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Decision support for the deployment of hydrogen technologies at the scale of a territory

Anaëlle Jodry

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THÈSE DE DOCTORAT
DE L'UNIVERSITÉ PSL

Préparée à Mines Paris-PSL

**Aide à la décision pour le déploiement de l'hydrogène
comme vecteur énergétique à l'échelle d'un territoire**
*Decision support for the deployment of hydrogen
technologies at the scale of a territory*

Soutenue par

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Contents

Remerciements	ix
Resumé en Français	x
Summary	xii
Abbreviations	
1 Introduction	1
1.1 Context	1
1.2 Hydrogen and energy transition	2
1.3 Technico-economic analysis of hydrogen supply chain: production, storage and transportation	3
1.3.1 Hydrogen production technologies	3
1.3.2 Hydrogen storage technologies	5
1.3.3 Transportation of hydrogen	7
1.4 Energy system modelling literature	8
1.4.1 Operational analysis models	8
1.4.2 Optimal dispatch models	8
1.4.3 Optimal planning models	9
1.5 Modelling hydrogen demand and its evolution	10
1.5.1 Hydrogen for industrial uses	10
1.5.2 Oil refining	10
1.6 Synthesis of the state-of-the-art	12
1.7 Problem definition and objectives	12
1.8 Challenges	13
Méthode et outils - Résumé	
2 Methods and tools	15
2.1 The three-step methodology	15
2.2 Generic model	16
2.2.1 Sets	17
2.2.2 Objective function	18

2.2.3	Decision variables	19
2.2.4	Conversion technologies capacity constraints	20
2.2.5	Storage constraints	21
2.2.6	Supply/demand constraint	22
2.2.7	Other constraints	22
2.2.8	Computational tools	22
2.3	Techno-economic parameters	22
2.3.1	Construction of time series for resource import prices	23
2.3.2	Evolution of technologies	25

Trajectoire optimale de déploiement dans un cluster industriel - Résumé

3	Optimal deployment trajectory of an industrial cluster	30
3.1	Fos-sur-Mer case study	30
3.1.1	Context	30
3.1.2	Demand evolution in the cluster	31
3.2	Description of the reference scenario	32
3.3	Description of the indicators used	35
3.3.1	Levelised cost of hydrogen	36
3.3.2	Carbon emissions	36
3.3.3	Installed capacity, produced energy and load factors	37
3.4	Results for the reference scenario	37
3.4.1	Production cost model (France scale)	37
3.4.2	Capacity expansion model (local scale)	39
3.5	Conclusion	

Analyses de sensibilités et robustesse du système - Résumé

4	Sensitivity analyses and robustness of the system	47
4.1	Sensitivity analyses	48
4.1.1	Weighted average cost of capital (WACC)	48
4.1.2	Electrolysis CAPEX learning rate	49
4.1.3	Natural gas prices	51
4.1.4	CO ₂ treatment price	54
4.1.5	Biomethane prices	55
4.1.6	Renewable potential	58
4.1.7	Geological storage	59
4.1.8	Hydrogen imports	60
4.1.9	Discussion	62
4.2	Robustness of the different scenarios	63
4.3	Conclusion	

Valeur d'hybridation des SMR - Résumé

5	SMR hybridisation value	70
5.1	Defining the hybridisation value indicator	70
5.2	SMR hybridisation value in the reference scenario	70
5.3	Limiting factor to hybridisation value	72
5.4	Conclusion	74

Schéma de raccordement optimal des EnR et des électrolyseurs - Résumé

6	Electrolysis and renewables optimal connection scheme	76
6.1	Description of the scenarios	76
6.2	Network costs	78
6.3	Results and discussion	79
6.4	Effect of electricity and hydrogen transmission costs	81
6.5	Sensitivity to the distance between the industrial cluster and the renewable electricity production	82
6.6	Sensitivity to the electricity network tax	83
6.7	Conclusion	83

Conclusions et perspectives - Résumé

7	Conclusion and perspectives	85
7.1	Conclusion	85
7.1.1	Contributions	85
7.1.2	Synthesis of the analyses	86
7.2	Ongoing work and perspectives	87
7.2.1	Ongoing work	87
7.2.2	Perspectives	87

