high because of the initial investment. This configuration differs from the three mono-criterion cases especially in the production technology type and a lower number of tanker trucks and flow rate links compared to the cost mono-optimisation case. Average 30% of the total demand is imported from one region to another one.

By 2030 (Figure 6.11-2030), a mix of production technologies such as biomass gasification, wind electrolysis and SMR is involved. Gasification produces 86% of the total demand, electrolysis 3% and SMR 11%. This option leads to a cost of $6.1 per kg H_2, an environmental impact of 4.7 kg CO_2 per kg H_2 and a low risk. The cost slightly increases because of the investment on 5 new gasification production plants and 26 storage units, but at the same time, an important decrease in the GWP results from this configuration (7.5 kg CO_2-equiv per kg H_2 in 2020 to 4.7 in 2030). By 2040 and 2050 (Figure 6.12), biomass gasification produces more the 97% of the total demand. In 2050, the chosen

solution involves a cost of \$3.9 per kg H_2, an environmental impact of 4 kg CO_2 per kg H_2 (as in 2040) and a low risk.

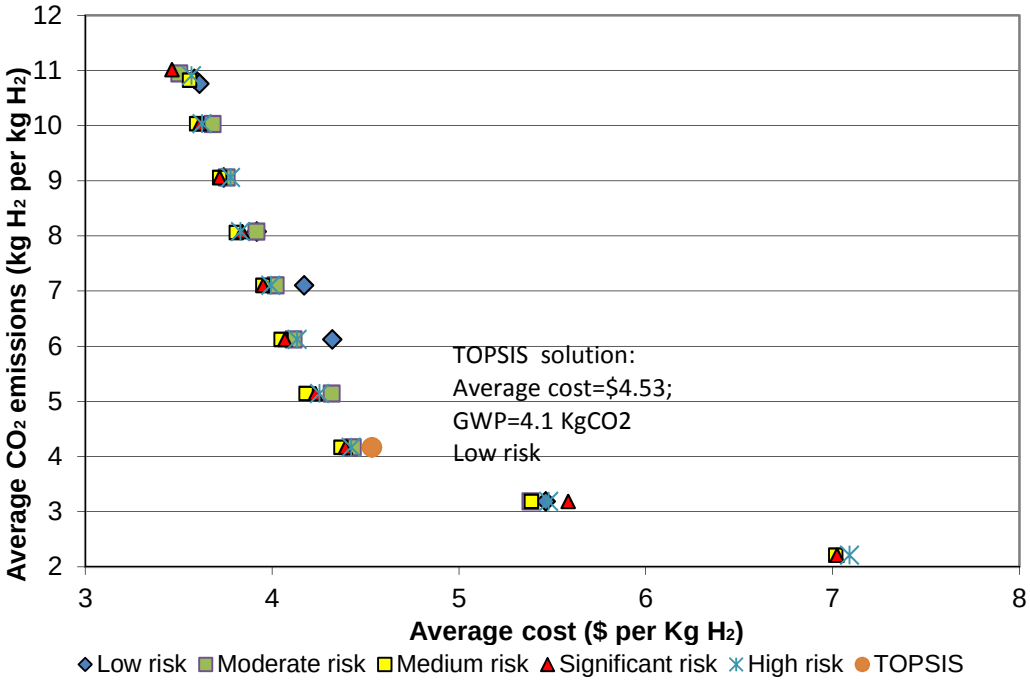


Figure 6.10 Pareto solutions for the multi-objective optimisation to the French case Pareto solutions for the multi-objective optimisation to the French case

Table 6.9 Multi-objective optimisation results of the hydrogen supply chain

Year	2020	2030	2040	2050
Demand (t per day)	160.30	1202.24	2805.23	4007.47
Number of total production facilities	21	26	31	31
Number of new production facilities	11	5	5	0
Number of total storage facilities	37	63	94	127
Number of new storage facilities	22	26	31	33
Number of transport units	9	83	104	140
Capital cost				
Plants and storage facilities (10^3 \$)	*1352414*	*11995098*	*11977694.4*	*2031702.2*
Transportation modes (10^3 \$)	*4500*	*41500*	*52000*	*70000*
Operating cost				
Plants and storage facilities (10^3 \$ per day)	728.8	4417.1	10284.1	14675.9
Transportation modes (10^3 \$ per day)	6.0	78.7	95.1	129.4
Total operating cost (10^3 \$ per day)	734.9	4495.8	10379.2	14805.2
Total network cost (10^3 \$ per day)	1049.7	7311.6	13250.1	15457.1
Cost per kg H_2 (\$)	***6.5***	***6.1***	***4.7***	***3.9***
Production facilities (t CO_2-equiv per day)	1072.7	4618.0	9037.9	12859.5
Storage facilities (t CO_2-equiv per day)	112.9	846.4	1974.9	2821.3
Transportation modes (t CO_2-equiv per day)	13.9	182.5	217.0	293.6
Total GWP (t CO_2-equiv per day)	1199.4	5646.8	11229.8	15974.4
Kg CO_2-equiv per kg H_2	***7.5***	***4.7***	***4.0***	***4.0***
Production facilities	24	54	83	83
Storage facilities	105	253	435	595
Transportation modes	46	443	452	601
Total Risk (Units-level)	***174***	***750***	***971***	***1280***

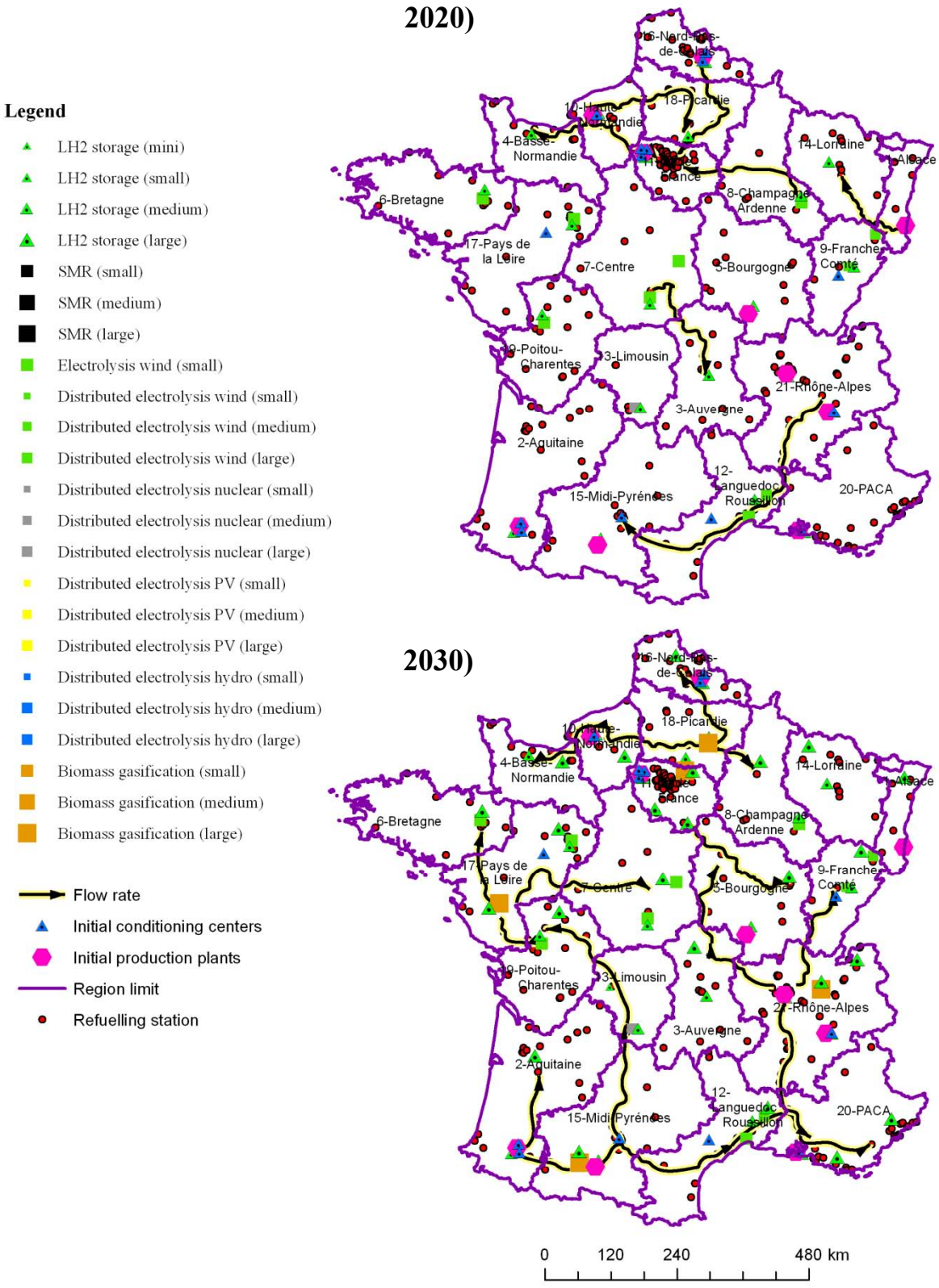


Figure 6.11 Network structure of liquid hydrogen distributed via tanker trucks for the case B1 (multi-objective, Ɛ-constraint) in 2020-30.

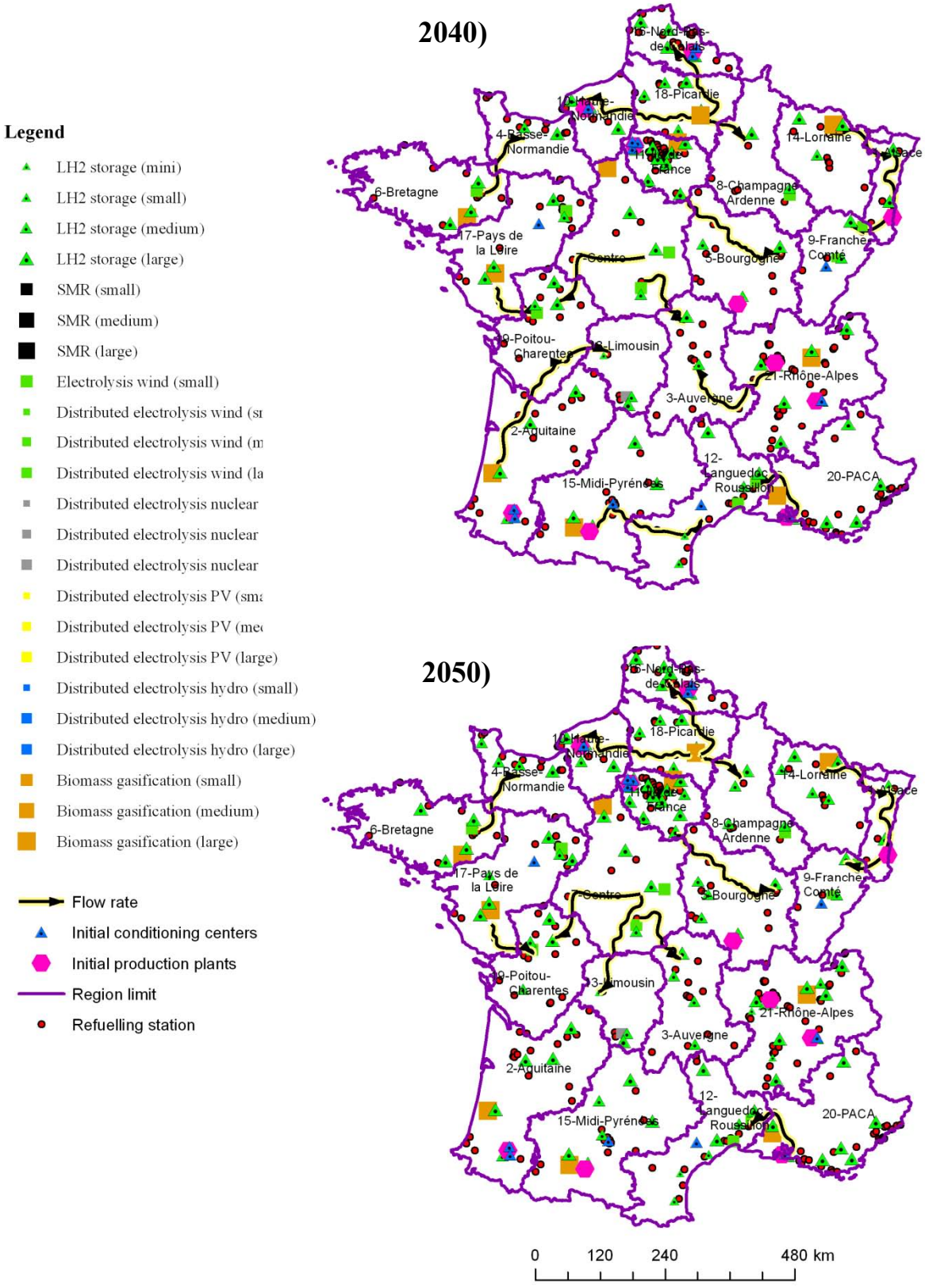


Figure 6.12 Network structure of liquid hydrogen distributed via tanker trucks for the case B1 (multi-objective, Ɛ-constraint*) in 2040-50.*

6.4.6 Case 3: Economic cycle. Multi-objective optimisation (Lexicographic method)

The underlying idea is here to examine if a strategy based on cost minimisation in the first period in order to launch the hydrogen market without being penalized by a high initial cost due to the investment phase is consistent with the target of low CO_2 emissions in the following periods. Then, for 2030, the objective is to optimise GWP. TDC and GWP are again optimised in 2040 and 2050 respectively (see Figure 6.13). For this approach, the lexicographic optimisation is applied. Then, the priority objective in each period is first optimised and the optimised result is then used as a constraint to optimise the two other objective functions.

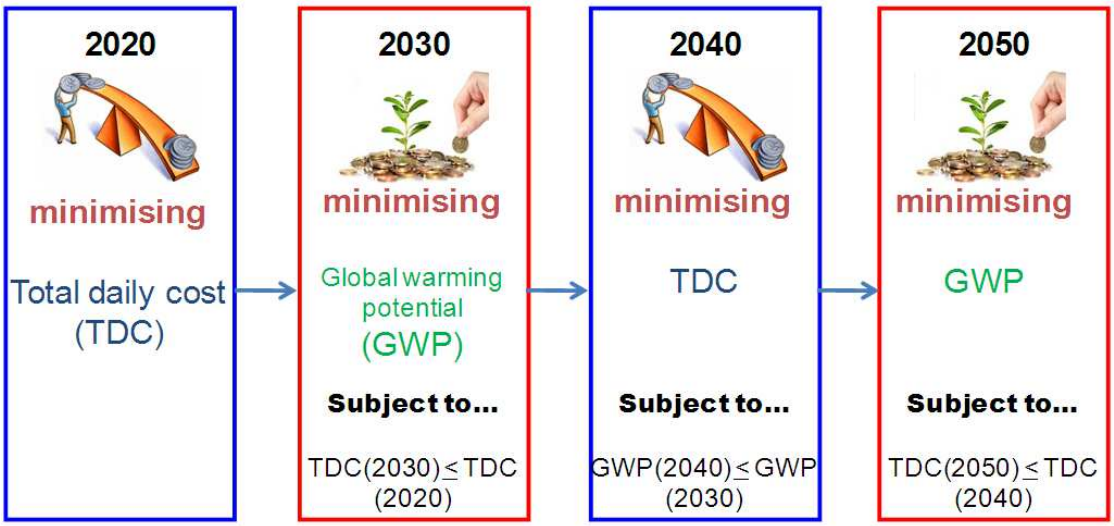


Figure 6.13. Economic cycle approach.

The results show a cost of \$4.5 per kg H_2 with 11.1 kg CO_2-equiv kg H_2 and a risk of 306 units (see Table 6.10) for 2020. Two new production plants are installed in regions nº 9 and 13 corresponding to small SMR units while the 10 already installed plants produce 99% of H_2. Seventy new storage units are positioned and 25 tanker truck transport 65% of the total demand. Exporter regions are nº 10 (60%), 21 (16%) and 20 (14%) while regions nº 11 and 15 export low amounts (see Figure 6.14-2020). Even if the cost can be viewed as competitive from this period, the environmental impact is high due to the production from natural gas and the risk is also high because of the important number of transportation links.

The obtained network is inserted as an initial configuration in 2030, for this stage, the GWP is optimised. The cost for this minimisation is \$8.5 per kg H_2 with 1.9 kg CO_2 per kg H_2 and a risk of 802 units. The cost impact is significant and almost the double of that in 2020. How could the society accept to pay two times more for a kg of H_2 fuel ten years after of its launch and when demand is higher? The investment cost that is necessary to change the production technology type in the second period will postpone the depreciation phase but if the environmental regulations forces the diminution of GHG, the SMR established in 2020 will be underutilized. To cope with this problem, an optimisation run is carried out in order to minimise GWP in 2030 with a boundary value for cost set at

$4.5 per kg H_2 (see Table 6.10). In this case, the HSC has one large size gasification plant in region nº 11 which is the main exporter in 2030 (see Figure 6.14-2030). Then, 78 new storage units are distributed (all sizes) and 148 tanker truck deliver almost 60% of the demand. The total risk is 1799 units and 80% of this risk is due to transportation. The gasification plant produces 70% of hydrogen, for this reason, the CO_2 emissions (6.2 kg CO_2-equiv per kg H_2) represent a 37% decrease compared to 2020. 92% of the imported demand is supplied from region nº 11 even if a high population density is established.

In 2040, GWP is set at 6.2 kg CO_2 per kg H_2 and the cost is optimised. The cost ranges from $4.5 to $4.1 per kg H_2. Five new production plants, 124 storage units and 271 tanker trucks are installed. The risk is 2980 and 70% is due to transportation. Three of the new production plants are small size electrolysis units using wind energy, one is a large size gasification plant and the other is of SMR type. The imported demand is 58% and the suppliers are regions nº 21 (40%), 11 (33%) and 17 (27%) (see Figure 6.15-2020).

Finally, in 2050, the GWP minimisation with an upper bound for cost equal to $4.1 per kg H_2 is carried out. The CO_2 emissions decrease of 22% from the previous period resulting in 4.1 kg CO_2-equiv per kg H_2. Two new large size gasification plants are installed, with 106 storage units and 368 tanker trucks distribute H_2. The total risk of the network is 3621 units from which 66% is associated to transportation. Exportation regions are nº 1 (34%), 21 (23%), 2 (22%), 11 (15%) and 17 (6%).

Table 6.10 Results of the multi-objective optimisation of the HSC for a economic cycle in a mono-period treatment.

Mono-period	Min cost	Min GWP + constraint cost	Min cost + constraint GWP	Min GWP + constraint cost
Year	2020	2030	2040	2050
Demand (t per day)	160.30	1202.24	2805.23	4007.47
Number of production facilities	12	13	18	20
Number of new production facilities	2	1	5	2
Number of storage facilities	85	163	287	381
Number of new storage facilities	70	78	124	106
Number of transport units	25	148	271	368
Total network cost (10^3 $ per day)	717.1	5410.1	11595.6	16430.6
Cost per kg H_2 ($)	***4.5***	***4.5***	***4.1***	***4.1***
Production facilities (t CO_2-equiv per day)	1618.67	6275.37	14794.36	15364.18
Storage facilities (t CO_2-equiv per day)	112.85	846.38	1974.88	2821.26
Transportation modes (t CO_2-equiv per day)	47.04	345.23	623.16	855.49
Total GWP (t CO_2-equiv per day)	1778.56	7466.98	17392.41	19040.92
kg CO_2-equiv per kg H_2	***11.1***	***6.2***	***6.2***	***4.8***
Production facilities risk	18	26	41	49
Storage facilities risk	130	383	836	1156
Transportation modes risk	159	1390	2103	2416
Total risk (units)	***306***	***1799***	***2980***	***3621***

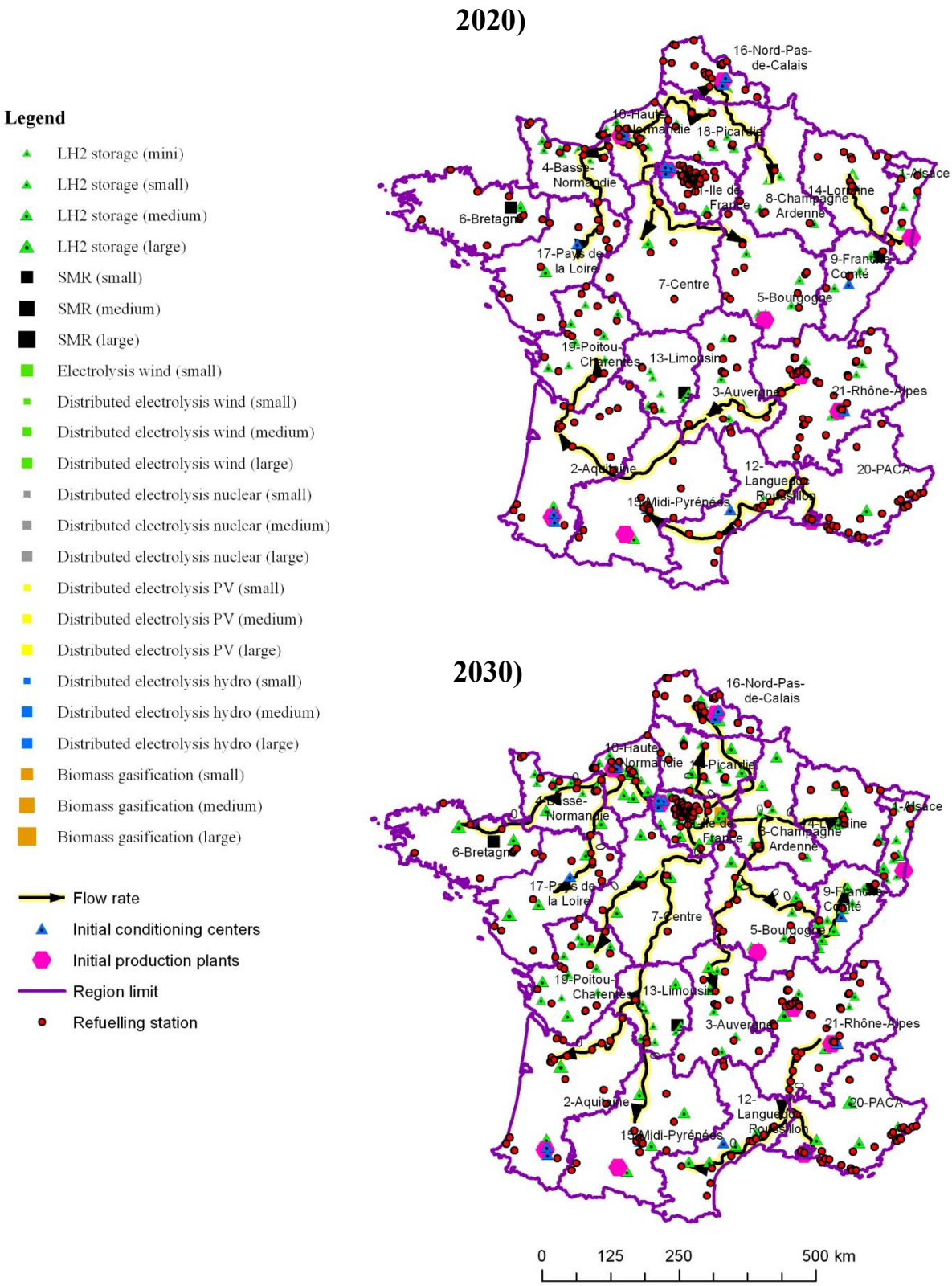


Figure 6.14 Network structure of liquid hydrogen distributed via tanker trucks for the case B2 (multi-objective-mono-period) in 2020-30.