List of Figures

1.1	Hydrogen value chain	3
2.1	Presentation of the three-step methodology.	16
2.2	Structure of the modelled energy system.	17
2.3	Nested time scales	18
2.4	Gas day-ahead market prices for year 2019.	25
2.5	Electrolysis learning curves obtained with IRENA assumptions [1] for different learning rates. The blue lines represents the cumulative capacities in 2030 and 2050 projected by the IRENA and the green line the cost projected by the Hydrogen Council [2]	26
2.6	Electrolysis learning curves with the IRENA assumptions [1] for different learning rates. The blue lines show the projected costs of the IEA and the green line the projected costs of RTE in 2030 and 2050.	27
2.7	Simplified conventional SMR process	28
2.8	Simplified SMR process with possibilities of CO ₂ capture.	28
3.1	Estimated industrial hydrogen demand evolution in Fos-sur-mer cluster between 2020 and 2060.	32
3.2	Grid electricity price duration curve from simulation for period 2020-2030. The black dotted line represent the observed curve for 2019 (which was taken as a reference for the meteorological data).The annotations show the cost of the marginal production plant.	38
3.3	Grid electricity price duration curves from simulation for all periods. The black dotted line represent the observed curve for 2019 (which was taken as a reference for the meteorological data).	39
3.4	Investment trajectory in the hydrogen and electricity production assets for between 2010 and 2050. The percentage on the bars represent the load factor for each technology for the following operation period (if the capacity is over 10 MW).	40
3.5	Hydrogen production by technology. The percentages on the bars represent the share of the demand that is supplied by the considered technology (if over 10%).	41
3.6	Carbon content of hydrogen evolution (left axis and blue line) and cumulative CO ₂ emissions (right axis) from 2020 to 2060. In grey, cumulative emissions for a "business as usual" scenario allowing only conventional SMR.	42

3.7	Stock inventory for gaseous storage in tank (data has been smoothed with a 20 h rolling-average window).	43
3.8	Stock inventory for gaseous storage in tank.	44
3.9	Levelised cost of hydrogen production and storage (LCOH) for alkaline electrolysis and steam methane reforming technologies, and for importations between 2020 and 2060.	45
3.10	Weekly hydrogen production by technology for the 2050-2060 operation period. . . .	45
4.1	Contribution of the assets to the hydrogen supply for the horizon period for different values of the WACC.	49
4.2	Average LCOH and average carbon content of hydrogen, hydrogen imported quantities and biomethane imported quantities for different values of the WACC.	50
4.3	Average LCOH and average carbon content of hydrogen, electrolysis CAPEX and electrolysis installed capacities for different learning rates.	51
4.4	Contribution of the assets to the hydrogen supply for the horizon period for different values of LR.	52
4.5	Average LCOH and average carbon content of hydrogen, hydrogen imported quantities and biomethane imported quantities for different prices of natural gas.	53
4.6	Contribution of the assets to the hydrogen supply for the horizon period for different prices of natural gas.	54
4.7	Comparison of hydrogen production by technology for different captured CO ₂ post-treatment prices. To the left 10€/tCO ₂ , in the middle the reference scenario with 50€/tCO ₂ and to the right 100€/tCO ₂	55
4.8	Comparison of carbon content for different captured CO ₂ post-treatment prices. In blue 10€/tCO ₂ , in orange the reference scenario with 50€/tCO ₂ and in green 100€/tCO ₂	56
4.9	Comparison of hydrogen production by technology for different biomethane prices. On the left 60 €/MWh, in the middle the reference scenario with 75 €/MWh and on the right 90 €/MWh. The percentage on the bars represents the share of the demand supplied by the technology (if greater than 10%).	57
4.10	Hydrogen cost distribution for the last operation period (2050-2060) for electrolysis and SMR for different prices of biomethane.	57
4.11	Comparison of hydrogen production by technology for different levels of renewable potential. On the left, the reference scenario, in the middle the doubled potential scenario, and on the right the unlimited renewable potential scenario. The percentages on the bars represent the share of hydrogen demand supplied by the technology (if greater than 10%).	59
4.12	Comparison of electrolysis capacity investment trajectory for different renewable potential levels. The dotted lines represent the electrolysis load factors.	60