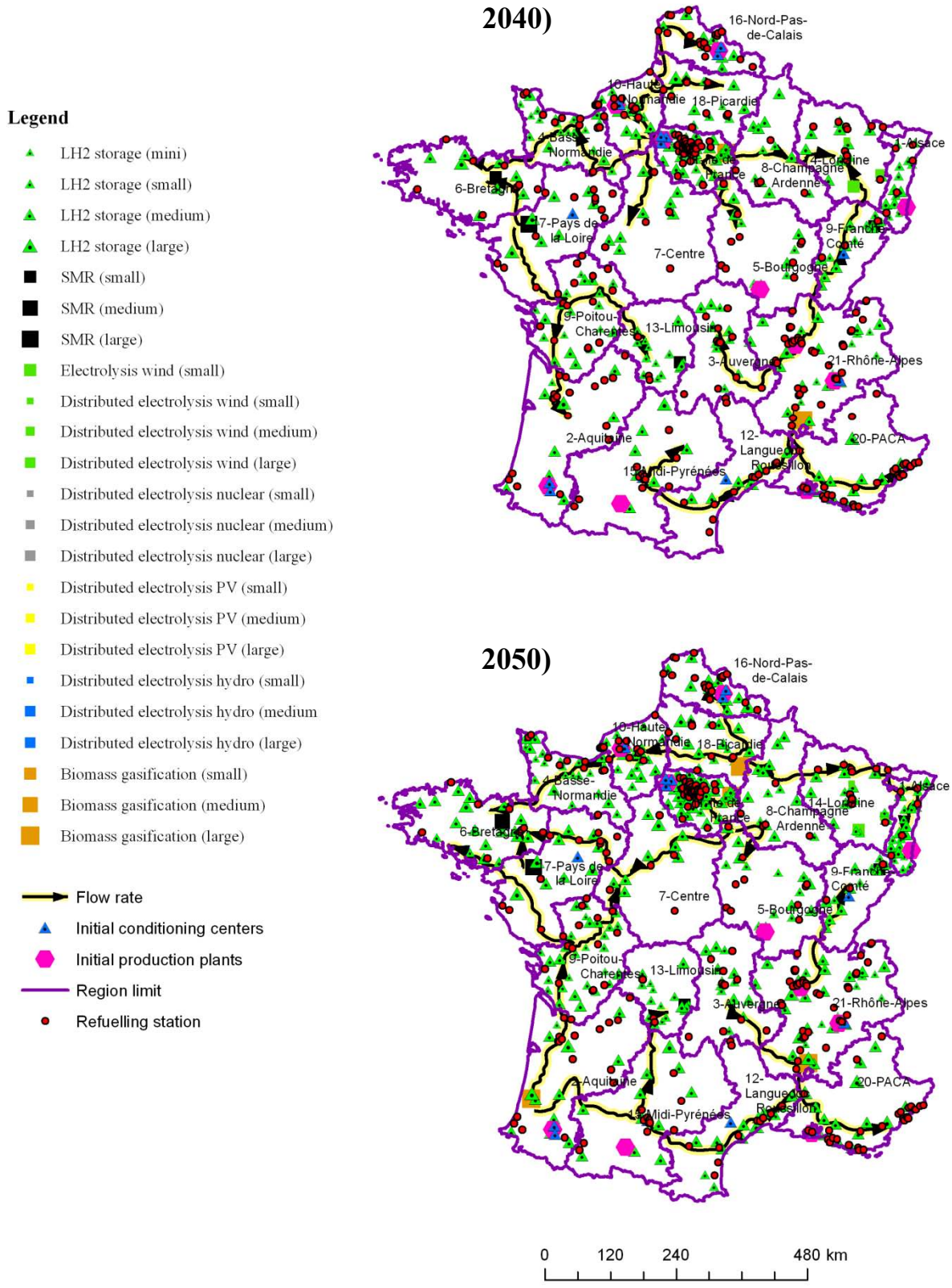


Figure 6.15 Network structure of liquid hydrogen distributed via tanker trucks for the case B2 (multi-objective-mono-period) in 2040-50.

6.4.7 Comparison

All the results are summarised in Table 6.11. In economic terms, the most interesting option to promote the hydrogen economy in 2020 is found in the case B2 (economic cycle) followed by case A1 (cost minimisation) (see Figure 6.16). In both cases, the environmental and safety criteria exhibit high values.

Table 6.11 Comparison between mono-objective and multi-objective results for approaches B1 and B2

		Mono-objective			Multi-objective					
	Solution strategy	**Case A**: Pay-off table obtained by mono-objective optimisation.			**Case B1.** Ɛ-constraint	Difference between B.1 and A1-3			**Case B2**. Economic cycle	Difference between cases B2 and B1
Year	Minimise:	TDC	GWP [39]	Risk	All criteria	TDC	GWP	Risk	TDC and GWP	
2020	Cost per kg H_2 ($)	**4.7**	9.7	7.0	6.5	41%	-32%	-7%	4.5	-31%
	Kg CO_2-equiv per kg H_2	11.1	**4.7**	9.8	7.5	-33%	59%	-23%	11.1	48%
	Total risk (Units)	285	175	**142**	174	-39%	0%	23%	306	76%
2030	Cost per kg H_2 ($)	**4.2**	8.6	7.8	6.1	46%	-29%	-22%	4.5	-26%
	Kg CO_2-equiv per kg H_2	11.0	**2.2**	5.6	4.7	-57%	110%	-17%	6.2	32%
	Total risk (Units)	1153	703	**301**	750	-35%	7%	149%	1799	140%
2040	Cost per kg H_2 ($)	**3.4**	7.0	6.3	4.7	40%	-32%	-25%	4.1	-13%
	Kg CO_2-equiv per kg H_2	11.0	**2.1**	4.6	4.0	-64%	87%	-12%	6.2	55%
	Total risk (Units)	2561	1622	**493**	971	-62%	-40%	97%	2980	207%
2050	Cost per kg H_2 ($)	**3.2**	6.5	6.1	3.9	20%	-41%	-37%	4.1	6%
	Kg CO_2-equiv per kg H_2	11.0	**2.1**	4.7	4.0	-64%	86%	-15%	4.8	20%
	Total risk (Units)	3436	1953	**663**	1280	-63%	-34%	93%	3621	183%
	Number of production plants (2050)	16	67	60	31				20	
	Number of storage units (2050)	261	118	118	127				106	
	Number of transport units (2050)	363	195	0	140				368	
	% Imported demand (2050)	61%	32%	0%	31%				58%	

The multi-objective solution selected in case B1 offers a compromise between the three objectives. The cost in the first period is compared for the different cases in Figure 6.16. Four of five analysed cases are under the maximal target defined in the HyWays roadmap since 2020. This is a very optimistic scenario compared to the Midi-Pyrénées case where the target is reached only in the latest maturity date of 2050. The national scale and the consideration of initial number of storage and production plants have impacted the final results for case B1. Case A2 (CO_2 minimisation) is the more expensive but it can reach the economic targets in 2040. In France, the gasoline price (unleaded 95) on July 2013 was US$7.73 per gallon)[40] and for Diesel US$/6.73 per gallon) (U.K. Drive Alive, 2013)[41].

[39] Bi-criteria results, see Table 6.3.

[40] 19 March 2012 US$1.317 = 1.00 Euro.

Let us remember that one kilogram of hydrogen is approximately equivalent to one gallon of gasoline based on lower heating value energy content.

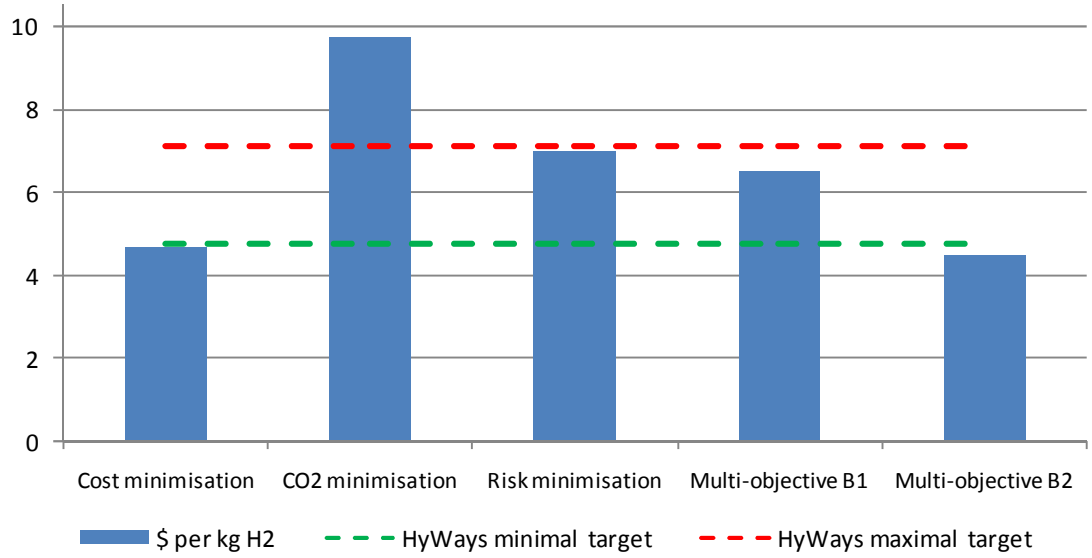


Figure 6.16 Average cost ($ per kg H_2) per case in 2020.

Figure 6.17 compares CO_2 emissions with gasoline and diesel fuels. Only well-to-tank emissions are considered for FCEV and they have been computed from the integration of all the HSC items at each optimisation stage. The HSC would fulfil with the planned EU regulation for all the studied cases (under 113 g CO_2 per km) as it was already observed in Midi-Pyrénées case: the most important contribution results from configuration obtained from the GWP minimisation. In this case, the values relative to approaches B1 and B2 are very high compared to the Midi-Pyrénées case where the production mix promotes the use of RES. For France, the production mix starts with the use of SMR in 2020 and the installation of different types of technologies but the total GWP is higher than in Midi-Pyrénées. This impact decreases over the time horizon and reaches its minimal value by 2050 for both cases with 4 kg CO_2 per kg H_2 for case B1 and 4.8 kg CO_2 per kg H_2 in case B2 (using biomass gasification).

Besides, the risk is mainly associated to transportation. The degree of centralisation can be measured here by the percentage of imported demand. Cases A1 and B2 are the more centralised networks with around 60% of hydrogen to be transported (more than 360 tanker truck are needed by 2050). Similar results for case A2 and B1 are observed with around 32% of hydrogen to be transported. A 100% decentralised network is involved when risk minimisation is considered. In a national case study, the transportation via pipeline could represent an interesting option.

[41]Date: July 18th 2013. The data is collected from various sources, some from official government websites, some from fuel companies' sites, and some from price comparison sites in the respective countries.

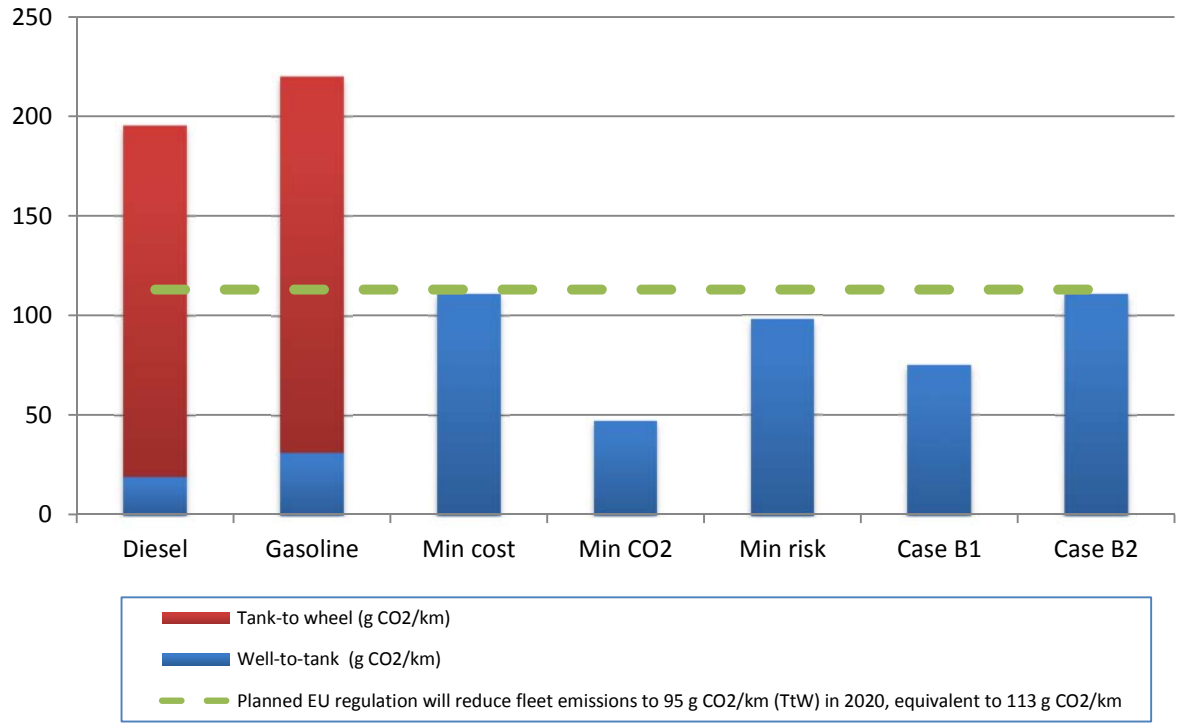


Figure 6.17 Comparison of emissions by sector in 2020 (Data from gasoline and diesel: (ADEME, 2010))

The comparison between approaches is given in Table 6.12. For the studied scenarios, we can conclude that the multi-objective optimisation treated in case B1 offers a good trade-off among the three objectives and is almost competitive since 2020 with low risk and a medium to low digressive environmental impact.

Table 6.12 Comparison between mono-objective and multi-objective results for approaches B1 and B2

Case	TDC	GWP	Risk	B1	B2
Centralisation degree	Centralised production network	Centralised production network	Decentralised network	Mostly decentralised network	Centralised production network
Cost	Competitive since 2020	High investment capital cost in 2020, low digressive cost over the time period.	Low digressive cost over the time period	Almost competitive in 2020	Most competitive cost in 2020
Energy sources	Natural gas	RES for H_2 production	Natural gas and nuclear electricity	Biomass, natural gas and wind	Natural gas and biomass and wind
Risk	Very significant risks associated with the intensification of transport	Significant risk associated to transportation	Low risk mainly due to the lack of transportation	Low risk	Very significant risks
Emissions	Significant environmental impact due to production via SMR	The major benefit obtained from the high volume produced via wind electrolysis	High environmental impact, due to the use of natural gas	Medium-low environmental impact due to the use of biomass and wind	High to medium environmental impact

This configuration resulted in production via biomass gasification (producing 97% of the total demand in 2050) followed by SMR and wind-electrolysis. This is mostly a decentralised network because only the 30% of the total demand is exported from one region to other.

6.5 Conclusion

In this chapter, the optimisation of the HSC was applied to the case of France. The objective was twofold: on the one hand, to examine if the methodology is robust enough to tackle a different geographic scale and second, to see if the regional approach is consistent with the national scale.

New data collection, demand prediction and assumptions were involved but the same model as the one applied to the Midi-Pyrénées region was used here with minor differences. In this case study, the ArcGIS® spatial tool was used before optimisation to identify the geographic items that were further used in the optimisation step. The GIS approach was used to assess potential HSC configurations, by using detailed GIS data, and this database is input as parameters in the MILP model. The mapping of the snapshot solution per time period was also done by Arc-GIS.

Several cases have been analysed. First, the mono-objective optimisation strategy defined as case A (three cases: cost, GWP and risk). Second, the multi-optimisation approach referred to case B1 with Ɛ-constraint. Finally, a new scenario considering the decision maker preferences was described following the economic cycle (case B2).

This chapter ends with a brief comparison between the results obtained with these three approaches. It was concluded that the multi-objective optimisation treated in case B1, offers the best option for production and storage of hydrogen in France because of the good trade-off among the three optimised objectives. In this option, hydrogen is competitive since 2020 with low risk and a medium to low environmental impact. This configuration resulted in production mix lead by biomass gasification (producing 97% of the total H_2 demand by 2050) and followed by SMR and wind-electrolysis. This is a mostly decentralised network which exports 30% of the total demand from one region to other.

In the case B2 that followed the economic cycle simulating the decision maker preferences, even if the cost can be viewed as competitive, the environmental impact is high due to the production from natural gas and the risk is also high because of the important number of transportation links. In the next years, the use of biomass gasification will decrease the CO_2 emissions in the future periods but the optimisation preference given in 2020 impacted strongly the next periods. We have highlighted that if the optimisation preference change in 2030 to GWP, the cost impact is almost the double of that in 2020 (the second period will postpone the depreciation phase because of the change of production technology) but if the environmental regulations forces the diminution of GHG, the SMR established

in 2020 will be underutilized. To cope with this problem, an optimisation run was carried out in order to minimise GWP in 2030 with a boundary value for cost.

One question asked at the beginning of this chapter was: is it possible to find competitive targets for a national case compared to a regional study? Effectively, in the national case, a competitive cost can be found since 2020 for all the analysed cases except for the GWP minimisation. This can be related firstly to the consideration of initial production plants and storage units in the French case and in a second place to the bigger geographic scale divided into regions because this division represents a higher demand volume per region than in the Midi-Pyrénées case. The region/district size represents an important issue for the flow rate and the use of trucks because the tanker truck capacity per trip is 3500 kg of H_2 and in the Midi-Pyrénées case study (divided in districts), the demand per district was lower than the 3.5 t in the first time periods, then, instead to established a distribution link, the optimiser found the installation of a decentralised production plant. This result could change if other transportation modes are assessed. It was surprising that for the national case, results locate plants even in very densely populated regions (e.g. Ile de France). This point needs to be studied in detail before next optimisation to verify if the weight given to the region size is adequate.

The methodology probed that is robust enough to tackle different geographic scales but some differences between the regional and national cases were found:

1. Input data. The amount of energy sources in the Midi-Pyrénées region exists compared to the dedicated study to Midi-Pyrénées that was conducted in the previous chapter. The order of magnitude about the availability for RES is different in regional and national cases. We are aware that this difference could influence the results. No correction was yet performed in order to maintain the same orders of magnitude for all the regions.
2. Output data. In order to compare main results for regional and national cases, we contrast only the chosen option for each case: Case B2 for Midi-Pyrénées and B1 for France (see Table 6.13).

In the French case, multiple regions tend to assume that each geographic area in the model follows exactly the same evolution in demand and energy source evolution. This is a questionable assumption, both because it ignores regional differences in economic and physical geography, and also because it ignores the infrastructure and marketing strategies already being developed by business, which focus planning on clusters around certain locations (Agnolucci and McDowall, 2013). Finding uniform data for all regions is also difficult but it remains an essential task because this will influence the final configuration as shown in the Midi-Pyrénées-France cases where the potential RES of the Midi-Pyrénées region are not used.

Table 6.13 Comparison between regional and national cases.

Case	Midi-Pyrénées	France
Energy sources	Wind, hydro, nuclear (biomass was not evaluated in the regional case because of the lack of data)	Biomass, natural gas and wind
Production type	Electrolysis	Gasification, SMR and electrolysis
Cost	High investment capital cost in 2020 ($13.9 per kg H_2), competitive in 2050 ($7.3 per kg H_2)	Almost competitive since 2020 ($6.5 per kg H2 in 2020 and $3.9 per kg H_2 in 2050)
Risk	Low risk	Low risk
Emissions	The major benefit obtained from the high volume produced via wind and hydro electrolysis	Medium to low environmental impact
Centralisation degree	Decentralised network (15% of the demand is exported)	Mostly decentralised network (30% of the demand is exported)
Flow rate	Demand independent region	In 2020, the Midi-Pyrénées region import H_2 from Rhône-Alpes, in 2030-40 is demand independent exporting product to other regions and in 2050 is demand independent without H_2 exportation.
ArcGIS® tool	Post-optimal spatial analysis	Pre and post-optimal spatial analysis

These differences support the importance to study different spatial scales. Focussing on a single sub-national geographic region as Midi-Pyrénées, allowed to find more refined results because the collected data was more detailed and consistent for all districts but, the use of the ArcGIS® tool only in the post-optimal stage is incomplete.

Chapter 7

GENERAL CONCLUSIONS AND PERSPECTIVES

7.1 Conclusions

The introduction to the market of new propulsion systems such as the fuel cell electric vehicle (FCEV) can be one of promising alternatives to treat problems as energy security, urban air quality and global warming potential. The FCEV power trains use hydrogen as fuel and are competitive to the internal combustion engines in the well-to-wheel efficiency point of view and kilometre range. Hydrogen offers many advantages as a potential fuel and the way as hydrogen economy could be developed is very flexible because many energy sources, production processes, transportation and storage modes exist. It must be yet emphasized that to our knowledge these options are not really interconnected and well-studied and one of the main objective of this research work was to propose a generic modelling framework to embed all these items since the lack of infrastructure may constitute one of the main barriers in the hydrogen and FCEV path. One of the most significant obstacles to achieve the hydrogen transition is the general perception that the cost associated to the infrastructure would be prohibitory expensive compared to the current fuels. According to the HyWays roadmap (European Commission, 2008), H_2 cost must be lower than US$5.3 per kg in periods 2020 and 2030, and H_2 must cost less than US$7.11 per kg in 2050 to reach competitive targets. This fuel can offer a CO_2 reduction in a well-to-wheel comparison with other fossil fuels. One of the main advantages of the FCEV is that is zero pollutant at consumer use. Regarding safety, hydrogen is actually no more dangerous than other flammable fuels such as gasoline and natural gas. Nevertheless, under specific conditions, hydrogen can behave dangerously. To ensure the safely use of hydrogen, risk management must be rigorously appreciated.

Currently, a large amount of literature related to hydrogen can be found. The roadmaps as HyWays and H_2 mobility are guiding many projects in Europe. They establish a certain number of targets in a very general perspective. In some cases, not all the network is considered but a particular activity (e.g. to install a certain number of refuelling stations). Moreover, some transition plan scenarios study different ways as the hydrogen economy could be reached and they evaluate external variables as competitors and demand. Engineering tools can be linked to the abovementioned studies to give detailed results.

The scientific objective of this thesis was to model the whole hydrogen supply chain (HSC) and to consider the different objectives that are involved in the design problem, i.e. cost, environmental impact, safety. The scientific aim was to develop a generic framework that can take into account the design of a HSC for fuel use in the time horizon 2020-2050 considering national and regional scales with many energy sources and that can embed the various production and storage technologies while considering the transportation modes to link hydrogen demand to its supply. More practically, an optimisation tool that could allow the generation of quantitative information when all the nodes of the supply chain are defined and integrated was developed. Particular emphasis was devoted to address the multi-objective formulation in which cost, environmental impact and safety must be simultaneously taken into account at the earlier design stage.

Problem formulation is based on mathematical programming. The work reported in (Almansoori and Shah, 2006) constitutes a consistent way to model the typical items of the supply chain and their interconnection in a mono-objective way considering only cost minimisation. The novelty of our work was to extend the model to new constraints and objectives related to environmental and safety aspects in order to treat the multi-objective problem. To our knowledge, these aspects have not yet been simultaneously treated in the dedicated HSC literature. The problem corresponds to a location-routing type to design at a strategic level the HSC using deterministic data in multi-period formulations for the long term scenario defined to the year 2050. The problem is referred to a mixed integer linear programming (MILP).The proposed framework takes into account the geographic and infrastructure constraints through the use of a geographic information system (GIS). Very few contributions have reported to date considering hydrogen infrastructure modelling across spatial scales; we address here the national and regional scale by linking geographic constraints found by GIS model to the MILP model. The resulting hydrogen network would heavily depend on the country/region-specific conditions.

All the activities of the HSC (i.e. energy source, production, storage, transportation and refuelling stations) used in this manuscript were presented in the dedicated chapters. The steam methane reforming is the leader process nowadays. Some technologies that are considered in the literature as possible technologies are only at a development stage and technical and/or economic aspects are not

proven or available (for example the thermo-chemical cycles or storage via metal hydrides). This explains why they have not been considered in this thesis. Sequestration and capture methods could be used to reduce emissions, but will induce additional costs. Pipelines were not considered in this work mainly for two reasons: first, they are considered to become relevant once a significant market penetration of hydrogen vehicles and second they are associated with a high capital cost.

The developed methodology is described below:

A. Mono-objective optimisation. The mathematical model described in (Almansoori and Shah, 2006) work addressed the optimal design of a steady-state HSC network with cost as an optimisation criterion. This model served as a validation step in the GAMS environment with the CPLEX solver. The model was extended to the consideration of safety and environmental criteria.
B. Multi-objective optimisation. This constitutes a key point of the proposed methodological framework: the minimal values of each objective function allow generating a pay-off table through lexicographic optimisation. The utopia and nadir points are also found and the Pareto front via ε-constraint method can be built in order to analyse the compromise solutions.
C. Multi criteria decision making (MCDM) via M-TOPSIS technique to identify a good compromise solution.
D. The last step consists in the spatial analysis using ArcGIS® to design the HSC.

Three case studies were treated as summarised in Table 7.1. The case study proposed in (Almansoori and Shah, 2006) is relative to a HSC in Great Britain. As abovementioned, this case study serves to validate the developed model for mono-objective optimisation in a mono-period problem. It is then extended to the multi-optimisation case. From the case study analysis, it must be highlighted that the model can identify the optimal HSC including the number, location, capacity, and type of production, transport and storage facilities, production rate of plants and average inventory in storage facilities, hydrogen flow rate and type of transportation links to be established. The main differences found between the mono- and multi-objective approaches are related to the degree of the production decentralisation that increases as risk criterion and CO_2 emissions are taken into account. We concluded that a geographic division based on states, regions or districts instead of grid squares would be more realistic to facilitate data collection and that the model must be extended to treat electrolysis production process and a panel of renewable energy sources. According to the data, compressed hydrogen turned out to be cost prohibitive due to high transportation and storage costs (without considering the possibility to use pipeline) under low demand rates.

Table 7.1 Comparison between multi-objective case studies.

Case	**Great Britain**	**Midi-Pyrénées**	**France**
Energy sources	Natural gas and biomass	Wind, hydro, nuclear (biomass was not evaluated in the regional case because of the lack of data)	Biomass, natural gas and wind
Production technology	SMR and gasification (electrolysis was not evaluated)	Electrolysis	Gasification, SMR and electrolysis
Cost	Competitive in 2050 ($7.1 per kg H_2)	High investment capital cost in 2020 ($13.9 per kg H_2), almost competitive in 2050 ($7.3 per kg H_2)	Almost competitive since 2020 ($6.5 per kg H_2, HyWays target= $5.3 per kg H_2) but competitive in 2050 ($3.9 per kg H_2)
Risk	Low risk	Low risk	Low risk
Emissions	Medium environmental impact	Low environmental impact	Medium to low environmental impact
Centralisation degree	Decentralised network	Decentralised network	Mostly decentralised network
Geographic division	Grids	Districts	Regions
ArcGIS® tool	-	Post-optimal spatial analysis	Pre and post-optimal spatial analysis
Data base	Academic case	More precision	Less precision
Approach type	Process engineering approach, different from the roadmaps and planning scenarios	Process engineering approach, with regional real application and spatial analysis	Process engineering approach in a national scale with spatial analysis before and after optimisation
Scale	National	Regional	National
Difficulties	Data collection	Problem size, data collection	Data collection and problem size
Use type	Multi-objective validation	Model augmentation, scale validation and communication	Scale validation, different scenarios including decision maker preferences and communication.

At the regional level, the HSC was designed for the Midi-Pyrénées region through the project "Green H_2 fuel" in the time horizon from 2020 to 2050. The mathematical model presented in Chapter 4 was adapted to the region and considered two new nodes: energy sources and refuelling stations. Two approaches were taken into account involving mono- and multi-objective optimisation. For the latter one, case B1 (Ɛ-constraint method in a multi-period problem) and case B2 (lexicographic+Ɛ -constraint method in four mono-period problems) were compared when three objectives (cost, CO_2 and risk) were optimised. From the given data, it was observed that if all the RES would be available to produce H_2, 89% of them would be necessary in 2050 to cover H_2 fuel demand: more RES investment or the use of other type of energy to cover the electrical grid need are then required. This topic was also tackled in the National Debate of the Energetic Transition. For case B1, cost in the first

time period is prohibitive in Midi-Pyrénées. A better option for the 2020 period is given by the case B2 exhibiting good results for GWP and risk while hydrogen cost remains high ($13.9 per kg H_2). It must be highlighted that the risk is mainly attributed to transportation. The use of PV energy source for hydrogen production is not so developed because of the CO_2 emissions linked to the grey energy involved in the panel design and does not succeed in the competition with wind, hydro or nuclear-electrolysis.

A spatial-based approach was used to have a more realistic snapshot in the Midi-Pyrénées HSC. ArcGIS® allowed the integration of geographic and demographic data of the region: the results show that the production centers (small, medium and large) and the refuelling stations are near as possible from the main road. This post-optimisation step allows analysing the feasible and the best solutions considering geographic criteria. We concluded that it would be better to use ArcGIS® in the pre-optimising stage by considering the real distances between each main city in order to evaluate a more realistic value of the optimal HSC. Based on these results, this regional scale case is then compared to the case of France.

For the national case study, the ArcGIS® spatial tool was used before optimisation to identify the geographic items that were further used in the optimisation step. The mapping of the snapshot solution per time period was also carried out. Several cases were analysed. The multi-optimisation approaches were referred as case B1 (Ɛ-constraint) and new scenarios considering the decision-maker preferences were considered following an economic cycle (case B2). It was emphasized that the multi-objective optimisation treated in case B1 offers the best option for production and storage of hydrogen in France because of the good trade-off among the three optimised objectives. In this option, hydrogen is almost competitive since 2020 with low risk and a medium to low environmental impact. In the case B2, the optimisation preference of 2020 impacted strongly the next periods.

One question asked was if is it possible to find competitive targets for a national case compared to a regional study: in the national case, a lower cost can be found in 2020 for all the analysed cases except for the GWP minimisation. This can be related firstly to the consideration of initial production plants and storage units in the French case and second to the larger geographic scale divided into regions. The region/district size represents an important issue for the flow rate and the use of trucks because the tanker truck capacity per trip is 3500 kg of H_2 and in the Midi-Pyrénées case study (divided in districts), the demand per district was lower than the 3.5 t in the first time periods. This explains a decentralised production plant network is found by optimisation. This result could change if other transportation modes are assessed. Surprisingly, for the national case, optimisation results lead to locate plants even in very populated regions (e.g. Ile de France). Hydrogen and FCEV reach the environmental targets for all the treated cases.

7.2 Lessons learned

The multi-period problem is larger and difficult to be solved by the lexicographic methodology but this difficulty led us to seek new ways of solution. The four mono-period problem turns out to be an interesting option that helps also in the first investment stage. We are aware that the analysis was performed with constant cost and that a discounted analysis would be more consistent. This could be further improved for investment assessment.

The input configuration requires a hard and detailed analysis and needs to be validated by an expert diversified team. The current hydrogen infrastructure must be integrated to find competitive costs in the first time period and to launch the market.

The geographic scale strongly influences the decision:

- the Midi-Pyrénées case provides a more optimistic assessment of renewable energy sources (RES) based on electrolysis due to the detailed technical and locating data for RES sites and energy availability;
- in the national case, the scale economy plays a major role in making biomass hydrogen competitive.

Compared to the reported roadmaps and transition plan scenarios, the work presented here gives a more reliable estimation of cost, CO_2 emissions and risk due to the systemic approach involving the supply chain management.

The methodology proved to be robust enough to tackle different geographic scales but some inconsistencies between the regional and national cases were found. The order of magnitude about the availability for RES is different in regional and national cases. We are aware that this difference could influence the results. No correction was yet performed in order to maintain the same order of magnitude for all the regions.

In the French case, multiple regions tend to assume that each geographic area in the model follow exactly the same evolution in demand and energy source evolution. This is a questionable assumption, both because it ignores regional differences in economic and physical geography, and also because it ignores the infrastructure and marketing strategies already being developed by business, which focus planning on clusters around certain locations (Agnolucci and McDowall, 2013). Finding uniform data for all regions was difficult but it remains an essential task because this will influence the final configuration as shown in the Midi-Pyrénées/France cases.

These differences support the importance to study different spatial scales. Focussing on a single sub-national geographic region as Midi-Pyrénées allowed finding more refined results because the collected data was more detailed and consistent for all districts.

From Table 7.1, it can be observed that the multi-objective optimisation tends to the decentralisation of the network so that the transportation risk is decreased. Depending on the input configuration, the technology mix leads to the use of renewable energy. Yet, the input configuration and assumptions are a limiting factor in the optimisation process. A competitive cost can be found in 2050 for all cases. The geographic scale affects the cost, but also the consideration of current production and storage H_2 facilities. The investment phase can be minimised for the first time by solving four mono-period problems. The use of ArcGIS is highly recommended both in pre- and post-optimisation phases.

7.3 Main contributions

The main contributions of this research work can be highlighted as follows:

- a multi-objective model addressing three objective functions to take into account sustainability minimising cost, CO_2 emissions and risk was developed.
- as the HSC problem is very large, three different solution approaches were proposed: mono-objective optimisation, multi-objective through Ɛ-constraint and finally multi-objective through a hybrid method (lexicographic+Ɛ-constraint).
- the optimisation framework was applied across a range of spatial scales. We have compared regional and national models. To our knowledge and as reported in (Agnolucci and McDowall, 2013), a few infrastructure optimisation studies tested the sensitivity of their analysis to assumptions about the spatial and temporal dynamics of demand. Yet the transition rate has an important effect on both costs and choice of the infrastructure, and there is some evidence from historical analogies that the transition rates widely assumed in the literature may be optimistic. The coupling of ArcGIS® analysis in pre- and post-optimisation stages can be very useful for this purpose.
- Time evolution constraints (related to the initial production plants and storage units) allow for the transfer of production and storage plants across time periods.
- The developed tool can be useful to assess different HSC scenarios and gives detailed results to aid the decision-making process.

7.4 Perspectives

Finally, several perspectives can be suggested in order to improve the proposed framework.

- This study was devoted to strategic planning. An operational HSC level integrating the three criteria using ArcGIS® could be investigated considering the intra grid/region transport. This issue will be addressed in the thesis of Christophe Salingue (October 2013).

- Demand modelling can be improved. The spatial model considered here takes an exogenously demand scenario as an input. Spatial variations in hydrogen demand have simply assumed constant penetration rates across regions.
- New energy sources such as biogas can be taken into account. The consideration in future periods of new technologies that currently are in development stage can be suggested: for instance carbon capture and storage, pipelines for high volume scenarios using the current natural gas pipeline to inject a H_2 percentage. The possibility to use the by-produced hydrogen integrating the additional costs associated to the purification step can be studied.
- The Power-to-Gas system modelling can be a natural extension to H_2 supply chain, in this system, hydrogen produced can be fed into the existing natural gas network for further use and replace natural gas on a like-for-like basis. Gas storage is not subject to the same limitations associated with hydrogen storage.
- Concerning optimisation, the use of dynamic programming (DP) can be a more appropriate way to model the problem.
- A rigorous treatment of uncertainty, going beyond the attempts we have seen so far in the literature, would a very useful improvement for policy maker and private investors alike.
- Concerning the production cost in the mathematical model, the unit production cost (UPC) remains static for all the time periods for a production plants p varying only for the size j. In the reality, the cost and availability of feedstock are critical and not fixed. We propose to change the UPC considering: fixed facilities costs (maintenance, labour cost), electricity cost and feedstock cost with variations for each time period.



A. DATABASE AND RESULTS FOR GREAT BRITAIN CASE

APPENDIX A.1 SUPPLY CHAIN DECISION DATABASE

Table A.1.1 – Total demand for product form *i* in grid *g* (kg per day)

Grid	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**
Liquid H_2	102000	80000	158000	198000	41000	130000	173000	7000	85000	316000	385000	9000	635000	902000
Grid	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**
Liquid H_2	143000	24000	489000	997000	500000	41000	63000	624000	1000000	861000	356000	63000	394000	879000
Grid	**29**	**30**	**31**	**32**	**33**	**34**	**Total (kg per day)**							
Liquid H_2	3000000	200000	208000	252000	200000	136000	**13395000**							

Table A.1.2 – Parameters for hydrogen supply chain components: (a) general data, (b) production, (c) storage, and (d) transportation modes.

	(a) General data	
α	Network operating period	365 days per year
CCF	Capital change factor -payback period of capital investment	3 years
WFP_g	Weigh factor risk population in each grid	units (see Table A.2.6)

(b) Production plants				
Plant type, *p*	Steam methane reforming	Biomass gasification	Coal gasification	Reference
Minimum production capacity of plant type *p* for product form *i* . $Pcapmin_{pi}$ (t/d)	10	10	10	(Almansoori and Shah, 2006)
Maximum production capacity of plant type *p* for product form *i* . $Pcapmax_{pi}$ (t/d)	480	480	480	(Almansoori and Shah, 2006)
Capital cost of establishing plant type *p* producing product form *i*. PCC_{pi} ($10+6)	535	1412	958	(Almansoori and Shah, 2006)
Unit production cost for product form *i* produced by plant type *p*. UPC_{pi} ($ per kg)	1,53	3,08	1,71	(Almansoori and Shah, 2006)
Production global warming potential by plant type *p*. GW^{Prod}_{p} gCO_2-eq per kg H_2	10100	3100	10540	(*Detailed California Modified GREET Pathway for Compressed Gaseous Hydrogen from North American Natural Gas*, 2009; Rivière, 2007; Utgikar and Thiesen, 2006)
Risk level of the production facility *p*. RP_p level	III	III	III	(Kim and Moon, 2008)

(c) Storage data		
Storage type, *s*	Liquid storage	Reference
Minimum storage capacity of storage type *s* for product form *i* . $Scap^{min}_{si}$ (kg)	10000	(Almansoori and Shah, 2006)
Maximum storage capacity of storage type *s* for product form *i*. $Scap^{max}_{si}$, (kg)	540000	(Almansoori and Shah, 2006)
Capital cost of establishing storage type *s* storing product form *i*. $SCC_{si\ (\$)}$	122000000	(Almansoori and Shah, 2006)
Unit storage cost for product form *i* at storage type *s*. $USC_{si\ (\$\ per\ kg\ per\ day)}$	0.005	(Almansoori and Shah, 2006)
Storage holding period-average number of days worth of stock . β (days)	10	(Almansoori and Shah, 2006)
Storage global warming potential form *i*. GW^{Stock}_{i} (g CO_2-eq per kg of H_2)	5241	(*Detailed California Modified GREET Pathway for Compressed Gaseous Hydrogen from North American Natural Gas*, 2009)
Risk level in storage facility *s*. RS_s (units)	III	(Kim and Moon, 2008)
(d) Transportation Modes		
Transportation mode, *l*	Tanker truck	Reference
Transport unit capacity, $Tcap_{il}$ (kg/mode)	4082	(Almansoori and Shah, 2006)
Fuel economy between grids, FE_l (km/L)	2.55	(Almansoori and Shah, 2006)
Average speed between grids, SP_l (km/hr)	55	(Almansoori and Shah, 2006)
Tanker truck weight, w_l tons	40	(McKinnon and Piecyk, 2011)
Mode availability between grids, TMA_l (hr/d)	18	(Almansoori and Shah, 2006)
Load/unload time, LUT_l (hr)	2	(Almansoori and Shah, 2006)
Driver wage, DW_l ($/hr)	23	(Almansoori and Shah, 2006)
Fuel price, FP_l ($/L)	1.16	(Almansoori and Shah, 2006)
Maintenance expenses, ME_l ($/km)	0.0976	(Almansoori and Shah, 2006)
General expenses, GE_l ($/d)	8.22	(Almansoori and Shah, 2006)
Transport mode cost, TMC_{il} ($/mode)	500	(Almansoori and Shah, 2006)
Minimum flow rate of product form i , $Qmin_{il}$ (kg/d)	4082	(Almansoori and Shah, 2006)
Maximum flow rate of product form i, $Qmax_{il}$ (t/d)	960	(Almansoori and Shah, 2006)
Global warming potential $GWTrans_l$ (g CO_2 per ton-km)	62	(McKinnon and Piecyk, 2011)
Risk level of transportation mode *l*, RT_l (Level)	III	(Kim and Moon, 2008)

Table A.1.3 Delivery distances within and between different grids squares (km per trip).

Grid	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
1	**65**	108	108	152	206	216	241	344	328	341	415	404	446	482	536	664	587	580	631	730	706	682	682	723	831	791	788	785	821	843	972	899	837	852
2	108	**65**	152	152	197	247	247	352	346	351	459	408	457	492	529	673	597	587	648	746	715	691	691	749	835	802	795	795	827	853	983	909	848	861
3	108	152	**65**	108	162	108	152	248	222	241	323	298	344	389	421	563	487	482	539	637	655	581	580	628	736	743	689	685	723	749	870	796	735	751
4	152	152	108	**65**	54	152	108	216	222	216	282	290	323	349	390	533	457	449	496	596	577	553	552	590	663	663	656	656	688	710	843	769	709	722
5	206	197	162	54	**65**	194	120	228	241	228	291	314	332	361	399	548	471	461	509	609	590	566	565	602	675	677	670	670	701	723	856	783	723	735
6	216	247	108	152	194	**65**	108	170	120	152	241	197	248	305	345	476	400	389	457	551	510	492	484	539	617	606	597	597	629	658	787	713	650	662
7	241	247	152	108	120	108	**65**	108	120	108	174	194	216	241	283	427	351	341	389	488	469	445	444	482	555	556	550	550	580	602	736	662	602	614
8	344	352	248	216	228	170	108	**65**	120	76	76	194	170	170	194	368	292	275	314	415	403	381	381	410	482	502	488	488	511	531	679	605	542	550
9	328	346	222	222	241	120	120	120	**65**	54	162	76	130	194	241	359	283	271	345	435	401	375	366	421	502	489	448	480	514	540	670	596	533	537
10	341	351	241	216	228	152	108	76	54	**65**	108	54	108	152	194	323	247	241	305	399	365	343	341	389	466	451	444	444	482	508	629	555	497	511
11	415	459	323	282	291	241	174	76	162	108	**65**	222	152	108	130	323	247	216	248	344	361	341	323	341	411	451	444	431	444	460	629	555	485	488
12	404	408	298	290	314	197	194	194	76	54	222	**65**	162	228	278	390	314	302	377	467	423	406	406	453	533	507	500	500	542	571	686	612	552	568
13	446	457	344	323	332	248	216	170	130	108	152	162	**65**	108	162	229	152	152	241	323	271	247	247	305	390	359	351	351	389	421	540	466	404	410
14	482	492	389	349	361	305	241	170	194	152	108	228	108	**65**	54	229	152	108	152	248	271	241	216	241	361	349	341	323	341	361	522	448	377	381
15	536	529	421	390	399	345	283	194	241	194	130	278	162	54	**65**	269	194	120	120	224	305	269	222	222	343	381	361	328	328	341	535	461	381	377
16	664	673	563	533	548	476	427	368	359	323	323	390	229	229	269	**65**	76	170	275	323	54	76	170	275	381	130	170	229	314	361	389	315	269	305
17	587	597	487	457	471	400	351	292	283	247	247	314	152	152	194	76	**65**	108	216	276	120	108	152	241	341	197	216	241	305	345	416	343	290	314
18	580	587	482	449	461	389	341	275	271	241	216	302	152	108	120	170	108	**65**	108	174	194	152	108	152	241	269	241	216	241	269	416	343	269	275
19	631	648	539	496	509	457	389	314	345	305	248	377	241	152	120	275	216	108	**65**	108	290	241	152	108	174	361	305	241	216	224	464	389	290	275
20	730	746	637	596	609	551	488	415	435	399	344	467	323	248	224	323	276	174	108	**65**	328	275	170	76	76	392	314	229	170	162	464	381	269	241
21	706	715	655	577	590	510	469	403	401	365	361	423	271	271	305	54	120	194	290	328	**65**	54	162	269	377	76	120	194	290	341	347	273	229	269
22	682	691	581	553	566	492	445	381	375	343	341	406	247	241	269	76	108	152	241	275	54	**65**	108	216	323	120	108	152	241	290	315	241	194	229
23	682	691	580	552	565	484	444	381	366	341	323	406	247	216	222	170	152	108	152	170	162	108	**65**	108	216	222	152	108	152	194	315	241	162	170
24	723	749	628	590	602	539	482	410	421	389	341	453	305	241	222	275	241	152	108	76	269	216	108	**65**	108	328	241	152	108	120	389	305	194	170
25	831	835	736	663	675	617	555	482	502	466	411	533	390	361	343	381	341	241	174	76	377	323	216	108	**65**	434	341	241	152	130	484	415	269	229
26	791	802	743	663	677	606	556	502	489	451	451	507	359	349	381	130	197	269	361	392	76	120	222	328	434	**65**	120	222	328	381	365	291	247	290
27	788	795	689	656	670	597	550	488	448	444	444	500	351	341	361	170	216	241	305	314	120	108	152	241	341	120	**65**	108	216	269	248	174	130	174
28	785	795	685	656	670	597	550	488	480	444	431	500	351	323	328	229	241	216	241	229	194	152	108	152	241	222	108	**65**	108	162	241	174	54	76
29	821	827	723	688	701	629	580	511	514	482	444	542	389	341	328	314	305	241	216	170	290	241	152	108	152	328	216	108	**65**	54	341	276	120	76
30	843	853	749	710	723	658	602	531	540	508	460	571	421	361	341	361	345	269	224	162	341	290	194	120	130	381	269	162	54	**65**	392	329	170	120
31	972	983	870	843	856	787	736	679	670	629	629	686	540	522	535	389	416	416	464	464	347	315	315	389	484	365	248	241	341	392	**65**	108	222	275
32	899	909	796	769	783	713	662	605	596	555	555	612	466	448	461	315	343	343	389	381	273	241	241	305	415	291	174	174	276	329	108	**65**	162	216
33	837	848	735	709	723	650	602	542	533	497	485	552	404	377	381	269	290	269	290	269	229	194	162	194	269	247	130	54	120	170	222	162	**65**	54
34	852	861	751	722	735	662	614	550	537	511	488	568	410	381	377	305	314	275	275	241	269	229	170	170	229	290	174	76	76	120	275	216	54	**65**

Table A.1.4. Total relative road risk matrix (units).