4.13	Comparison of the hydrogen production by technology for scenarios with and without geological storage. On the left, the reference scenario without geological storage, in the middle, the scenario with geological storage, and on the right, the unlimited renewable potential with geological storage scenario. The percentages on the bars represent the share of hydrogen demand supplied by the technology (if greater than 10%).	61
4.14	Comparison of the average LCOH for scenarios with and without geological storage.	62
4.15	Comparison of hydrogen production by technology for different price of hydrogen importation. On the left, the reference scenario with 6 € / kg, in the middle, the hydrogen imports scenario with a progression decreasing from 6 to 2 € / kg, and on the right the cheap hydrogen imports scenario with a price of 2 €/kg. The percentage on the bars represents the share of the demand supplied by the technology (if > 10%).	63
4.16	Matrix of costs for the robustness analysis. Each case represents the average LCOH of the considered scenario.	66
4.17	Matrix of cost differences between the perfectly optimised scenario and the optimised operation only scenarios. Each case represents the average LCOH difference between the two scenarios.	67
4.18	Distribution of the LCOH (upper graph), the carbon content of hydrogen (middle graph), and the hydrogen imported quantities (lower graph) for the eight anticipated scenarios. The black diamond shows the value for the perfectly anticipated optimisation.	68
5.1	Average LCOH and carbon content evolution over the planning horizon for the reference scenario and the scenarios without SMR.	71
5.2	Cumulative CO ₂ emissions over the planning horizon for the reference scenario and scenarios without SMR.	72
5.3	SMR average hybridisation value for the planning horizon for the unlimited renewables potential scenario, the geological storage scenario and the unlimited potential + geological storage scenario, with variant with carbon tax more expensive and carbon treatment less expensive.	74
5.4	SMR hybridisation value per period for the unlimited renewables potential scenario, the geological storage scenario and the unlimited potential + geological storage scenario, with variant with carbon tax more expensive and carbon treatment less expensive.	74
6.1	Graphic representation of the four investigated connection schemes.	77
6.2	Optimised production capacities with load factors for electrolysis.	80
6.3	Optimised distribution of the hydrogen production.	80
6.4	Comparison of the levelised cost of hydrogen breakdown between the different scenarios.	81
6.5	Sensitivity analysis of the levelised cost of hydrogen to the distance between the industrial zone and the renewable zone	82
6.6	Sensitivity of the levelised cost of hydrogen to network taxes.	83

List of Tables

1.1	Hydrogen production technologies costs and CO ₂ emissions	6
2.1	List of decision variables.	20
2.2	Main efficiency parameters for SMR processes [3].	
3.1	Values of the main technical parameters for the technologies considered.	33
3.2	Values of the main parameters for the reference scenario.	35
3.3	France installed capacities for the electric system according to the RTE's N1 scenario (GW) [4].	37
3.4	Electricity prices for the reference scenario.	44
4.1	Synthesis of the scenarios for the WACC analysis.	48
4.2	Synthesis of the scenarios for the learning rate sensitivity analysis.	49
4.3	Synthesis of the scenarios for the natural gas sensitivity analysis.	52
4.4	Synthesis of the scenarios for the CO ₂ treatment price sensitivity analysis.	54
4.5	Synthesis of the scenarios for the biomethane price sensitivity analysis. The biomethane prices are in €/MWh	56
4.6	Synthesis of all the different scenarios for the renewable potential sensitivity analysis.	58
4.7	Synthesis of all the different scenarios for the geological storage sensitivity analysis.	60
4.8	Synthesis of all the different scenarios for hydrogen importation sensitivity analysis. Hydrogen prices are given in €/kgH ₂	62
5.1	Synthesis for SMR hybridisation value analysis.	73
6.1	Location of the technologies for all scenarios.	78
6.2	Distribution of networks costs for each scenario.	81