Grid	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34
1	0	3	4	6	7	6	8	9	7	9	11	8	13	15	17	16	15	18	20	22	19	18	21	23	25	20	20	24	27	29	24	22	26	28
2	3	0	5	3	4	7	5	6	8	7	9	9	10	12	14	16	15	15	17	21	19	18	21	24	26	20	20	24	27	29	30	28	26	28
3	4	5	0	4	5	4	6	7	5	8	10	6	11	13	15	16	15	16	18	24	19	18	21	22	24	20	20	24	25	27	30	28	26	26
4	6	3	4	0	3	6	4	5	7	6	8	8	9	12	14	14	13	15	17	23	17	16	18	20	22	19	18	21	23	25	27	25	23	24
5	7	4	5	3	0	7	5	6	9	7	9	10	10	12	14	18	17	15	17	22	21	20	18	21	23	23	21	21	24	26	27	25	23	25
6	6	7	4	6	7	0	4	5	3	6	8	4	9	11	13	12	11	14	16	22	15	14	17	20	22	16	16	20	23	25	19	18	22	24
7	8	5	6	4	5	4	0	3	5	4	6	6	7	10	12	10	9	13	14	20	13	12	16	19	21	15	14	19	22	24	24	23	24	23
8	9	6	7	5	6	5	3	0	6	5	3	7	8	6	8	11	10	9	11	17	14	13	12	15	17	16	15	15	18	20	21	19	17	19
9	7	8	5	7	9	3	5	6	0	3	5	2	6	8	10	9	8	11	13	19	12	11	14	17	19	13	13	17	20	22	23	21	19	20
10	9	7	8	6	7	6	4	5	3	0	4	5	5	8	10	8	7	11	13	19	11	10	14	17	19	13	12	17	20	22	22	21	19	20
11	11	9	10	8	9	8	6	3	5	4	0	6	8	5	7	11	10	8	10	16	15	14	11	14	16	17	16	14	17	19	20	18	16	18
12	8	9	6	8	10	4	6	7	2	5	6	0	7	10	12	10	9	13	15	21	20	19	16	19	21	22	21	19	22	24	25	23	21	23
13	13	10	11	9	10	9	7	8	6	5	8	7	0	6	8	6	5	9	11	17	16	15	12	15	17	18	17	15	18	20	21	19	17	19
14	15	12	13	12	12	11	10	6	8	8	5	10	6	0	5	9	8	6	8	14	13	12	9	12	14	15	14	12	15	17	18	16	14	16
15	17	14	15	14	14	13	12	8	10	10	7	12	8	5	0	11	10	8	4	10	15	14	11	7	9	17	16	14	10	12	20	18	16	11
16	16	16	16	14	18	12	10	11	9	8	11	10	6	9	11	0	3	6	8	14	7	6	9	12	14	9	8	11	14	16	15	13	13	14
17	15	15	15	13	17	11	9	10	8	7	10	9	5	8	10	3	0	5	7	13	6	5	8	11	13	8	7	10	13	15	14	12	12	13
18	18	15	16	15	15	14	13	9	11	11	8	13	9	6	8	6	5	0	5	11	9	8	6	9	11	11	10	9	12	14	15	13	13	14
19	20	17	18	17	17	16	14	11	13	13	10	15	11	8	4	8	7	5	0	8	11	10	8	5	7	13	12	11	8	10	17	15	13	14
20	22	21	24	23	22	22	20	17	19	19	16	21	17	14	10	14	13	11	8	0	13	12	9	6	3	14	14	12	9	5	18	16	14	15
21	19	19	19	17	21	15	13	14	12	11	15	20	16	13	15	7	6	9	11	13	0	4	7	10	12	2	4	7	10	12	11	9	9	10
22	18	18	18	16	20	14	12	13	11	10	14	19	15	12	14	6	5	8	10	12	4	0	6	9	11	6	5	9	12	14	15	13	11	12
23	21	21	21	18	18	17	16	12	14	14	11	16	12	9	11	9	8	6	8	9	7	6	0	6	8	9	8	6	9	11	12	10	8	9
24	23	24	22	20	21	20	19	15	17	17	14	19	15	12	7	12	11	9	5	6	10	9	6	0	5	12	11	9	6	8	15	13	11	7
25	25	26	24	22	23	22	21	17	19	19	16	21	17	14	9	14	13	11	7	3	12	11	8	5	0	14	13	11	8	10	17	15	13	9
26	20	20	20	19	23	16	15	16	13	13	17	22	18	15	17	9	8	11	13	14	2	6	9	12	14	0	3	6	9	11	10	8	8	9
27	20	20	20	18	21	16	14	15	13	12	16	21	17	14	16	8	7	10	12	14	4	5	8	11	13	3	0	5	8	10	9	7	7	8
28	24	24	24	21	21	20	19	15	17	17	14	19	15	12	14	11	10	9	11	12	7	9	6	9	11	6	5	0	6	8	9	7	5	6
29	27	27	25	23	24	23	22	18	20	20	17	22	18	15	10	14	13	12	8	9	10	12	9	6	8	9	8	6	0	5	12	10	8	4
30	29	29	27	25	26	25	24	20	22	22	19	24	20	17	12	16	15	14	10	5	12	14	11	8	10	11	10	8	5	0	14	12	10	6
31	24	30	30	27	27	19	24	21	23	22	20	25	21	18	20	15	14	15	17	18	11	15	12	15	17	10	9	9	12	14	0	4	6	7
32	22	28	28	25	25	18	23	19	21	21	18	23	19	16	18	13	12	13	15	16	9	13	10	13	15	8	7	7	10	12	4	0	4	5
33	26	26	26	23	23	22	24	17	19	19	16	21	17	14	16	13	12	13	13	14	9	11	8	11	13	8	7	5	8	10	6	4	0	3
34	28	28	26	24	25	24	23	19	21	20	18	23	19	16	11	14	13	14	14	15	10	12	9	7	9	9	8	6	4	6	7	5	3	0
Total	531	526	515	469	514	434	414	372	386	374	377	462	402	373	390	367	335	360	385	492	391	389	378	428	487	421	400	420	472	530	565	507	475	487

Table A.1.5 – Level risk according to harmfulness for people, the environment and facilities for hydrogen activities.

Harmfulness for	Level II	Level III	Level IV
People	Medical treatment and lost time injury	Permanent disability	Several fatalities
Environment	Damage of short duration (<1 month)	Time for restitution of ecological resource (<1 year)	Time for restitution of ecological resource (1–3 years)
Facilities	Minor structural damage and minor influence on operations.	Considerable structural damage and operation interrupted for weeks	Loss of main part of system and operation interrupted for months.
Weighted scoring method	3	5	7

Table A.1.6 – Example of external effect factors gained during transportation from grid 1 to 33.

From grid 1 to 33				
grid	size	grid safety level	weight factor of adjacency level	total
1	Med	2	1	2
2	Small	1	0.5	0.5
3	Med	2	0.5	1
4	Med	2	1	2
5	Small	1		0
6	Med	2		0
7	Med	2	1	2
8	Small	1		0
9	Small	1		0
10	Med	2	1	2
11	Med	2		0
12	Small	1		0
13	Large	3	1	3
14	Large	3		0
15	Med	2		0
16	Small	1		0
17	Med	2	1	2
18	Large	3	0.5	1.5
19	Med	2		0
20	Small	1		0
21	Small	1		0
22	Large	3	0.5	1.5
23	Large	3	1	3
24	Large	3		0
25	Med	2		0
26	Small	1		0
27	Med	2		0
28	Large	3	1	3
29	Large	3		0
30	Med	2		0
31	Med	2		0
32	Med	2		0
33	Med	2	1	2
34	Small	1		0
			Total	25.5

APPENDIX A2: DETAILED RESULTS

Table A.2.1 - Flow rate of liquid hydrogen via tanker truck for cases 1 to 4.

Case 1. Mono-objective optimisation. Min **TDC**.		
From grid	To grid	Flow rate, $Q_{ilgg'}$ (kg d^{-1})
3	1	102130
3	2	80020
3	4	12396
3	6	123203
7	4	185544
7	5	41060
7	6	6297
7	8	7370
7	9	67059
10	9	18221
10	12	9480
10	13	136359
11	13	9761
11	15	87377
14	13	8910
14	15	48850
22	16	24450
22	17	8520
22	18	36640
22	21	63170
22	23	87490
22	26	62810
22	33	14101
24	15	6693
24	19	11453
24	30	80824
25	19	5977
25	20	40610
25	30	74212
27	33	86270
28	33	66036
28	34	15424
29	30	32924
29	34	120506
32	31	207720
32	33	18623
	TOTAL	2008490

Case 2. Mono-objective optimisation. Min **GWP**.		
From grid	To grid	Flow rate, $Q_{ilgg'}$ (kg d^{-1})
9	12	9480
11	8	7370
16	17	8520
	TOTAL	25370

Case 3. Mono-objective optimisation. Min **Risk**.		
From grid	To grid	Flow rate, $Q_{ilgg'}$ (kg d^{-1})
9	12	9480
11	8	7370
16	17	8520
	TOTAL	25370

Case 4. Multi-objective optimisation. Min **TDC+GWP+Risk.**		
From grid	To grid	Flow rate, $Q_{ilgg'}$ (kg d^{-1})
9	12	9480
11	8	7370
16	17	8520
	TOTAL	25370

Table A.2.2 - Summary of results for cases 1 to 4

Case 1.					*Case 2, 3 and 4*		
Variable	**DL_{ig}** (kg d^{-1})	**DI_{ig}** (kg d^{-1})	**PT_{ig}** (kg d^{-1})	**ST_{ig}** (t)*	**DL_{ig}** (kg d^{-1})	**DI_{ig}** (kg d^{-1})	**PT_{ig}** (kg d^{-1})
G.1	-	102130	-	1021.3	102130	-	102130
G.2	-	80020	-	800.2	80020	-	80020
G.3	157930	-	475679	1579.3	157930	-	157930
G.4	-	197940	-	1979.4	197940	-	197940
G.5	-	41060	-	410.6	41060	-	41060
G.6	-	129500	-	1295	129500	-	129500
G.7	172670	-	480000	1726.7	172670	-	172670
G.8	-	7370	-	73.7	-	7370	
G.9	-	85280	-	852.8	85280	-	94760
G.10	315940	-	480000	3159.4	315940	-	315940
G.11	382810	-	479948	3828.1	382810	-	390180
G.12	-	9480		94.8	-	9480	
G.13	480000	155030	480000	6350.3	635030	-	635030
G.14	902240	-	960000	9022.4	902240	-	902240
G.15	-	142920	-	1429.2	142920	-	142920
G.16	-	24450	-	244.5	24450	-	32970
G.17	480000	8520	480000	4885.2	480000	8520	480000
G.18	960000	36640	960000	9966.4	996640	-	996640
G.19	480000	17430	480000	4974.3	497430	-	497430
G.20	-	40610	-	406.1	40610	-	40610
G.21	-	63170	-	631.7	63170	-	63170
G.22	623950	-	921131	6239.5	623950	-	623950
G.23	960000	87490	960000	10474.9	1047490	-	1047490
G.24	861030	-	960000	8610.3	861030	-	861030
G.25	356500	-	477299	3565	356500	-	356500
G.26	-	62810	-	628.1	62810	-	62810
G.27	393730	-	480000	3937.3	393730	-	393730
G.28	878540	-	960000	8785.4	878540	-	878540
G.29	2726570	-	2880000	27265.7	2726570	-	2726570
G.30	-	187960	-	1879.6	187960	-	187960
G.31	-	207720	-	2077.2	207720	-	207720
G.32	252230		478573	2522.3	252230	-	252230
G.33	-	185030	-	1850.3	185030	-	185030
G.34	-	135930	-	1359.3	135930	-	135930

*ST_{ig} is only given for network case 1 since networks 2, 3 and 4 have the same values.

Table A.2.3 - Comparison between results in TOPSIS and M-TOPSIS

	CRITERIA VALUE			TOPSIS		M-TOPSIS	
Alternatives	Total risk (units)	TDC (M$ per day)	Total GWP (Thousand tons CO_2-eq per day)	Ratio **TOPSIS**	Rank	Ratio **M-TOPSIS**	Rank
1	5970	132.05	111.85	0.4539	25	0.0462	24
2	5970	126.86	113.59	0.4363	22	0.0494	21
3	5970	124.07	115.33	0.4272	14	0.0513	16
4	5970	122.09	117.07	0.4212	11	0.0525	13
5	5970	120.10	118.81	0.4148	8	0.0540	11
6	5970	118.11	120.55	0.4081	7	0.0555	8
7	5970	116.93	122.29	0.4053	6	0.0562	6
8	5970	109.01	132.74	0.3838	3	0.0617	3
9	5970	103.49	143.19	0.3786	1	0.0632	2
10	5970	97.97	153.63	0.3790	2	0.0634	1
11	5970	93.26	164.08	0.3896	4	0.0608	4
12	5970	88.54	174.52	0.4039	5	0.0568	5
13	5970	83.83	184.97	0.4197	9	0.0522	14
14	5970	79.11	195.41	0.4350	20	0.0479	23
15	5970	73.65	205.60	0.4459	23	0.0460	26
16	8132	110.89	113.59	0.4321	19	0.0492	22
17	8132	109.70	115.33	0.4297	16	0.0501	20
18	8132	109.01	117.07	0.4299	17	0.0503	19
19	8132	108.30	118.81	0.4301	18	0.0505	18
20	8132	107.11	120.55	0.4278	15	0.0514	15
21	8132	105.42	122.29	0.4227	12	0.0531	12
22	8132	100.22	132.74	0.4210	10	0.0555	9
23	8132	95.50	143.19	0.4262	13	0.0558	7
24	8132	90.79	153.63	0.4356	21	0.0544	10
25	8132	86.57	164.08	0.4505	24	0.0506	17
26	8132	81.36	174.52	0.4609	26	0.0460	25
27	8132	76.68	184.89	0.4732	27	0.0402	27
28	8132	71.92	195.41	0.4837	28	0.0347	28
29	8132	67.05	205.75	0.4913	29	0.0318	29
30	10293	108.88	113.59	0.5104	30	0.0262	35
31	10293	108.02	115.33	0.5114	32	0.0260	36
32	10293	106.81	117.07	0.5111	31	0.0264	32
33	10293	106.47	118.81	0.5142	34	0.0258	37
34	10293	105.26	120.55	0.5139	33	0.0262	33
35	10293	104.91	122.29	0.5170	35	0.0258	38
36	10293	99.87	132.74	0.5247	36	0.0266	31
37	10293	95.13	143.19	0.5340	37	0.0268	30
38	10293	89.93	153.63	0.5402	38	0.0262	34
39	10293	85.29	164.08	0.5475	40	0.0236	39
40	10293	80.51	174.47	0.5517	43	0.0197	41
41	10293	75.43	184.40	0.5510	41	0.0159	42
42	10293	70.72	194.70	0.5513	42	0.0140	43
43	10293	64.57	205.86	0.5461	39	0.0201	40

Appendix B

B. DATABASE AND RESULTS FOR MIDI-PYRÉNÉES REGION

APPENDIX B1: SUPPLY CHAIN DECISION DATABASE

Table B.1.1 - Number of vehicles in Midi-Pyrénées by district
(Insee, 2010; Ministère du développement durable et de l'énergie, 2010; Salingue, 2012)

District	Main city	Population	Private vehicles	Buses	Light-good-vehicles			Forklifts
					GVWR< 1,5 t	1,5 t < GVWR < 2.5 t	GVWR< 3.5 t	
1	Gourdon	43831	23903	62	369	2506	1433	57
2	Figeac	53847	29775	123	453	3079	1760	112
3	Cahors	75884	41540	171	639	4338	2480	156
4	Villefranche de Rouergue	64200	37367	89	476	3772	2207	81
5	Rodez	141753	81559	282	1050	8329	4872	257
6	Millau	71095	41261	151	526	4177	2444	138
7	Castres	191394	102664	301	1117	8733	5346	275
8	Albi	182624	94940	287	1065	8333	5102	262
9	Montauban	164825	92857	328	1252	8135	5582	299
10	Castelsarrasin	74466	42780	138	565	3675	2522	126
11	Condom	65102	37403	169	666	4138	2316	154
12	Auch	83805	44114	217	857	5327	2982	198
13	Mirande	38274	22044	99	391	2434	1362	90
14	Tarbes	143348	78429	306	883	6167	4286	279
15	Argelès-Gazost	39858	22575	83	246	1715	1192	76
16	Bagnères de Bigorre	46464	26235	97	286	1998	1389	89
17	Saint Gaudens	77373	42528	97	466	3272	2021	89
18	Muret	198376	109038	281	1194	8389	5183	256
19	Toulouse	955071	524957	1370	5750	40387	24953	1250
20	Pamiers	70833	38205	132	459	3129	2236	120
21	Saint Girons	27819	15665	51	180	1229	878	47
22	Foix	52465	28457	97	340	2317	1656	89
	Total	2862707	1578296	4931	19230	135579	84202	4500

Table B.1.2 - Total demand for product form *i* in district *g* during time period *t* -D^{T}_{igt}- (kg per day)

Scenario	*1*				*2*			
District/ Period	*2020*	*2030*	*2040*	*2050*	*2020*	*2030*	*2040*	*2050*
1	124	910	2140	3050	235	1800	4220	6040
2	157	1200	2800	3990	318	2360	5480	7820
3	221	1670	3910	5570	442	3280	7650	10930
4	196	1430	3340	4790	378	2810	6600	9430
5	428	3230	7570	10810	841	6380	14880	21250
6	219	1660	3840	5500	431	3240	7550	10790
7	509	3840	8970	12820	1002	7570	17650	25220
8	468	3570	8360	11950	951	7060	16450	23510
9	480	3660	8520	12170	964	7180	16750	23930
10	229	1660	3880	5540	440	3270	7630	10880
11	211	1570	3660	5210	403	3070	7150	10210
12	243	1910	4440	6330	496	3710	8670	12400
13	116	940	2160	3070	237	1810	4210	6000
14	398	3000	7000	10000	781	5900	13720	19600
15	115	850	1990	2850	225	1670	3900	5570
16	126	1000	2320	3320	257	1940	4540	6490
17	196	1500	3520	5010	398	2970	6920	9910
18	518	3900	9110	12990	1021	7670	17920	25610
19	2507	18780	43840	62620	4943	37030	86390	123430
20	208	1470	3450	4920	379	2910	6780	9680
21	93	590	1400	1990	154	1180	2760	3910
22	136	1090	2570	3670	277	2160	5030	7200
Total	*7898*	*59430*	*138790*	*198170*	*15573*	*116970*	*272850*	*389810*

Table B.1.3 – Parameters for hydrogen supply chain components: general data

α	Network operating period	365 days / year
CCF	Capital change factor -payback period of capital investment	12 years
LR_t	Learning rate	Increasing 2% each period*
WFP_g	Weigh factor risk of population in each grid or district	Table B.2.2

* Assumption based on McKinsey & Company, 2010

Table B.1.4a – Production (Almansoori and Shah, 2011)

Liquid H_2 (*i*)	$PCap^{min}_{pij}$ Minimum production capacity of plant type *p* size *j* for product form *i*				$PCap^{max}_{pij}$ Maximum production capacity of plant type *p* size *j* for product form *i*			
Technology (*p*)	small	medium	large	unit	small	medium	large	unit
Steam methane reforming	300	10000	200000	(kg per day)	9500	150000	960000	(kg per day)
Electrolysis	300	10000	0		9500	150000	0	
Electrolysis (distributed)	50*	450*	1050*		400*	1000*	2500*	
Biomass gasification	-	10000	200000		-	150000	960000	
Liquid H_2 (*i*)	PCC_{pji} Capital cost of establishing plant type *p* size *j* producing product form *i*				UPC_{pij} Unit production cost for product form *i* produced by plant type *p* and size *j*			
Technology (*p*)	small	medium	large	unit	small	medium	large	unit
Steam methane reforming	29000000	224000000	903000000	($)	3.36	1.74	1.43	($ per kg)
Electrolysis	61000000	663000000	0		4.69▲	4.59 ▲	0	
Electrolysis (distributed)	4026385•	9018000•	20198000•		6.24	5.38	4.94	
Biomass gasification	-	575000000	1836000000		-	3.52	2.15	
Liquid H_2 (*i*)	RP_{pj} Risk level of the production facility *p* size *j*■				γ_{epj} Rate of utilization of primary energy source *e* by plant type *p* and size *j*			
Technology (*p*)	small	medium	large	unit	small	medium	large	unit
Steam methane reforming	0.27	1.33	2.70	units	4.02	3.34	3.16	kgs/kg H_2
Electrolysis	0.30	0.75	0		52.49	52.49	0	kWhelec/kg H_2
Electrolysis (distributed)	0.15	0.23	0.30					
					$NP0_{pjig}$	Initial number of plants of type *p* and size *j* producing product form *i* in grid *g*		0 units

* Size suggested in this study, similar to that provided in the McKinsey and Co. (2010)

▲McKinsey&Co, 2010 (4,4-5,5€/KgH_2)

• We extrapolated the formula presented by Murthy Konda et al. (2011) for determining the cost of distributed electrolysis plants for the proposed capacity: $\frac{I_2}{\$4900000} = \left(\frac{C_2 *}{500 kgH2/day}\right)^{0.88}$

These costs generally include facilities, permits and start engineering, contingencies and working capital, land and other costs.

■Calculated using the methodology of Kim and Moon (2011) (see Table Appendix B2)

Table B.1.4b – Production global warming potential by plant type *p* - GW^{Prod}_{ep} - (*g CO_2-eq per kg of H_2*)

Production type / energy source	Gaz naturel	PV	Wind	Hydro	Nuclear	Biomass
SMR	10100	-	-	-	-	-
Electrolysis	-	6206*	1034*	2068*	3100*	-
Gasification	-	-	-	-	-	3100
Ref.	Stromman and Hertwich (2004) reported in (Rivière, A. 2007)	(Utgikar & Thiesen, 2006) *approximate values				

Table B.1.5 - Storage (Almansoori and Shah 2011)

Liquid H_2 (*i*)		mini	small	medium	large
$SCap^{min}_{sji}$ - Minimum storage capacity of storage type *s* size *j* for product form *i* (kg)		50*	500*	10000	200000
$SCap^{max}_{sji}$ - Maximum storage capacity of storage type *s* size *j* for product form *i* (kg)		450*	9500	150000	540000
SCC_{sij} - Capital cost of establishing storage type *s* size *j* storing product form *i* ($)		802165*	5000000	33000000	122000000
USC_{sij} - Unit storage cost for product form *i* at storage type *s* size *j* ($ per kg per d)		0.064	0.032	0.01	0.005
RS_{sj} - Risk level in storage facility *s* size *j* ◙		0.3	0.9	2.1	3
GW^{Stock}_{i}	Storage global warming potential form *i*			(704 g CO_2-eq per kg of H_2) ▲	
β	Storage holding period-average number of days worth of stock			(10 days)	
$NS0_{sjiq}$	Initial number of storage facilities of type *s* and size *j* storing product form *i* in grid *g*			(0 units)	

* Size suggested in this study, similar to that provided in the McKinsey and Co. (2010)
◙ Calculated using the methodology of Kim and Moon (2011)
▲ This value was calculated for the *French energy mix* based on data base of liquefaction and compresion presented in Grol et al. NETL (2005) based on Bossel U. :
1 kWh → 0.083 kg CO_2, fossil (Ecoinvent Database v2.2)
For liquefaction of H_2 → 8.42 kWh/kgH_2 → 0.704 kg CO_2/kgH_2
For compression of H_2 → 4.17 kWh/kgH_2 → 0.349 kg CO_2/kgH_2

Table B.1.6 - Transportation data base (tanker truck).

Parameter		units		Reference
W_l	Weight of transportation mode *l*	40	ton	(AFH2, 2011, p. 2)
DW_l	Driver wage of transportation mode *l*	14.57	US$ per hour	CNR - Enquête Longue Distance 2010
FE_l	Fuel economy of transportation mode *l*	2.3	km per liter	Almansoori and Shah, 2011
FP_l	Fuel price of transportation mode *l*	1.5	US$ per liter	Almansoori and Shah, 2011=1,16$/L. Murthy Konda, 2011 =1,3$/L
GE_l	General expenses of transportation mode *l*	8.22	US$ per day	Almansoori and Shah, 2011= US$ 8.22 per day. Murthy Konda, 2011 =$8,22/d
LUT_l	Load and unload time of product for transportation mode *l*	2	hours per trip	Almansoori and Shah, 2011
ME_l	Maintenance expenses of transportation mode *l*	0.126*	US$ per km	CNR - Enquête Longue Distance, 2010
SP_l	Average speed of transportation mode *l*	66.8	km per hour	CNR - Enquête Longue Distance, 2010
TMA_l	Availability of transportation mode *l*	18	hours per day	Almansoori and Shah, 2011
GW^{Trans}_{l}	Global warming potential of transportation mode *l*	62	g CO_2 per tonne-km	McKinnon, A., Piecyk M. 2011.
RT_l	Risk level of transportation mode *l*	1.33	Units	Calculated using the methodology of Kim and Moon (2011) (see Appendix B.2)
$TCap_{il}$	Capacity of transportation mode *l* transporting product form *i*	3500	kg per trip	Dagdougui, 2012
Q^{min}_{il}	Minimum flow rate of product form *i* by transportation mode *l*	3500	kg per day	As the capacity of the transportation mode
Q^{max}_{il}	Maximum flow rate of product form *i* by transportation mode *l*	960000	kg per day	Almansoori and Shah, 2011
TMC_{il}	Cost of establishing transportation mode *l* transporting product form *i*	500000	US$	Based on : Almansoori and Shah (2011)=500000$; Hawkins (2006) ; AIE (2006a) ; Ogden (1999a); Amos (1998))=590000$; Nagore et al. (2011): 434236€ or 355931,14$; Bento (2010)=300000-400000$; Murthy Konda et al. (2011) = 800 000$

* Definition of maintenance expenses of transportation mode *l:* repair=0,0919 $/km (0,072 €/km)+ pneumatic=0,0345 $/km (0,027 €/km). Total 0,126 $/km (0,099 €/km)

Table B.1.7 Average delivery distance between districts *g* and *g'* (km per trip). MAPPY. March 2012.

District	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	-	63	46	97	128	197	198	175	102	139	148	191	222	306	338	297	243	174	155	222	246	240
2	63	-	70	34	65	134	146	103	133	170	220	226	293	341	373	332	278	205	186	253	277	242
3	46	70	-	59	112	173	156	133	60	97	127	148	180	264	295	254	201	132	113	180	204	198
4	97	34	59	-	53	114	111	69	76	113	192	165	197	280	312	271	218	148	131	197	220	232
5	128	65	112	53	-	70	115	71	131	208	287	230	262	309	341	300	247	177	151	216	249	234
6	197	134	173	114	70	-	135	104	186	261	339	266	300	345	377	336	289	216	187	312	292	330
7	198	146	156	111	115	135	-	43	99	140	214	157	189	226	258	217	164	94	71	124	180	141
8	175	103	133	69	71	104	43	-	75	133	187	155	186	234	266	225	172	102	75	141	174	158
9	102	133	60	76	131	186	99	75	-	23	117	88	112	206	238	197	143	73	55	123	146	140
10	139	170	97	113	208	261	140	133	23	-	83	75	100	218	250	209	156	87	68	135	159	152
11	148	220	127	192	287	339	214	187	117	83	-	43	54	102	137	125	141	135	146	188	169	205
12	191	226	148	165	230	266	157	155	88	75	43	-	24	73	108	91	86	83	80	147	124	136
13	222	293	180	197	262	300	189	186	112	100	54	24	-	49	84	68	72	92	104	135	138	145
14	306	341	264	280	309	345	226	234	206	218	102	73	49	-	35	23	66	135	158	163	111	173
15	338	373	295	312	341	377	258	266	238	250	137	108	84	35	-	35	99	168	191	196	144	206
16	297	332	254	271	300	336	217	225	197	209	125	91	68	23	35	-	58	134	150	155	103	165
17	243	278	201	218	247	289	164	172	143	156	141	86	72	66	99	58	-	72	93	100	49	102
18	174	205	132	148	177	216	94	102	73	87	135	83	92	135	168	134	72	-	23	51	75	102
19	155	186	113	131	151	187	71	75	55	68	146	80	104	158	191	150	93	23	-	70	94	87
20	222	253	180	197	216	312	124	141	123	135	188	147	135	163	196	155	100	51	70	-	55	20
21	246	277	204	220	249	292	180	174	146	159	169	124	138	111	144	103	49	75	94	55	-	44
22	240	242	198	232	234	330	141	158	140	152	205	136	145	173	206	165	110	102	87	20	44	-

Table B.1.8 $RR_{gg'}$*:* Road risk between grids *g* and *g'* (units)

District	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	-	3	2	3	4	5	9	6	4	5	3	5	6	9	10	9	8	9	7	9	11	10
2	3	-	2	2	3	4	6	4	4	5	6	7	8	12	13	11	10	9	7	9	10	10
3	2	2	-	2	3	4	8	5	3	4	5	5	6	11	12	10	9	8	6	8	9	9
4	3	2	2	-	2	3	5	3	3	4	5	4	5	11	12	10	9	8	5	6	9	7
5	4	3	3	2	-	2	5	3	4	5	6	7	8	11	12	10	9	8	6	7	9	8
6	5	4	4	3	2	-	3	3	5	6	10	7	8	11	12	10	9	8	6	7	9	8
7	9	6	8	5	5	3	-	4	7	8	9	6	7	10	11	9	8	7	5	5	8	6
8	6	4	5	3	3	3	4	-	4	5	6	6	7	10	11	9	8	7	5	6	8	7
9	4	4	3	3	4	5	7	4	-	3	4	5	6	10	11	9	8	7	5	6	8	7
10	5	5	4	4	5	6	8	5	3	-	2	2	3	9	10	8	7	6	4	5	7	6
11	3	6	5	5	6	10	9	6	4	2	-	2	3	3	4	4	3	9	7	8	10	9
12	5	7	5	4	7	7	6	6	5	2	2	-	2	3	4	4	3	6	4	5	7	6
13	6	8	6	5	8	8	7	7	6	3	3	2	-	2	3	3	3	3	4	5	4	6
14	9	12	11	11	11	11	10	10	10	9	3	3	2	-	2	2	2	5	8	5	4	5
15	10	13	12	12	12	12	11	11	11	10	4	4	3	2	-	2	4	6	9	6	5	7
16	9	11	10	10	10	10	9	9	9	8	4	4	3	2	2	-	2	4	7	4	3	5
17	8	10	9	9	9	9	8	8	8	7	3	3	3	2	4	2	-	3	6	3	2	3
18	9	9	8	8	8	8	7	7	7	6	9	6	3	5	6	4	3	-	5	5	5	5
19	7	7	6	5	6	6	5	5	5	4	7	4	4	8	9	7	6	5	-	4	6	5
20	9	9	8	6	7	7	5	6	6	5	8	5	5	5	6	4	3	5	4	-	2	2
21	11	10	9	9	9	9	8	8	8	7	10	7	4	4	5	3	2	5	6	2	-	2
22	10	10	9	7	8	8	6	7	7	6	9	6	6	5	7	5	3	5	5	2	2	-
Total	*136*	*144*	*130*	*118*	*132*	*139*	*145*	*127*	*122*	*114*	*117*	*98*	*100*	*145*	*165*	*134*	*118*	*133*	*121*	*116*	*138*	*132*

Table B.1.9 –Refuelling stations

$Fcap_i$ Capacity of fuelling station for product form *i* (kg per day)	2500	McKinsey and Co (2010) considered 3 types of refuelling stations where the H_2 is taken as liquid (30 bar) or gaseous (250 or 450bar) and is compressed to 350 or 700 bar ; the stations sizes are : small (2 dispensers) = 0.4 t H_2 /d, medium (4 dispensers) = 1 t H_2/d, large (10 dispensers) = 2.5 t H_2/d
UFC_i Unit fuelling cost of product form *i* ($ / kg)	0,39	Almansoori and Shah, 2011

Table B.1.10 - Installed capacity in 2010 and strategic objectives 2020 in Midi-Pyrénées (Salingue, 2012 and SRCAE, 2012).

Objective per type	*Situation 2010*	*Objective min.2020*	*Objective maxi.2020*
Hydraulic	5000 MW	5300 MW	5400 MW
PV	80 MW	750 MW	1000 MW
Wind	322 MW	850 MW	1600 MW

Table B.1.11 – Initial availability of energy sources in Midi-Pyrénées (2020-2050) (Salingue 2012)

Scenario **2020**

Renewable energy/district	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**kWh/d**
PV (kWh/d)	148691	148691	173896	178691	156252	148691	148691	148691	155540	148691	228691	148691	148691	0	0	0	4726	162253	197595	26575	0	0	2473747
Wind (kWh/d)	0	0	0	529148	685860	1242901	1444490	675175	529148	529148	529148	529148	0	0	0	0	0	0	840080	0	0	0	7534246
Hydraulic (kWh/d)	0	177275	379786	189923	95402	0	0	550197	92937	1019786	0	0	0	0	2281507	999726	1019178	775129	120060	86575	500164	1067424	9355069

Scenario **2030** (increasing PV (250 MWc) and wind (500 MW)*

Renewable energy/district	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**kWh/d**
PV (kWh/d)	203486	203486	228691	233486	211047	203486	203486	203486	210335	203486	283486	203486	203486	0	0	0	4726	217048	252390	26575	0	0	3295672
Wind (kWh/d)	0	0	0	871614	1028326	1585367	1786956	1017641	871614	871614	871614	871614	0	0	0	0	0	0	1182546	0	0	0	10958906
Hydraulic (kWh/d)	0	177275	379786	189923	95402	0	0	550197	92937	1019786	0	0	0	0	2281507	999726	1019178	775129	120060	86575	500164	1067424	9355069

Scenario **2040** (increasing PV and wind 2%)*

Renewable energy/district	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**kWh/d**
PV (kWh/d)	207556	207555	233264	238155	215267	207555	207555	207555	214541	207555	289155	207556	207556	0	0	0	4726	221388	257437	26575	0	0	3360959
Wind (kWh/d)	0	0	0	889046	1048892	1617074	1822695	1037993	889046	889046	889046	889046	0	0	0	0	0	0	1206196	0	0	0	11178085
Hydraulic (kWh/d)	0	177275	379786	189923	95402	0	0	550197	92937	1019786	0	0	0	0	2281507	999726	1019178	775129	120060	86575	500164	1067424	9355069

Scenario **2050** (increasing PV and wind 2%)*

Renewable	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**kWh/d**
PV (kWh/d)	211706	211706	237930	242918	219573	211706	211706	211706	218832	211706	294938	211706	211706	0	0	0	4726	225816	262586	26575	0	0	3427552
Wind (kWh/d)	0	0	0	906827	106987	1649415	1859149	1058753	906827	906827	906827	906827	0	0	0	0	0	0	1230320	0	0	0	11401646
Hydraulic (kWh/d)	0	177275	379786	189923	95402	0	0	550197	92937	1019786	0	0	0	0	2281507	999726	1019178	775129	120060	86575	500164	1067424	9355069

* Team assumptions

+ Nuclear is available in district 4= 51210000 (kWh/d)

**Natural gas is available in all grids

Scenario in 2020:

Increase of wind production from 380MW in 2012 to a maximum of 1600 MW in 2020 (will be used in the calculations 1100 MW). Production is estimated based on an annual schedule of 2500 h (ICPE classification of turbines)

Increase of PV from 80 MW to 750 MWp (minimum capacity) or 1000 MWp (maximum). For this study, calculation for 750 MWp (minimum) is used. Production is estimated on an hourly annual basis of 1200 h

Increase of hydro + 200 GWh in 2020 (initially 600 GWh in 2020, but only 28.5% taking into account because it corresponds to "run of river" centrals

APPENDIX B2: SAFETY RELATIVE RISK (DETAILED CALCULATION)

(Kim and Moon, 2008)(Kim et al., 2011) proposed a methodology to determine the relative safety risk of a hydrogen supply chain (HSC). They assesed risks for the different HSC activities and we have integrated their results to our mathematical model to measure the total relative risk of the network and that way, it is possible to optimise the HSC minimising the safety risk. The steps of the analysis are:

- process specification and breakdown;
- hazard identification with FMEA. With the help of an FMEA (failure mode effect analysis), the safety plan identifies failure modes of equipment and processes and establishes the consequences of such failures frequency and consequence estimation;
- risk evaluation with relative risk index matrix (see Table B.2.1). he results presented in the risk ranking matrix of (Kim et al., 2011) were taken into account in our database;
- total relative risk index (TRRI) calcultation (**This last step is the only one considered in our mathematical model**).

Table B.2.1. Risk ranking matrix (Kim et al. 2011)

Table 4 – Risk ranking matrix for case study.

Consequence					
Likelihood	Catastrophic (C3)			Critical (C2)	Marginal (C1)
Frequent (F3)				12, 23	9,17
Probable (F2)	11			2, 7, 10, 15, 16	19, 21
Remote (F1)	5, 6, 8, 14			3, 4, 13, 20	1,18, 22
Consequence (Index)		**Likelihood**		**Decision criteria according to ranking value**	
C3	Several damage and fatalities (≥1000)	F3	High ($\geq 10^{-4}$)	RV1	Unacceptable
C2	Considerable damage and injury (≥500)	F2	Medium ($\geq 10^{-6}$)	RV2	Undesirable
C1	Minor damage and lost time (≥100)	F1	Low ($\geq 10^{-8}$)	RV3	Acceptable with existing control & protections
Hydrogen activity					
Electrolysis plant	1, 2, 3, 4, 5, 6			SMR plant	1, 5, 7, 8, 9, 10
LH_2 storage facility	1, 5, 11, 12, 13, 14			CH_2 storage facility	5, 8, 12, 15, 16, 17
Tank truck	5, 18, 19, 20, 21, 22			Tube trailer	5, 18, 19, 20, 21, 23

The equations to calculate the relative risk level of production, storage and transport units are:

Production

$$RP_{pj} = \alpha_p \frac{1}{c_p} \sum_{f=1}^{c_p} RV_{pf}$$

Storage

$$RS_{sj} = \alpha_s \frac{1}{c_s} \sum_{f=1}^{c_s} RV_{sf}$$

Transportation

$$RT_t = \alpha_t \frac{1}{c_t} \sum_{f=1}^{c_t} RV_{tf}$$

where

f : potential risks (example in Kim et al. 2011)
p: production technology
s: storage technology
t: transport type
c : constant which is the number of the selected failure modes used to compare H_2 activities with the same basis.
RP_{pj} : inherent risk factor of plant type *p* size *j* (see Table B.2.4)
RS_{sj} : inherent risk factor of storage type *s* size *j* (see Table B.2.4)
RT_l : inherent risk factor of transportation mode *l* (see Table B.2.4)
RV_f : ranking value assessed with the risk ranking method (based on Table B.2.1, see Table B.2.6)
α : weight factor according to the production and storage units scale, values between 0-1; the value one is assigned to the plant producing the maximum flow rate of hydrogen at any given time –see Table B.2.3.

Table B.2.2 –Weigh factor risk of population in each grid or district in the Midi-Pyrénées region -WFP_g- (calculated similarly to that of Kim and Moon (2011).

District	**Main city**	**Population** [(1)]	**Size**	**WFP_g (units)** [(2)]
1	Gourdon	43831	Small	1
2	Figeac	53847	Small	1
3	Cahors	75884	Small	1
4	Villefranche de Rouergue	64200	Small	1
5	Rodez	141753	Small	1
6	Millau	71095	Small	1
7	Castres	191394	Medium	2
8	Albi	182624	Medium	2
9	Montauban	164825	Medium	2
10	Castelsarrasin	74466	Small	1
11	Condom	65102	Small	1
12	Auch	83805	Small	1
13	Mirande	38274	Small	1
14	Tarbes	143348	Small	1
15	Argelès-Gazost	39858	Small	1
16	Bagnères de Bigorre	46464	Small	1
17	Saint Gaudens	77373	Small	1
18	Muret	198376	Medium	2
19	Toulouse	955071	Large	3
20	Pamiers	70833	Small	1
21	Saint girons	27819	Small	1
22	Foix	52465	Small	1
(1) INSEE 2009:http://www.insee.fr/fr/ppp/bases-de-donnees/recensement/populations-legales/				
(2) > 201000=3; 151000-200000=2; 0-150000=1				

Table B.2.3 - Factor α defined for the different production and storage technologies and sizes (units).

α	mini	small	medium	large
Steam methane reforming	-	0.1	0.5	1
Electrolysis	-	0.2	0.5	-
Electrolysis distributed	-	0.1	0.15	0.2
Storage	0.1	0.3	0.7	1

Table B.2.4 - Results of inherent risks factors for the activities of the hydrogen supply chain. Midi-Pyrénées case study (units).

Size	mini	small	medium	large
$RP_{\text{Steam methane reforming}}$	-	0.27	1.33	2.67
$RP_{\text{Electrolysis (distributed)}}$	-	0.15	0.23	0.3
$RP_{\text{Electrolysis}}$	-	0.3	0.75	-
$RS_{\text{Super-insulated spherical tanks}}$	0.3	0.9	2.1	3
$RT_{\text{Tanker truck}}$		1.33		

Table B.2.5 - Example of calculation of the road risk between grids *g* and *g'*

District	Size	WFP_g (units) (see table B.2.2)	Weight factor that indicates the adjacency level *	Road risk between districts 2 and 19
1	Small	1		0
2	Small	1	1	1
3	Small	1		0
4	Small	1	1	1
5	Small	1		0
6	Small	1		0
7	Medium	2		0
8	Medium	2		0
9	Medium	2	1	2
10	Small	1		0
11	Small	1		0
12	Small	1		0
13	Small	1		0
14	Small	1	1	1
15	Small	1		0
16	Small	1	1	1
17	Small	1	1	1
18	Medium	2	1	2
19	Large	3	1	3
20	Small	1		0
21	Small	1		0
22	Small	1		0
			Total	12

* It takes a rating value between 0.1 and 1.0 according to the adjacency level.