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Resumé en Français

Pour tenter de maintenir le réchauffement climatique en dessous des 2°C, nous devons faire la transition d'un système basé sur les énergies fossiles vers un système neutre en émission de gaz à effet de serre. Une étape importante pour la réalisation de cet objectif est la décarbonation du secteur industriel pour lequel les émissions directes de CO₂ mondiales s'élèvent à 8,4 Gt en 2020. L'hydrogène a été identifié comme un composant intéressant dans la transition énergétique, particulièrement dans les secteurs de la raffinerie et de la chimie de base où il est aujourd'hui déjà largement utilisé. Des usages dans d'autres secteurs sont également envisagés pour le futur. Cependant, l'hydrogène n'est pas naturellement disponible en grande quantité à notre connaissance, il est donc nécessaire de le produire à partir d'autres ressources énergétiques. Aujourd'hui, l'hydrogène est produit sur site à partir de ressources fossiles avec des procédés fortement émetteurs de gaz à effet de serre. De plus, les infrastructures de stockage, transport et distribution n'existent pas encore. Il y a donc de nombreux challenges à relever pour utiliser l'hydrogène à grande échelle pour décarboner le système. La production et l'utilisation de l'hydrogène impliquant des couplages énergétiques, les investisseurs et planificateurs ont besoin d'outils pour mesurer les impacts de leurs décisions. Pour cela, nous avons développé un modèle d'optimisation intégré et flexible, suffisamment détaillé pour prendre en compte le stockage des ressources et la variabilité des énergies renouvelables. L'optimisation se fait en minimisant les coûts totaux du système sous un certain nombre de contraintes techniques ou économiques. L'apport de cette thèse réside principalement dans la modélisation détaillée des réseaux interconnectés de gaz et d'électricité ainsi que dans la construction de scénarios de données cohérents. Nous avons testé notre méthodologie sur un cas d'étude autour du rôle des unités existantes de reformage du méthane (SMR) dans la transition. Les résultats montrent que l'électrolyse devrait devenir une technologie incontournable dans la production d'hydrogène bas carbone. La capture du CO₂ (CCUS) peut aussi devenir une technologie clef en fonction du prix de traitement du CO₂ capté. Nous trouvons que la limite de compétitivité se trouve autour de 50€ par tonne de CO₂ capté. Nous avons également trouvé une limite de la compétitivité du reformage du biométhane autour de 75€/MWh de gaz. La combinaison de la capture du CO₂ et de l'utilisation du biométhane dans les SMR permet des émissions nulles. De plus, les unités de reformage permettent d'apporter de la flexibilité dans la production d'hydrogène, mais cette flexibilité est en compétition avec le stockage d'hydrogène à grande échelle, par exemple en cavernes souterraines. Cependant, ni la capture du carbone, ni le biométhane ne semblent en compétition directe avec l'électrolyse. Cette constatation nous a permis d'établir l'impact décisif des prix de l'électricité sur le développement de l'électrolyse. En faisant le lien entre l'évolution des prix

de l'électricité à l'échelle nationale et l'opération des électrolyseurs à l'échelle locale, nous avons trouvé qu'alimenter les électrolyseurs avec l'électricité du réseau n'est pas compétitif la majorité du temps. La trajectoire optimale de déploiement implique la construction de parcs renouvelables dédiés, cependant, le manque d'espace dans certaines régions peut être un facteur limitant. A l'aide de la version simple nœud de notre modèle, nous avons pu faire de nombreuses analyses sur le territoire d'intérêt. Cependant, il serait intéressant de pouvoir placer notre territoire dans un contexte plus international. La modélisation développée est particulièrement adaptée à l'étude des ports, il est donc essentiel de pouvoir considérer les importations et le transport de l'hydrogène sur de longues distance.