Table B.2.6 - Calculation of the Risk Value (RV)

Technology	Electrolysis		Steam methane reforming		Super-insulated spherical tanks		Pressurized cylindrical vessels		Tanker trucks		Tube trailers	
Failure mode	Combined risk	RV	Combined risk	RV	Combined risk	RV	Combined risk	RV	Combined risk	RV	Combined risk	RV
1	C1xF1	1	C1xF1	1	C1xF1	1						
2	C2xF2	3										
3	C2xF1	1										
4	C2xF1	1					C2xF1	1				
5	C3xF1	3	C3xF1	3	C3xF1	3			C3xF1	3	C3xF1	3
6	C3xF1	3										
7			C2xF2	3			C2xF2	3				
8			C3xF1	3								
9			C1xF3	3								
10			C2xF2	3								
11					C3xF2	5						
12					C2xF3	5	C2xF3	5				
13					C2xF1	1						
14					C3xF1	3						
15							C2xF2	3				
16							C2xF2	3				
17							C1xF3	3				
18									C1xF1	1	C1xF1	1
19									C1xF2	1	C1xF2	1
20									C2xF1	1	C2xF1	1
21									C1xF2	1	C1xF2	1
22									C1xF1	1		
23											C2xF3	5
Total		12		16		18		18		8	Total	12

	Level	The combinations (consequence x likelihood) :	Index
RV1	High-risk	C3xF2, C2xF3 and C3xF3	5
RV2	Moderate-risk	C3xF1, C1xF3 and C2xF2	3
RV3	Low-risk	C2xF1, C1xF2 and C1xF1	1

APPENDIX B3: DETAILED RESULTS

B.3.1. Results for case B1. Midi-Pyrénées.

Table B.3.1a - Comparison between results in M-TOPSIS. Case B.1: Midi-Pyrénées (2020-2050)

	CRITERIA VALUE			MCDM						
Altern.	Cost ($ per kg H_2)	GWP (kg CO_2 per kg H_2)	Risk (units)	MATRIZ V [A*wj]			D+	D-	Ratio M-Topsis	Rank
x1	-	-	-	-	-	-	-	-	-	-
x2	-	-	-	-	-	-	-	-	-	-
x3	-	-	-	-	-	-	-	-	-	-
x4	6.58	8.51	342	0.22	0.25	0.16	0.14	0.2	0.09	13
x5	6.5	9.18	341.8	0.22	0.27	0.16	0.13	0.22	0.07	17
x6	**7.81**	**1.94**	**405.9**	0.26	0.06	0.19	0.27	0.11	0.25	1
x7	7.06	4.15	395	0.24	0.12	0.18	0.22	0.1	0.22	5
x8	6.54	6.24	400.6	0.22	0.18	0.18	0.17	0.14	0.16	10
x9	5.76	8.54	399.9	0.19	0.25	0.18	0.13	0.2	0.09	14
x10	5.26	10.74	397.9	0.18	0.32	0.18	0.12	0.26	0.03	19
x11	7.76	1.94	459.8	0.26	0.06	0.21	0.27	0.11	0.24	2
x12	6.88	4.15	468.4	0.23	0.12	0.21	0.21	0.11	0.2	6
x13	6.35	5.96	459.3	0.21	0.18	0.21	0.16	0.14	0.16	9
x14	5.61	8.57	469.2	0.19	0.25	0.21	0.11	0.21	0.08	15
x15	5.03	10.61	457	0.17	0.31	0.21	0.11	0.26	0.03	20
x16	7.76	1.94	459.8	0.26	0.06	0.21	0.27	0.11	0.24	2
x17	6.88	4.15	521.8	0.23	0.12	0.24	0.2	0.13	0.19	7
x18	6.31	6.36	493.9	0.21	0.19	0.23	0.15	0.16	0.14	11
x19	5.49	8.38	529.5	0.18	0.25	0.24	0.11	0.21	0.07	16
x20	4.77	10.74	528.2	0.16	0.32	0.24	0.11	0.27	0.01	21
x21	7.76	1.94	459.8	0.26	0.06	0.21	0.27	0.11	0.24	2
x22	6.88	4.15	521.8	0.23	0.12	0.24	0.2	0.13	0.19	7
x23	6.31	6.36	493.9	0.21	0.19	0.23	0.15	0.16	0.14	11
x24	5.39	8.57	572.9	0.18	0.25	0.26	0.1	0.22	0.06	18
x25	4.9	10.68	594.2	0.16	0.32	0.27	0.1	0.28	0	22
			A+=max	0.26	0.32	0.27				
			A-=min	0.16	0.06	0.16				

Table B.3.1b - Summary of results for Case B.1

Variable	DL_{ig} (kg d^{-1})				D_{ig} (kg d^{-1})			
	2020	2030	2040	2050	2020	2030	2040	2050
G.1	124	910	2140	3050	-	-	-	-
G.2	157	1200	2800	350	-	-	-	3640
G.3	221	1670	250	250	-	-	3660	5320
G.4	196	1430	3340	4790	-	-	-	-
G.5	428	3230	7570	10810	-	-	-	-
G.6	219	1660	3840	5500	-	-	-	-
G.7	509	3840	8970	12820	-	-	-	-
G.8	468	3570	8360	11950	-	-	-	-
G.9	480	3660	8520	12170	-	-	-	-
G.10	229	1660	3880	5540	-	-	-	-
G.11	211	1570	3660	5210	-	-	-	-
G.12	243	1910	4440	6330	-	-	-	-
G.13	116	940	2160	3070	-	-	-	-
G.14	398	3000	300	300	-	-	6700	9700
G.15	115	850	1990	2850	-	-	-	-
G.16	126	1000	2320	3320	-	-	-	-
G.17	196	1500	3520	350	-	-	-	4660
G.18	518	100	100	100	-	3800	9010	12890
G.19	2507	18780	43840	62620	-	-	-	-
G.20	208	1470	3450	350	-	-	-	4570
G.21	93	590	1400	1990	-	-	-	-
G.22	136	1090	2570	3670	-	-	-	-

Table B.3.1c - Flow rate of liquid hydrogen via tanker truck for the multi-objective optimisation (2020-2050). Case B.1

From district	To district	Flow rate, $Q_{ilgg'}$ (kg d^{-1})			
		2020	*2030*	*2040*	*2050*
4	2	-	-	-	3640
4	3	-	-	3660	5320
12	14	-	-	6700	9700
12	17	-	-	-	4660
19	18	-	3800	9010	12890
19	20	-	-	-	4570

B.3.2. Results for case B2. Midi-Pyrénées.

Table B.3.2a - Comparison between results in M-TOPSIS. Case B.2. Midi-Pyrénées (2020).

	CRITERIA VALUE			MCDM						
Altern.	Cost	GWP	Risk	MATRIZ V [A*wj]			D+	D-	**Ratio** M-Topsis	Rank
	($ per kg H_2)	(kg CO_2 per kg H_2)	(units)							
x1	15.52	2.14	34.5	0.168	0.261	0.199	0.025	0.165	0	2
x2	15.51	2.51	34.5	0.168	0.222	0.199	0.046	0.127	0.05	8
x3	15.51	2.5	34.5	0.168	0.223	0.199	0.045	0.128	0.04	7
x4	15.51	2.23	34.5	0.168	0.25	0.199	0.027	0.154	0.01	3
x5	15.51	3.09	34.5	0.168	0.18	0.199	0.084	0.088	0.1	14
x6	15.51	3.98	34.5	0.168	0.14	0.199	0.123	0.053	0.15	20
x7	15.51	4.13	34.5	0.168	0.135	0.199	0.128	0.05	0.16	22
x8	15.6	3.35	34.5	0.167	0.166	0.199	0.098	0.075	0.12	16
x9	14.18	5.14	34.4	0.184	0.108	0.199	0.153	0.04	0.18	23
x10	14.68	5.6	34.1	0.177	0.099	0.201	0.162	0.039	0.19	26
x11	**13.94**	**2.14**	**37.7**	0.187	0.261	0.182	0.02	0.164	0	**1**
x12	13.93	2.24	37.7	0.187	0.249	0.182	0.023	0.152	0.01	4
x13	13.94	2.28	37.7	0.187	0.244	0.182	0.026	0.147	0.02	6
x14	13.93	2.88	37.7	0.187	0.193	0.182	0.07	0.098	0.08	11
x15	13.93	3.22	37.7	0.187	0.173	0.182	0.09	0.078	0.11	15
x16	13.94	3.36	37.7	0.187	0.166	0.182	0.097	0.072	0.12	17
x17	13.94	3.93	37.7	0.187	0.142	0.182	0.12	0.05	0.15	21
x18	13.84	4.83	37.6	0.188	0.115	0.183	0.147	0.032	0.18	24
x19	13.68	5.19	37.7	0.19	0.107	0.182	0.155	0.03	0.19	27
x20	13.68	5.19	37.7	0.19	0.107	0.182	0.155	0.03	0.19	27
x21	13.79	2.14	41.6	0.189	0.261	0.165	0.036	0.163	0.02	5
x22	13.79	2.52	41.6	0.189	0.221	0.165	0.054	0.124	0.05	9
x23	13.79	2.78	41.6	0.189	0.2	0.165	0.07	0.103	0.08	10
x24	13.95	2.98	41.8	0.187	0.187	0.164	0.083	0.09	0.1	12
x25	13.81	3.52	41.7	0.188	0.158	0.165	0.109	0.063	0.14	18
x26	13.84	3.73	41.9	0.188	0.15	0.164	0.117	0.054	0.15	19
x27	13.84	2.99	41.9	0.188	0.186	0.164	0.084	0.089	0.1	13
x28	13.64	4.83	41.5	0.191	0.115	0.165	0.15	0.029	0.19	25
x29	13.53	5.19	41.6	0.192	0.107	0.165	0.158	0.027	0.2	29
x30	13.53	5.19	41.6	0.192	0.107	0.165	0.158	0.027	0.2	29
			A+=max	0.192	0.261	0.201				
			A-=min	0.167	0.099	0.164				

Table B.3.2b - Summary of results for case B.2 (2020)

Variable	**DL_{ig}** (kg d^{-1})	**DI_{ig}** (kg d^{-1})	**PT_{ig}** (kg d^{-1})	**ST_{ig}** (kg)*
G.1	124	-	124	1240
G.2	157	-	157	1570
G.3	221	-	221	2210
G.4	196	-	196	1960
G.5	428	-	428	4280
G.6	219	-	219	2190
G.7	509	-	509	5090
G.8	468	-	468	4680
G.9	480	-	480	4800
G.10	229	-	229	2290
G.11	211	-	211	2110
G.12	243	-	243	2430
G.13	116	-	116	1160
G.14	398	-	398	3980
G.15	115	-	115	1150
G.16	126	-	126	1260
G.17	196	-	196	1960
G.18	518	-	518	5180
G.19	2507	-	2507	25070
G.20	208	-	208	2080
G.21	93	-	93	930
G.22	136	-	136	1360

Table B.3.2c - Comparison between results in M-TOPSIS. Case B.2. Midi-Pyrénées (2030).

	CRITERIA VALUE						MCDM			
Altern.	Cost	GWP	Risk	MATRIZ V [A*wj]			D+	D-	Ratio M-Topsis	Rank
	($ per kg H_2)	(kg CO_2 per kg H_2)	(units)							
x8	8.7	7.88	91	0.2	0.12	0.24	0.31	0.06	0.39	14
x9	8.49	8.7	91	0.2	0.11	0.24	0.33	0.06	0.4	16
x10	8.43	9.52	90.9	0.21	0.1	0.24	0.33	0.06	0.4	18
x11	**9.09**	**2.14**	**102.2**	0.19	0.43	0.22	0.04	0.33	0	**1**
x12	8.9	2.96	104	0.2	0.31	0.21	0.13	0.22	0.15	3
x13	8.71	3.78	103.3	0.2	0.24	0.22	0.19	0.15	0.24	5
x14	8.51	4.6	102	0.2	0.2	0.22	0.23	0.11	0.3	7
x15	8.33	5.42	103.9	0.21	0.17	0.21	0.26	0.08	0.34	9
x16	8.2	6.24	103.5	0.21	0.15	0.21	0.28	0.06	0.37	11
x17	8.09	6.96	103.1	0.21	0.13	0.22	0.3	0.05	0.38	13
x18	7.98	7.87	101.8	0.22	0.12	0.22	0.31	0.04	0.4	17
x19	7.93	8.67	104	0.22	0.11	0.21	0.33	0.04	0.41	20
x20	7.92	9.28	103.9	0.22	0.1	0.21	0.33	0.04	0.42	21
x21	9.14	2.14	116.3	0.19	0.43	0.19	0.06	0.33	0.02	2
x22	8.83	2.96	116.9	0.2	0.31	0.19	0.13	0.21	0.15	4
x23	8.64	3.78	116.9	0.2	0.24	0.19	0.2	0.15	0.24	6
x24	8.45	4.6	116.7	0.21	0.2	0.19	0.24	0.1	0.3	8
x25	8.25	5.42	116.8	0.21	0.17	0.19	0.27	0.08	0.34	10
x26	8.09	6.24	116.7	0.21	0.15	0.19	0.29	0.06	0.37	12
x27	7.94	7.06	117	0.22	0.13	0.19	0.31	0.04	0.39	15
x28	7.82	7.88	116.9	0.22	0.12	0.19	0.32	0.04	0.41	19
x29	7.8	8.7	116.6	0.22	0.11	0.19	0.33	0.03	0.42	22
x30	7.8	8.75	116.6	0.22	0.11	0.19	0.33	0.03	0.42	23
			A+=max	0.22	0.43	0.24				
			A-=min	0.19	0.1	0.19				

Table B.3.2e - Summary of results for case B.2 (2030)

Variable	DL_{ig} (kg d^{-1})	DI_{ig} (kg d^{-1})	PT_{ig} (kg d^{-1})	ST_{ig} (kg)*
G.1	910	-	910	9100
G.2	1200	-	1200	12000
G.3	1670	-	1670	16700
G.4	1430	-	1430	14300
G.5	3230	-	3230	32300
G.6	1660	-	1660	16600
G.7	3840	-	3840	38400
G.8	3570	-	3570	35700
G.9	3660	-	3660	36600
G.10	1660	-	1660	16600
G.11	1570	-	1570	15700
G.12	1910	-	1910	19100
G.13	940	-	940	9400
G.14	3000	-	3000	30000
G.15	850	-	850	8500
G.16	1000	-	1000	10000
G.17	1500	-	1500	15000
G.18	3900	-	3900	39000
G.19	18780	-	18780	187800
G.20	1470	-	1470	14700
G.21	590	-	590	5900
G.22	1090	-	1090	10900

Table B.3.2f - Comparison between results in M-TOPSIS. Case B.2. Midi-Pyrénées (2040).

	CRITERIA VALUE			MCDM						
Altern.	Cost	GWP	Risk	MATRIZ V [A*wj]			D+	D-	**Ratio** M-Topsis	Rank
	($ per kg H_2)	(kg CO_2 per kg H_2)	(units)							
x1	-	-	-	-	-	-	-	-	-	-
x2	-	-	-	-	-	-	-	-	-	-
x3	-	-	-	-	-	-	-	-	-	-
x4	-	-	-	-	-	-	-	-	-	-
x5	-	-	-	-	-	-	-	-	-	-
x6	-	-	-	-	-	-	-	-	-	-
x7	8.62	5.28	167.1	0.16	0.16	0.26	0.28	0.12	0.3	9
x8	8.42	6.1	167.1	0.17	0.14	0.26	0.3	0.1	0.32	11
x9	8.35	6.54	167.1	0.17	0.13	0.26	0.31	0.1	0.33	13
x10	8.37	7.74	167.1	0.17	0.11	0.26	0.33	0.09	0.35	15
x11	**8.11**	**2**	**206.4**	0.17	0.43	0.21	0.09	0.34	0	**1**
x12	7.76	2.82	212.4	0.18	0.31	0.2	0.15	0.22	0.14	3
x13	7.52	3.64	212.3	0.19	0.24	0.21	0.21	0.15	0.23	5
x14	7.14	4.46	212.4	0.2	0.19	0.2	0.25	0.11	0.28	7
x15	6.8	5.28	210.2	0.21	0.16	0.21	0.28	0.09	0.31	10
x16	6.52	6.1	212.1	0.21	0.14	0.21	0.3	0.08	0.33	14
x17	6.26	6.92	212.5	0.22	0.12	0.2	0.31	0.08	0.35	16
x18	6.05	7.74	212.2	0.23	0.11	0.21	0.32	0.08	0.35	17
x19	5.95	8.56	212	0.23	0.1	0.21	0.33	0.08	0.36	20
x20	5.88	9.33	211.8	0.24	0.09	0.21	0.34	0.08	0.36	22
x21	8.11	2	213	0.17	0.43	0.2	0.09	0.34	0	2
x22	7.73	2.82	252.3	0.18	0.31	0.17	0.17	0.21	0.15	4
x23	7.49	3.64	256.1	0.19	0.24	0.17	0.22	0.15	0.24	6
x24	7.12	4.46	242.9	0.2	0.19	0.18	0.26	0.11	0.29	8
x25	6.75	5.28	255.5	0.21	0.16	0.17	0.28	0.08	0.32	12
x26	6.15	6.92	249.6	0.23	0.12	0.17	0.32	0.07	0.35	18
x27	6.15	6.92	249.6	0.23	0.12	0.17	0.32	0.07	0.35	18
x28	5.91	7.7	254.8	0.24	0.11	0.17	0.33	0.08	0.36	21
x29	5.8	8.56	253.4	0.24	0.1	0.17	0.34	0.08	0.36	23
x30	5.72	9.38	257.7	0.24	0.09	0.17	0.35	0.08	0.37	24
			A+=max	0.24	0.43	0.26				
			A-=min	0.16	0.09	0.17				

Table B.3.2g – Summary of results case B.2. Midi-Pyrénées (2040).

Variable	DL_{ig} (kg d^{-1})	DI_{ig} (kg d^{-1})	PT_{ig} (kg d^{-1})	ST_{ig} (kg)*
G.1	2140	-	2140	21400
G.2	2800	-	2800	28000
G.3	3910	-	3910	39100
G.4	3340	-	3340	33400
G.5	7570	-	7570	75700
G.6	3840	-	3840	38400
G.7	8970	-	8970	89700
G.8	8360	-	8360	83600
G.9	8520	-	8520	85200
G.10	3880	-	3880	38800
G.11	3660	-	3660	36600
G.12	4440	-	10290	44400
G.13	2160	-	2160	21600
G.14	1150	5850	1150	70000
G.15	1990	-	1990	19900
G.16	2320	-	2320	23200
G.17	3520	-	3520	35200
G.18	1550	7560	1550	91100
G.19	43840	-	51399	438400
G.20	3450	-	3450	34500
G.21	1400	-	1400	14000
G.22	2570	-	2570	25700

Table B.3.2h - Flow rate of liquid hydrogen via tanker truck for the multi-objective optimisation (2040).

From grid	To grid	Flow rate, $Q_{ilgg'}$ (kg d^{-1})
12	14	5850
19	18	7560

Table B.3.2i - Comparison between results in M-TOPSIS. Case B.2. Midi-Pyrénées (2050).

	CRITERIA VALUE			MCDM						
Altern.	Cost ($ per kg H_2)	GWP (kg CO_2 per kg H_2)	Risk (units)	MATRIZ V [A*wj]			D+	D-	**Ratio** M-Topsis	Rank
x1	-	-	-	-	-	-	-	-	-	-
x2	-	-	-	-	-	-	-	-	-	-
x3	7.16	3.55	246	0.16	0.22	0.23	0.19	0.16	0.2	5
x4	6.89	4.34	246	0.17	0.18	0.23	0.23	0.12	0.24	8
x5	6.75	5.13	246	0.17	0.15	0.23	0.25	0.1	0.28	11
x6	6.66	5.83	246	0.18	0.14	0.23	0.27	0.09	0.29	13
x7	6.64	6.14	246	0.18	0.13	0.23	0.28	0.09	0.3	18
x8	6.64	6.09	246	0.18	0.13	0.23	0.28	0.09	0.3	16
x9	6.66	6.04	246	0.18	0.13	0.23	0.28	0.09	0.3	14
x10	6.64	6.13	246	0.18	0.13	0.23	0.28	0.09	0.3	17
x11	**7.32**	**1.97**	**276.6**	0.16	0.4	0.2	0.08	0.32	0	**1**
x12	7.25	2.76	307.7	0.16	0.29	0.18	0.14	0.2	0.13	3
x13	6.8	3.55	308.8	0.17	0.22	0.18	0.19	0.14	0.21	6
x14	6.4	4.34	309	0.18	0.18	0.18	0.23	0.1	0.26	9
x15	6.25	5.13	307.3	0.19	0.15	0.18	0.25	0.08	0.29	12
x16	5.92	5.91	307.3	0.2	0.13	0.18	0.27	0.07	0.31	19
x17	5.8	6.7	307.9	0.2	0.12	0.18	0.29	0.06	0.33	23
x18	5.31	7.49	308.4	0.22	0.11	0.18	0.3	0.07	0.33	22
x19	5.2	8.28	308.6	0.22	0.1	0.18	0.31	0.07	0.33	25
x20	5.41	8.66	308.7	0.22	0.09	0.18	0.31	0.06	0.34	27
x22	7.15	2.76	366.7	0.16	0.29	0.15	0.15	0.2	0.14	4
x23	6.72	3.55	335.6	0.17	0.22	0.17	0.2	0.14	0.21	7
x24	6.36	4.34	355.8	0.18	0.18	0.16	0.23	0.1	0.27	10
x25	6.11	5.13	351	0.19	0.15	0.16	0.26	0.07	0.3	15
x26	5.94	5.91	339.7	0.2	0.13	0.16	0.28	0.06	0.32	20
x27	5.49	6.7	325.6	0.21	0.12	0.17	0.29	0.07	0.33	21
x28	5.23	7.49	325.6	0.22	0.11	0.17	0.3	0.07	0.33	24
x29	5.24	8.28	371.4	0.22	0.1	0.15	0.31	0.06	0.34	28
x30	4.96	9.06	362.7	0.24	0.09	0.15	0.32	0.08	0.34	26
			A+=max	0.24	0.4	0.23				
			A-=min	0.16	0.09	0.15				

Table B.3.2j - Summary of results for case B.2: Midi-Pyrénées (2050).