Summary

One of the biggest challenges of the century is to successfully make the transition from a fossil fuel based energy system to a carbon neutral one in order to keep the global warming below 2°C. A key step towards that goal is to decarbonise the industry sector, whose direct CO₂ emissions amounted to 8.4 Gt in 2020 worldwide. Hydrogen was identified as an interesting gas to help energy transition, especially in industrial sectors such as refineries and production of basic chemicals where it is already widely used. More innovative uses of hydrogen also need to be investigated for the future. However, since no significant natural reserves of hydrogen have been identified to date, it has to be produced from another energetic resource. Nowadays hydrogen is produced on site from fossil resources in small units, however, the different processes are emitting a significant amount of greenhouse gases (GHG). Moreover, the infrastructure needed to store, transport and distribute hydrogen are yet to be developed. That's why there are many challenges to overcome before we can use hydrogen in a way that would help decreasing GHG emissions. Because hydrogen scope is large and implies energy coupling, investors and decision makers need tools to understand the impacts of the evolution of the economic context on its deployment. With this in mind, we developed a flexible integrated optimisation model that can be adapted to any territory. We wanted it to be detailed enough to take into account resources storage and renewables variability. Our model works toward minimising the total costs of the system under different constraints like technical constraints or market constraints. The innovation lies in the detailed description of the interdependent gas and electricity networks and the building of coherent input data. Then, we tested our model on a use case about the role of existing steam methane reforming (SMR) units in the energy transition. The results show that electrolysis is expected to play a major role in low-carbon hydrogen production. Carbon capture (CCUS) could also be a key technology in order to decarbonise the production, depending on the CO₂ management price. The limit for CCUS competitiveness is around 50€ per ton of captured CO₂ in the reference scenario. We found that CCUS can be in competition with biomethane if its price drops below 75€/MWh. We emphasised the key role played by existing steam methane reformer in the transition to keep hydrogen competitive. The combination of carbon capture and biomethane, can lead to zero emission production. On the other hand, steam methane reforming brings flexibility to the hydrogen system, but this flexibility is in competition with large hydrogen storage flexibility. However, we note that neither carbon capture, neither biomethane are in direct competition with electrolysis. We also established the decisive impact of electricity prices on electrolysis deployment. By linking the evolution of grid electricity prices at national scale with electrolysis operation at local scale, we found that running electrolyzers with grid electricity is

not competitive most of the time. The optimal deployment trajectory involves building dedicated renewables to power electrolysers, although in constrained territories, space might be a limiting factor. Until now, thanks to the single-node version of the model, we were able to obtain a lot of insightful information about the territory of interest. However, it would be really interesting to view the studied territory in a broader context. The way we developed the modelling is particularly suitable for the study of hydrogen ecosystems in industrial ports, that's why it is essential to be able to consider abroad imports and long distance transportation of hydrogen.

Nomenclature

Indices

c	conversion technologies
s	storage technologies
r	resources
y	operation year
t	operation time step
h	subset of operation time step

General parameters

$\gamma_{y,r,t}$	importation cost of r at t for y [€/MWh]
ψ_h	fixed cost of withdrawal component of TURPE for h [€/MW]
τ	discount rate [%]
$\theta_{h,t}$	variable cost of withdrawal component of TURPE for t and h [€/MWh]
$d_{y,t,r}$	external consumption of r at t for y [MWh]
$g_y^{\text{CO}_2}$	maximum total CO ₂ emission for y [kgCO ₂]
$t_y^{\text{CO}_2}$	carbon tax value for y [€/kgCO ₂]
$t_{y,r}^{\text{net}}$	network tax for y [€/yr]

Conversion parameters

$\beta_{y,c}$	CAPEX of c [€/MW]
$\omega_{y,c}$	OPEX of c [€/MW/an]
$\lambda_{y,c}$	marginal cost for use of c [€/MWh]
$a_{y,t,c}$	availability of c at t for y [$\in [0, 1]$]

$k_{r,c}$ conversion factor of r by c (if $k_{r,c} \geq 0$ then r is produced, if $k_{r,c} \leq 0$ then r is consumed) [$\in \mathbb{R}$]

$q_{c1,c2}$ 1 if transformation of $c1$ in $c2$ is possible [$\in [0; 1]$]

$e_{y,c}^{\text{CO}_2}$ CO₂ emission for c [kgCO₂/MWh]