Variable	**DL_{ig}** (kg d^{-1})	**DI_{ig}** (kg d^{-1})	**PT_{ig}** (kg d^{-1})	**ST_{ig}** (kg)*
G.1	3050	-	3050	30500
G.2	3990	-	3990	39900
G.3	1600	3970	1600	55700
G.4	4790	-	8760	47900
G.5	10810	-	10810	108100
G.6	5500	-	5500	55000
G.7	12820	100	12820	128200
G.8	11950	-	11950	119500
G.9	12170	-	12170	121700
G.10	5540	-	5540	55400
G.11	5210	-	5210	52100
G.12	6330	-	15180	63300
G.13	3070	-	3070	30700
G.14	1150	8850	1150	100000
G.15	2850	-	2850	28500
G.16	3320	-	3320	33200
G.17	5010	-	5010	50100
G.18	1550	11440	1550	129900
G.19	62620	-	74060	626200
G.20	4920	-	4920	49200
G.21	1990	-	1990	19900
G.22	3670	-	3670	36700

Table B.3.2k - Flow rate of liquid hydrogen via tanker truck for the multi-objective optimisation (2050).

From grid	To grid	Flow rate, $Q_{ilgg'}$ (kg d^{-1})
4	3	3970
9	7	100
12	14	8850
19	18	11440

Appendix C

C. DATABASE AND RESULTS FOR FRANCE

APPENDIX C1: ENERGY SOURCES (analysed scenarios for France).

Table C.1.1- Global energy per sector per period (%) (WWF, 2011)

Source	2000	2010	2020	2030	2040	2050
Total electricity	17%	18%	20%	27%	37%	49%*
Industry fuels and heat	23%	24%	23%	23%	23%	23%
Building fuels and heat	28%	26%	25%	21%	17%	9%
Transport fuels	32%	31%	32%	29%	23%	19%
Grand total	100%	100%	100%	100%	100%	100%

*Higher electricity demand is listed for 2050

Table C.1.2 - Gross electricity production in France reference 2010. Projection 2020-2050 under different scenarios (TWh / year).

	2010[42]	2020[43]	2030[44]	2040[41]	2050[45]
Scénario de base (RTE)	564	543	545	756	967
RTE ref 2030	564	576	610	788	967
Global Chance-sortir du nuc,	564	438	335	651	967
AREVA prolong nuclear	564	582	623	795	967
AREVA sortie nuc ENR fort	564	551	561	764	967
CEA sortie du nuc	564	526	510	738	967

[42] Annual statistics RTE (2010)

[43] Hypothesis

[44] (Percebois & Centre d'analyse stratégique., 2012)

[45] (European Climate Fondation; GIEC 2011)

Table C.1.3 – Scenarios analysed to project the initial availability of the energy source for France (2020-2050)

Pessimistic regarding the RES in France:	**Optimistic regarding the RES in France:**
1. *RTE* 2030 3. *AREVA* prolongation nucléaire	2. *Global Chance*[46] (81% RES in France in 2050)
Promote the use of biomass, hydro and wind:	**Promote the use of PV:**
4. *AREVA* (nuclear off) 5. *CEA* (nuclear off) (60% wind in 2050 and 12% PV)	2. *Global Chance* 7. *WWF* [44] (29% of the electricity is produced by PV in 2050)
Projection close to Midi-Pyrénées (%):	**Average development of PV and wind technologies in France:**
2. *Global Chance* (15% PV, 35% wind and 31% hydro) Midi-Pyrénées (14% PV, 47% wind and 39% hydro) (Salingue, 2012)	6. *Syndicat des Energies Renouvelables*[44] (PV, wind and biomass) 8. *Project Master 3A*[44] (19% PV, 45% wind, 22% hydro and 14% biomass)

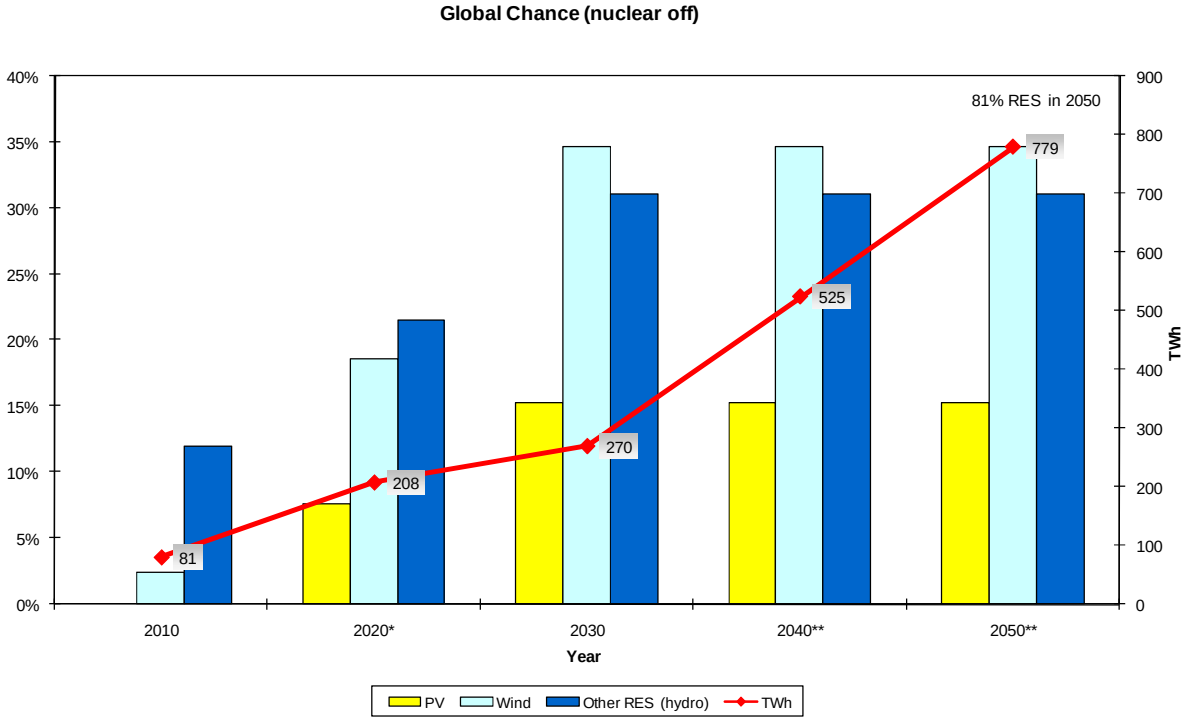


Figure C.1.1 - Scenario for electricity production from Global Chance based on (Percebois and Centre d'analyse stratégique., 2012)

[46] Scenarios analysed.

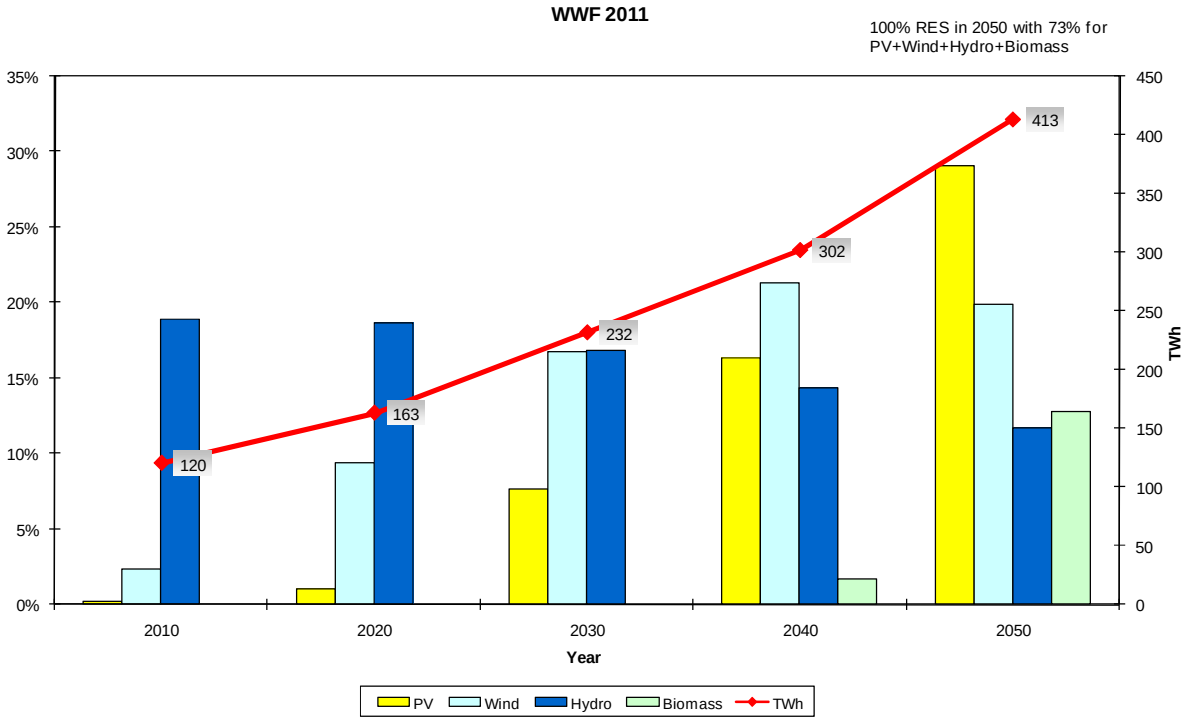


Figure C.1.2 - Scenario for RES electricity production (WWF, 2011).

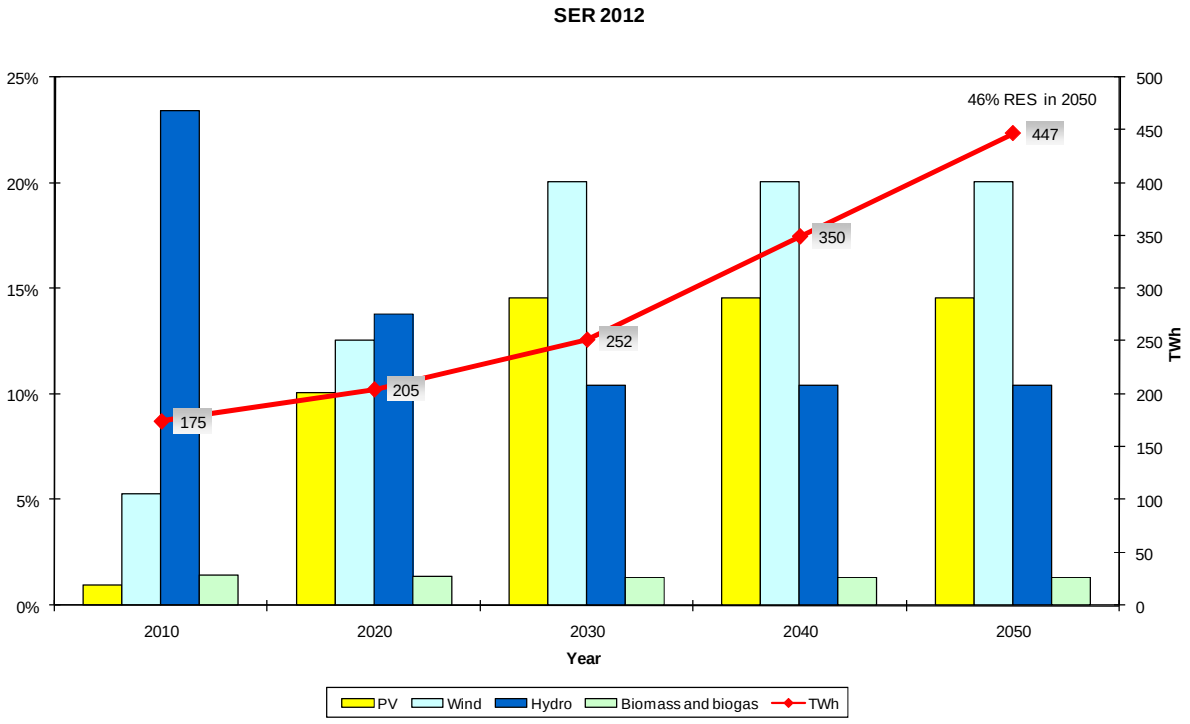


Figure C.1.3 - Scenario for RES electricity production based on the SER roadmap (2020-2030) (Syndicat des énergies renouvelables, 2012).

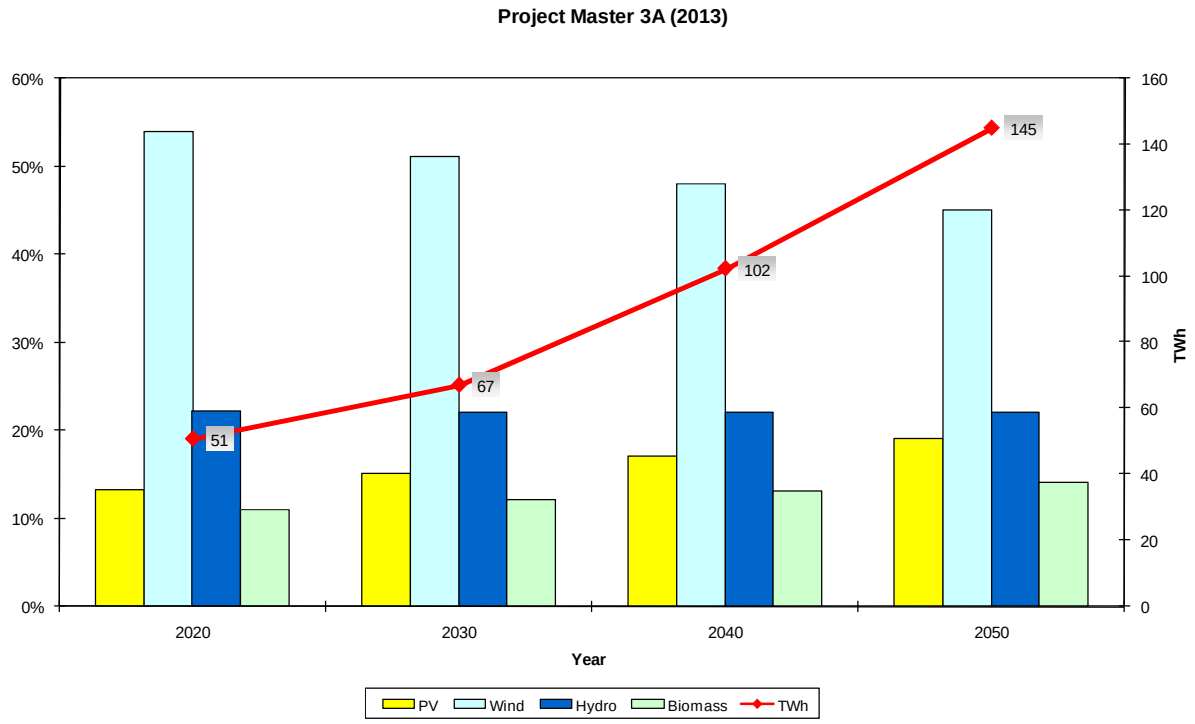


Figure C.1.4 - Scenario for RES electricity production. Researched by a group of students of the Eco-energy Master NTE in the ENSIACET University (2013)

Table C.2.1 - Total demand for product form *i* in district *g* during time period *t* -D^{T}_{igt}- (kg per day)

	kg per day in each time period			
Region/time	**2020**	**2030**	**2040**	**2050**
1	4653	34898	81430	116328
2	9091	68183	159093	227276
3	3682	27618	64441	92059
4	3934	29504	68842	98346
5	4483	33620	78448	112068
6	8823	66172	154402	220575
7	6805	51035	119081	170116
8	3791	28434	66345	94779
9	3192	23940	55860	79800
10	5130	38477	89779	128256
11	24040	180303	420707	601010
12	7140	53548	124945	178493
13	2088	15660	36539	52199
14	6089	45670	106564	152234
15	8070	60528	141232	201759
16	9189	68919	160811	229730
17	9484	71128	165966	237094
18	5728	42958	100235	143193
19	4854	36409	84953	121362
20	13108	98312	229394	327706
21	16923	126925	296159	423085
Total	160299	1202240	2805227	4007467

Table C.2.2 Average delivery distance between districts *g* and *g'* (km per trip). ArcGIS

Main city	Nº	*1*	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	*19*	*20*	*21*
Strasbourg	*1*	0	1099	682	797	500	681	693	363	253	632	551	730	891	156	956	601	1003	534	872	820	490
Bordeaux	*2*	1099	0	536	686	603	505	410	807	750	851	595	562	220	1002	263	913	406	783	227	721	580
Clermont-ferrand	*3*	682	536	0	669	465	681	272	669	428	670	457	238	310	680	274	753	582	768	430	521	191
Caen	*4*	797	686	669	0	370	181	397	399	617	164	212	907	587	640	861	392	280	262	459	1066	860
Dijon	*5*	500	603	465	370	0	602	193	204	247	371	158	724	383	352	657	442	503	329	387	635	484
Rennes	*6*	681	505	681	181	602	0	409	554	849	345	319	919	398	761	672	573	99	443	278	1078	757
Orléans	*7*	693	410	272	397	193	409	0	397	440	398	185	510	190	545	464	486	310	356	194	793	677
Châlons-en-Champagne	*8*	363	807	669	399	204	554	397	0	377	400	187	928	587	207	861	238	549	171	591	944	614
Besançon	*9*	253	750	428	617	247	849	440	377	0	728	405	477	630	252	904	615	750	548	634	567	237
Rouen	*10*	632	851	670	164	371	345	398	400	728	0	213	908	588	607	862	228	444	98	623	1027	697
Paris	*11*	551	595	457	212	158	319	185	187	405	213	0	695	375	394	649	301	362	171	379	972	642
Montpellier	*12*	730	562	238	907	724	919	510	928	477	908	695	0	548	729	299	1166	820	866	789	159	240
Limoges	*13*	891	220	310	587	383	398	190	587	630	588	375	548	0	794	274	676	300	546	120	831	501
Metz	*14*	156	1002	680	640	352	761	545	207	252	607	394	729	794	0	954	445	756	378	739	819	489
Toulouse	*15*	956	263	274	861	657	672	464	861	904	862	649	299	274	954	0	1099	573	820	394	458	465
Lille	*16*	601	913	753	392	442	573	486	238	615	228	301	1166	676	445	1099	0	672	130	697	1182	852
Nantes	*17*	1003	406	582	280	503	99	310	549	750	444	362	820	300	756	573	672	0	533	179	979	773
Amiens	*18*	534	783	768	262	329	443	356	171	548	98	171	866	546	378	820	130	533	0	550	1115	785
Poitiers	*19*	872	227	430	459	387	278	194	591	634	623	379	789	120	739	394	697	179	550	0	951	621
Marseille	*20*	820	721	521	1066	635	1078	793	944	567	1027	972	159	831	819	458	1182	979	1115	951	0	330
Lyon	*21*	490	580	191	860	484	757	677	614	237	697	642	240	501	489	465	852	773	785	621	330	0

Table C.2.3 $RR_{gg'}$: Road risk between grids *g* and *g'* (units)

Main city	Nº	*1*	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*	*13*	*14*	*15*	*16*	*17*	*18*	*19*	*20*	*21*
Strasbourg	*1*	0	7	4	9	3	13	9	4	3	8	8	13	9	3	11	7	10	5	10	8	7
Bordeaux	*2*	7	0	5	7	6	7	5	7	7	9	9	6	4	11	4	13	5	10	4	9	7
Clermont-ferrand	*3*	4	5	0	6	2	7	2	5	4	6	6	5	2	6	5	10	6	8	4	9	4
Caen	*4*	9	7	6	0	7	3	5	7	8	2	6	13	7	9	10	6	5	3	8	15	10
Dijon	*5*	3	6	2	7	0	11	5	2	2	6	5	7	5	4	6	6	7	3	5	9	4
Rennes	*6*	13	7	7	3	11	0	6	12	12	4	10	14	7	14	9	8	4	5	5	15	10
Orléans	*7*	9	5	2	5	5	6	0	6	6	3	5	10	3	8	6	8	5	6	3	10	8
Châlons-en-Champagne	*8*	4	7	5	7	2	12	6	0	3	6	5	9	7	3	9	5	9	2	6	8	5
Besançon	*9*	3	7	4	8	2	12	6	3	0	7	6	8	4	3	10	7	8	4	7	9	5
Rouen	*10*	8	9	6	2	6	4	3	6	7	0	5	11	4	5	7	5	4	2	7	13	9
Paris	*11*	8	9	6	6	5	10	5	5	6	5	0	13	6	7	9	7	8	4	6	12	8
Montpellier	*12*	13	6	5	13	7	14	10	9	8	11	13	0	8	13	4	17	9	14	7	5	8
Limoges	*13*	9	4	2	7	5	7	3	7	4	4	6	8	0	9	4	10	4	7	2	9	5
Metz	*14*	3	11	6	9	4	14	8	3	3	5	7	13	9	0	10	7	12	4	8	10	7
Toulouse	*15*	11	4	5	10	6	9	6	9	10	7	9	4	4	10	0	12	7	10	5	7	9
Lille	*16*	7	13	10	6	6	8	8	5	7	5	7	17	10	7	12	0	12	4	9	14	10
Nantes	*17*	10	5	6	5	7	4	5	9	8	4	8	9	4	12	7	12	0	5	3	12	9
Amiens	*18*	5	10	8	3	3	5	6	2	4	2	4	14	7	4	10	4	5	0	9	13	9
Poitiers	*19*	10	4	4	8	5	5	3	6	7	7	6	7	2	8	5	9	3	9	0	11	7
Marseilles	*20*	8	9	9	15	9	15	10	8	9	13	12	5	9	10	7	14	12	13	11	0	7
Lyon	*21*	7	7	4	10	4	10	8	5	5	9	8	8	5	7	9	10	9	9	7	7	0
Total		148	140	104	146	102	173	116	117	120	122	144	192	114	149	153	176	140	126	124	204	146

SAFETY RELATIVE RISK (DETAILED CALCULATION)

Table C.2.4 –Weigh factor risk of population in each grid or district in the Midi-Pyrénées region -WFP_g- (calculated similarly to that of Kim and Moon (2011).

N°	Region	Population	Type	Score
1	Alsace	1,845,687.00	small	1
2	Aquitaine	3,232,352.00	medium	2
3	Auvergne	1,347,387.00	small	1
4	Basse-Normandie	1,473,494.00	small	1
5	Bourgogne	1,642,115.00	small	1
6	Bretagne	3,199,066.00	medium	2
7	Centre	2,548,065.00	medium	2
8	Champagne-Ardenne	1,335,923.00	small	1
9	Franche-Comté	1,171,763.00	small	1
10	Haute-Normandie	1,836,954.00	small	1
11	Île-de-France	11,786,234.00	large	3
12	Languedoc-Roussillon	2,636,350.00	medium	2
13	Limousin	742,771.00	small	1
14	Lorraine	2,350,920.00	medium	2
15	Midi-Pyrénées	2,881,756.00	medium	2
16	Nord - Pas-de-Calais	4,038,157.00	large	3
17	Pays de la Loire	3,571,495.00	medium	2
18	Picardie	1,914,844.00	small	1
19	Poitou-Charentes	1,770,363.00	small	1
20	Provence-Alpes-Côte d'Azur	4,899,155.00	large	3
21	Rhône-Alpes	6,230,691.00	large	3

Table C.2.5 - Factor α defined for the different production and storage technologies and sizes (units).

α	mini	small	medium	large
Steam methane reforming	-	0.1	0.5	1
Electrolysis	-	0.2	0.5	-
Electrolysis distributed	-	0.1	0.15	0.2
Storage	0.1	0.3	0.7	1

Table C.2.6 - Results of inherent risks factors for the activities of the hydrogen supply chain. Midi-Pyrénées case study (units).

	mini	small	medium	large
RP steam methane reforming	-	0.27	1.33	2.67
RP Gasification*	-	-	1.33	2.67
RP Electrolysis (distributed)	-	0.20	0.30	0.40
RP Electrolysis	-	0.40	1.00	-
RS Super-insulated spherical tanks	0.30	0.90	2.10	3
RS Pressurized cylindrical vessels	-	-	-	3
RT Tanker truck	1.33			
RT Tube Trailer	2.00			

*Assumption

APPENDIX C3: DETAILED RESULTS

Table C.3.1a - Summary of results for case A.1 cost minimisation. France (2020-2050)

	DLig (kg d^{-1})				**Dlig (kg d^{-1})**			
Variable	2020	2030	2040	2050	2020	2030	2040	2050
G.1	4653	34898	81430	116328	-	-	-	-
G.2	300	300	300	300	8791	67883	158793	226976
G.3	-	-	-	-	3682	27618	64441	92059
G.4	-	-	-	-	3934	29504	68842	98346
G.5	300	300	300	300	4183	33320	78148	111768
G.6	-	-	-	-	8823	66172	154402	220575
G.7	-	-	-	-	6805	51035	119081	170116
G.8	-	-	-	-	3791	28434	66345	94779
G.9	3192	300	300	300	-	23640	55560	79500
G.10	5130	10000	10000	10000	-	28477	79779	118256
G.11	50	180303	420707	601010	23990	-	-	-
G.12	-	-	-	-	7140	53548	124945	178493
G.13	2088	300	300	300	-	15360	36239	51899
G.14	-	-	-	-	6089	45670	106564	152234
G.15	300	300	300	300	7770	60228	140932	201459
G.16	9189	10000	10000	10000	-	58919	150811	219730
G.17	-	-	-	-	9484	71128	165966	237094
G.18		42958	100235	143193	5728	-	-	-
G.19		36409	84953	121362	4854	-	-	-
G.20	13108	10000	11974	131498	-	88312	217420	196208
G.21	16923	126925	296159	423085	-	-	-	-

Table C.3.1b - Flow rate of liquid hydrogen via tanker truck for the cost minimisation (2020-2050).

Case A.1. France

From region	To region	Flow rate, $Q_{ilgg'}$ (kg d^{-1})			
		2020	*2030*	*2040*	*2050*
1	14	6089			
10	4	3934			
10	5	4183			
10	6	8823			
10	7	6805			
10	11	23990			
10	17	9484			
10	18	5728			
11	4		29504	68842	
11	5		33320	78148	111768
11	6				77156
11	7		51035	119081	170116
11	8		3500		
16	8	3791			
18	4				98346
18	6				22209
18	8		24934	66345	94779
18	10		28477	79779	118256
18	14		45670	106564	152234
18	16		58919	150811	219730
19	2		67883	158793	226976
19	6		66172	154402	121210
19	13		15360	36239	51899
19	15		60228	140932	201459
19	17		71128	165966	237094
20	12	7140			
20	15	7770			
21	2	8791			
21	3	3682	27618	64441	92059
21	9		23640	55560	79500
21	12		53548	124945	178493
21	19	4854			
21	20		88312	217420	196208

Table C.3.2a - Summary of results for case A.2 GWP minimisation. France (2020-2050)

	DLig (kg d^{-1})				**Dlig (kg d^{-1})**			
Variable	2020	2030	2040	2050	2020	2030	2040	2050
G.1	4653	11484	12806	102672	-	23415	68624	13656
G.2	300	300	300	300	8791	67883	158793	226976
G.3	3682	27618	49126	65217	-	-	15315	26842
G.4	3934	29504	60294	80043	-	-	8548	18304
G.5	4483	33620	78448	112068	-	-	-	-
G.6	8823	66172	154402	220575	-	-	-	-
G.7	6805	51035	119081	170116	-	-	-	-
G.8	3791	28434	66345	94779	-	-	-	-
G.9	3192	4451	6395	8489	-	19489	49465	71311
G.10	5130	38477	89779	116743	-	-		11513
G.11	4794	5984	8577	11896	19246	174319	412130	589114
G.12	7140	53548	124945	178493	-	-	-	-
G.13	2088	4896	7035	9338	-	-	-	-
G.14	742	45670	106564	152234	-	10764	29505	42861
G.15	8070	60528	141232	201759	5347	-	-	-
G.16	9189	68919	160811	229730	-	-	-	-
G.17	9484	71128	129538	171960	-	-	36428	65134
G.18	2228	42958	100235	143193	3500	-	-	-
G.19	4854	36409	84953	121362	-	-	-	-
G.20	13108	30194	79034	105187	-	68117	150360	222519
G.21	16923	41376	296159	423085	-	85549	-	-

Table C.3.2b - Flow rate of liquid hydrogen via tanker truck for the GWP minimisation (2020-2050).

Case A.2. France

From region	To region	Flow rate, $Q_{ilgg'}$ (kg d^{-1})			
		2020	*2030*	*2040*	*2050*
1	14	5347			
3	21		6567		
5	2				3870
5	11	14376	18721		
5	20			8965	
5	21		7641		
6	2			12418	
6	17			36428	49232
7	2			75232	87831
7	13		4300		
8	2			5574	5178
8	9			45965	
8	11			223851	353685
10	11	4870			
12	20		68117	125210	153581
12	21		52427		
14	1		23415	68624	13656
14	9		19489	3500	71311
14	21		18914		
15	2		47020	26757	116422
16	3			15315	
16	10				6228
16	11			11353	17163
16	13			5666	
16	18	3500			
18	2			32186	9831
18	4			8548	18304
18	10				5285
18	11		155598	176926	218266
18	13			23839	42861
18	17				15902
19	2	8791	20863	6626	
19	13		6464		
21	2				3844
21	3				26842
21	20			16186	68938

Table C.3.3a - Summary of results for case A.3 risk minimisation. France (2020-2050)

Variable	DLig (kg d^{-1})				Dlig (kg d^{-1})			
	2020	2030	2040	2050	2020	2030	2040	2050
G.1	4653	34898	81430	116328	-	-	-	-
G.2	9091	68183	159093	227276	-	-	-	-
G.3	3682	27618	64441	92059	-	-	-	-
G.4	3934	29504	68842	98346	-	-	-	-
G.5	4483	33620	78448	112068	-	-	-	-
G.6	8823	66172	154402	220575	-	-	-	-
G.7	6805	51035	119081	170116	-	-	-	-
G.8		28434	66345	94779	3791	-	-	-
G.9	3192	23940	55860	79800	-	-	-	-
G.10	5130	38477	89779	128256	-	-	-	-
G.11	24040	180303	420707	601010	-	-	-	-
G.12	7140	53548	124945	178493	-	-	-	-
G.13	2088	15660	36539	52199	-	-	-	-
G.14		45670	106564	152234	6089	-	-	-
G.15	8070	60528	141232	201759	-	-	-	-
G.16	9189	68919	160811	229730	-	-	-	-
G.17	9484	71128	165966	237094	-	-	-	-
G.18		42958	100235	143193	5728	-	-	-
G.19	4854	36409	84953	121362	-	-	-	-
G.20	13108	98312	229394	327706	-	-	-	-
G.21	16923	126925	296159	423085	-	-	-	-

Table C.3.3b - Flow rate of liquid hydrogen via tanker truck for the risk minimisation (2020-2050). Case A.3. France

From region	To region	Flow rate, $Q_{ilgg'}$ (kg d^{-1})			
		2020	*2030*	*2040*	*2050*
1	14	6089	-	-	-
10	18	5728	-	-	-
16	8	3791	-	-	-

Table C.3.4a - Comparison between results in M-TOPSIS. Multi-objective optimisation. Case B.1: France (2020-2050)

Altern.	Total daily cost ($ per day)	GWP (kg CO_2 per day)	Risk (units)	MATRIZ V [A*wj]			D+	D-	Ratio M-Topsis	Rank
x1	35331096.33	50049494.13	2410	0.145	0.124	0.038	0.232	0.084	0.267	6
x2	34097042.29	58049033.29	2405	0.139	0.144	0.038	0.227	0.102	0.311	8
x3	29287859.15	88658847.48	2405	0.120	0.220	0.038	0.222	0.175	0.441	19
x4	**37068448.13**	**34050415.79**	**3175**	**0.152**	**0.085**	**0.051**	**0.240**	**0.055**	**0.186**	**1**
x5	32016854.79	66048572.46	3175	0.131	0.164	0.051	0.214	0.121	0.361	12
x6	29508145.32	87941588.61	3175	0.121	0.218	0.051	0.211	0.174	0.452	21
x7	44665143.88	26050876.63	3782	0.183	0.065	0.060	0.236	0.073	0.236	3
x8	30571006.05	74048111.62	4600	0.125	0.184	0.073	0.194	0.144	0.425	17
x9	43992770.42	26050876.63	4769	0.180	0.065	0.076	0.226	0.077	0.254	4
x10	36216445.19	34050415.79	4797	0.148	0.085	0.076	0.223	0.064	0.222	2
x11	35301449.54	42049954.96	4795	0.144	0.104	0.076	0.213	0.076	0.264	5
x12	33628612.8	50049494.13	4791	0.138	0.124	0.076	0.206	0.091	0.306	7
x13	32845777.86	58049033.29	4798	0.134	0.144	0.076	0.199	0.108	0.352	10
x14	32008776.58	66048572.46	4700	0.131	0.164	0.075	0.195	0.126	0.392	14
x15	30707979.88	74048111.62	4760	0.126	0.184	0.076	0.192	0.144	0.429	18
x16	30087373.73	81999321.73	4783	0.123	0.204	0.076	0.190	0.163	0.463	23
x17	28631590.14	89485308.7	4799	0.117	0.222	0.076	0.192	0.181	0.485	27
x18	57364478.75	18051337.46	7901	0.235	0.045	0.126	0.205	0.148	0.418	16
x19	44033617.4	26050876.63	7907	0.180	0.065	0.126	0.197	0.111	0.360	11
x20	35704038.6	34050415.79	7994	0.146	0.085	0.127	0.194	0.102	0.345	9
x21	34179800.45	42049954.96	7900	0.140	0.104	0.126	0.184	0.109	0.371	13
x22	33090863.3	50049494.13	7900	0.135	0.124	0.126	0.174	0.120	0.407	15
x23	32286971.6	58049033.29	7900	0.132	0.144	0.126	0.166	0.133	0.446	20
x24	31119055.72	65910159.69	7900	0.127	0.164	0.126	0.161	0.148	0.480	25
x25	30391522.96	74048111.62	7900	0.124	0.184	0.126	0.156	0.164	0.513	29
x26	29391752.46	82023341.73	7900	0.120	0.204	0.126	0.156	0.181	0.538	31
x27	29074544.42	88501745.95	7900	0.119	0.220	0.126	0.155	0.196	0.557	36
x28	57412447.01	18051337.46	11000	0.235	0.045	0.175	0.186	0.181	0.494	28
x29	45645401.52	26050876.63	11020	0.187	0.065	0.176	0.174	0.156	0.472	24
x30	35901418.76	34050415.79	11002	0.147	0.085	0.175	0.174	0.146	0.457	22
x31	34584531.15	42049954.96	11000	0.141	0.104	0.175	0.161	0.152	0.485	26
x32	33253483.08	50049494.13	11000	0.136	0.124	0.175	0.151	0.160	0.514	30
x33	32306117.79	58049033.29	11001	0.132	0.144	0.175	0.141	0.170	0.546	34
x34	31379205.49	66048572.46	11000	0.128	0.164	0.175	0.134	0.182	0.575	38
x35	30397115.1	74048111.62	11000	0.124	0.184	0.175	0.130	0.195	0.600	40
x36	29525747.51	82047650.79	11000	0.121	0.204	0.175	0.129	0.210	0.620	41
x37	28311473	90047189.96	11000	0.116	0.224	0.175	0.132	0.225	0.631	43
x38	57954947.47	18051337.46	14200	0.237	0.045	0.226	0.179	0.224	0.556	35
x39	44794626.85	26050876.63	14229	0.183	0.065	0.227	0.168	0.201	0.545	33
x40	36156572.94	34050415.79	14200	0.148	0.085	0.226	0.165	0.195	0.541	32
x41	34761377.23	42049954.96	14200	0.142	0.104	0.226	0.152	0.199	0.566	37
x42	33787340.33	50049494.13	14200	0.138	0.124	0.226	0.140	0.205	0.594	39
x43	32632169.27	58049033.29	14200	0.133	0.144	0.226	0.131	0.213	0.620	42
x44	31307709.47	66048572.46	14200	0.128	0.164	0.226	0.124	0.223	0.642	44
x45	30876060.69	74048111.62	14202	0.126	0.184	0.226	0.118	0.234	0.665	45
x46	29628363.27	82029177.07	14200	0.121	0.204	0.226	0.118	0.246	0.677	46

Table C.3.4b - Summary of results for case B1: multi-objective optimisation. France (2020-2050)

	DLig (kg d^{-1})				**Dlig (kg d^{-1})**			
Variable	2020	2030	2040	2050	2020	2030	2040	2050
G.1	4653	34898	10000	12440			71430	103888
G.2	9091	300	159093	227276		67883		
G.3	-	-	-	-	3682	27618	64441	92059
G.4	-	-	-	-	3934	29504	68842	98346
G.5	4483	1719	3565	9105		31901	74883	102964
G.6	8823	2716	154402	220575		63456		
G.7	6805	17528	119081	170116		33506		
G.8	3791	1888	4405	300		26546	61940	94479
G.9	3192	3161	3057	1500		20779	52803	78300
G.10	5130	10000	10000	10000		28477	79779	118256
G.11	400	180303	420707	601010	23640			
G.12	7140	1777	9963	10753		51771	114982	167740
G.13	2088	3311	300	3036		12349	36239	49164
G.14			106564	152234	6089	45670		
G.15	3210	60528	141232	201759	4860			
G.16	9189	15459	11122	15889		53460	149689	213841
G.17	9484	71128	165966	237094	-	-	-	-
G.18		42958	100235	143193	5728			
G.19	4854	300	4335	6574		36109	80618	114788
G.20	13108	62485	229394	327706		35827		
G.21	16923	126925	296159	423085	-	-	-	-

Table C.3.4c - Flow rate of liquid hydrogen via tanker truck case B1: multi-objective optimisation. France (2020-2050)

From region	To region	Flow rate, $Q_{ilgg'}$ (kg d^{-1})			
		2020	*2030*	*2040*	*2050*
1	14	6089			
2	13			36239	
2	19			5050	
6	4			68842	98346
7	3	3682		57314	92059
7	13				49164
7	19			24205	3500
8	11	5709			
10	4	3934			
10	11	14432			
10	18	5728			
11	5		28081	74883	102964
12	15	4860			
14	1			71430	103888
14	9			52803	78300
15	2		67883		
15	12		51771	59068	
15	13		12349		
15	19		3760		
15	20		4010		
16	11	3500			
17	6		63456		
17	7		33506		
17	19		32348	51364	111288
18	4		29504		
18	8		26546	61940	94479
18	10		28477	79779	118256
18	14		45670		
18	16		53460	149689	213841
20	12			55913	167740
21	3		27618	7127	
21	5		3820		
21	9		20779		
21	20		31818		

Table C.3.5a - Summary of results for case B2: economic cycle. France (2020-2050)

	DLig (kg d^{-1})				**Dlig (kg d^{-1})**			
Variable	2020	2030	2040	2050	2020	2030	2040	2050
G.1	4653	34898	81430	10000	-	-	-	106328
G.2	300	300	300	227276	8791	67883	158793	-
G.3	-	-	-	-	3682	27618	64441	92059
G.4	-	-	-	-	3934	29504	68842	98346
G.5	300	300	300	300	4183	33320	78148	111768
G.6	-	-	-	-	8823	66172	154402	220575
G.7	-	-	-	-	6805	51035	119081	170116
G.8	-	-	-	-	3791	28434	66345	94779
G.9	3192	300	300	300	-	23640	55560	79500
G.10	5130	10000	10140	10000	-	28477	79639	118256
G.11	50	180303	420707	601010	23990	-	-	-
G.12	-	-	-	-	7140	53548	124945	178493
G.13	2088	300	300	300	-	15360	36239	51899
G.14	-	-	10819	853	6089	45670	95745	151381
G.15	300	300	300	300	7770	60228	140932	201459
G.16	9189	38878	150000	10000	-	30042	10811	219730
G.17	-	-	165966	237094	9484	71128	-	-
G.18	-	-	-	143193	5728	42958	100235	-
G.19	-	-	-	-	4854	36409	84953	121362
G.20	13108	98312	20635	10073	-	-	208759	317633
G.21	16923	126925	296159	423085	-	-	-	-

Table C.3.5b - Flow rate of liquid hydrogen via tanker truck for case B2:economic cycle. France (2020-2050)

From region	To region	Flow rate, $Q_{ilgg'}$ (kg d^{-1})			
		2020	*2030*	*2040*	*2050*
1	14	6089	-	-	-
2	6	-	-	-	3680
2	7	-	-	-	4179
2	12	-	-	-	120469
2	13	-	-	-	51899
2	15	-	-	-	201459
2	19	-	-	-	121362
10	4	3934	-	-	-
10	5	4183	-	-	-
10	6	8823	-	-	-
10	7	6805	-	-	-
10	11	23990	-	-	-
10	17	9484	-	-	-
10	18	5728	-	-	-
11	2	-	67883	-	-
11	3	-	27618	-	-
11	4	-	29504	68842	-
11	5	-	33320	78148	111768
11	6	-	66172		81335
11	7	-	51035	119081	165937
11	8	-	28434	66345	-
11	9	-	23640	-	-
11	10	-	28477	79639	-
11	13	-	15360	-	-
11	14	-	45670	16242	-
11	15	-	60228	-	-
11	16	-	30042	10811	-
11	17	-	71128	-	-
11	18	-	42958	100235	-
11	19	-	36409	-	-
17	2	-	-	158793	-
17	6	-	-	154402	131432
17	13	-	-	36239	-
17	19	-	-	84953	-
18	1	-	-	-	106328
18	4	-	-	-	98346
18	6	-	-	-	4128
18	8	-	-	-	94779
18	10	-	-	-	118256
18	14	-	-	-	151381
18	16	-	-	-	219730
20	12	7140	50048	-	-
20	15	7770	-	-	-
21	2	8791	-	-	-
21	3	3682	-	64441	92059
21	9	-	-	55560	79500
21	12	-	3500	124945	-
21	14	-	-	79504	-
21	15	-	-	140932	-
21	19	4854	-	-	-
21	20	-	-	208759	-
21	12	-	-	-	58023
21	20	-	-	-	317633

Appendix D

D. M-TOPSIS METHODOLOGY

TOPSIS is based upon the concept that the chosen alternative should have the shortest distance from the Positive Ideal Solution (PIS) and the furthest from the Negative Ideal Solution (NIS) (García-Cascales & Lamata, 2012) (Ren et al., 2007). The steps are:

1. Data treatment (max max or min min, all objectives in the same sence):

(i) the reciprocal ratio method ($X'_{ij}=1/X_{ij}$)

(ii) the difference method ($X'_{ij}=1-X_{ij}$)

2. Calculation of the normalized decision matrix. Different ways to normalize:

(i) $$A=\lfloor a_{ij}\rfloor_{nxm,}\ a_{ij}=X'_{ij}/Max_i(X'_{ij})$$

(ii) $$A=\lfloor a_{ij}\rfloor_{nxm,}\ a_{ij}=\left(X'_{ij}-Min_i(X'_{ij})\right)/\left(Max_i(X'_{ij})-Min_i(X'_{ij})\right)$$

(iii) $$A=\lfloor a_{ij}\rfloor_{nxm,}\ a_{ij}=X'_{ij}/\sqrt{\sum_{i=1}^{n}(X'_{ij})^2}$$

3. Calculation of the weighted normalized decision matrix

$$v_{ij}=w_j\otimes a_{ij}$$

4. Determination of the positive ideal and negative ideal.

$$A^+=\left\{v_1^+,\ldots,v_1^+\right\}=\left\{\left(\max_i v_{ij}, j\in J\right)\left(\min_i v_{ij}, j\in J'\right)\right\}$$

$$A^-=\left\{v_1^-,\ldots,v_1^-\right\}=\left\{\left(\min_i v_{ij}, j\in J\right)\left(\max_i v_{ij}, j\in J'\right)\right\}$$

Where J is associated with benefit criteria and J' is associated with cost criteria

5. Calculatation of the separation measures, using the n-dimensional Euclidean distance. The separation from the positive and negative ideals solution is given as

(i) $$D_i^+ = \sqrt{\sum_{j=1}^{m} w_j \left(a_{ij}^+ - a_{ij}\right)^2}$$

(ii) $$D_i^- = \sqrt{\sum_{j=1}^{m} w_j \left(a_{ij}^- - a_{ij}\right)^2}$$

6. Calculation of the relative closeness to the ideal solution

(i) $$R_i = \frac{d_i^-}{d_i^+ + d_i^-}$$ → Topsis

(ii) $$R_i = \sqrt{\left[D_i^+ - \min\left(D_i^+\right)\right]^2 + \left[D_i^- - \max\left(D_i^-\right)\right]^2}$$ → M-Topsis

Rank reversal is a phenomenon that occurs when a decision maker, in the process of selecting an alternative from a set of choices, is confronted with new alternatives that were not thought about when the selection process was initiated. It depends on the relationship between this new alternative and the old ones under each criterion (García-Cascales and Lamata, 2012).

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