$l_{y,c}$ life length of c [year]

$\bar{p}_{y,c}^{\text{max}}$ maximum capacity that can be invested during y [MW]

$\bar{p}_{y,c}^{\text{min}}$ minimum capacity that should be invested during y [MW]

$y_{y,c}^{\text{inv}}$ year when c should be installed for it to arrive at the end of its life during y

Storage parameters

$\beta_{y,s}$ power related CAPEX of technology s [€/MW]

$\sigma_{y,s}$ capacity related CAPEX of technology s [€/MWh]

$\omega_{y,s}$ OPEX of technology s [€/MW/an]

$\eta_{r,s}^{\text{in}}$ efficiency factor to put r or another resource into s [$\in [0, 1]$]

$\eta_{r,s}^{\text{out}} = \frac{1}{\text{efficiencyOut}}$ efficiency factor to take r or another resource out of s [$\text{efficiencyOut} \in [0, 1]$]

$\delta_{r,s}$ dissipation factor to hold r or another resource in s [% for one timestep]

$\bar{c}_{y,s}^{\text{max}}$ maximum storage capacity that can be invested during y [MWh]

$\bar{c}_{y,s}^{min}$	minimum storage capacity that should be invested during y [MWh]
$c_{y,s}^{max}$	maximum storage power that can be invested during y [MW]
$c_{y,s}^{min}$	minimum storage power that should be invested during y [MW]
$l_{y,s}$	life length of s [year]
$res_{y,s}$	resource stored by storage mean s

Investment variables

dy	investment period
$\bar{P}_{y,c}^{inv}$	capacity of c invested during y [MW]
$\bar{P}_{y1,y2,c}^{dem}$	capacity of c installed during $y1$ and removed during $y2$ [MW]
$\bar{P}_{y1,y2,c}^{del}$	capacity of c installed during $y1$ coming at the end of its life during $y2$ [MW]
$\bar{P}_{y,c1,c2}^{trans}$	capacity of $c1$ transformed in $c2$ during y [MW]
$\bar{P}_{y,c}^{tot}$	total capacity of c at the end of y [MW]
$\bar{C}_{y,s}^{inv}$	invested capacity in s during y [MWh]
$C_{y,s}^{inv}$	invested power in s during y [MW]
$\bar{C}_{y,s}^{del}$	removed capacity of s during y [MWh]

$C_{y,s}^{del}$	removed power of s during y [MW]
$\bar{C}_{y,s}^{tot}$	total capacity of s at the end of y [MWh]
$C_{y,s}^{tot}$	total power of s at the end of y [MW]

Operation Variables

dt	operation period
$PS_{y,h}$	contractual withdrawal power for h [MW]
$E_{y,t}^{CO_2}$	CO ₂ emission at t [kgCO ₂]
$I_{y,t,r}$	importation of r at t [MWh]
$P_{y,t,c}$	instant power of c at t [MW]
$S_{y,t,r,s}^{cons}$	amount of r consumed by s [MWh]
$S_{y,t,r,s}^{in}$	amount of r stored at t in s [MWh] (total amount removed from grid)
$S_{y,t,r,s}^{out}$	amount of r taken out of storage s at t [MWh] (total amount added to grid)
$S_{y,t,s}$	amount of r in s [MWh]

General cost variables

CAP_y	fixed capital cost of the system at year y
OPE_y	fixed operation cost of the system at year y
$VAR_{t,y}$	variable cost of the system at time t

Abbreviations

AEL	Alkaline Electrolysis
BF-BOF	Blast-Furnace Basic Oxygen Furnace
CAPEX	CAPital EXpenditure
CCUS	Carbon Capture, Utilization and Storage
DRI	Direct Reduction of Iron
EAF	Electric Arc Furnace
GHG	Greenhouse Gas
IEA	International Energy Agency
LCOE	Levelised Cost Of Electricity
LCOH	Levelised Cost Of hydrogen
LHV	Lower Heating Value
LOHC	Liquid Organic Hydrogen Carrier
MILP	Mixed-Integer Linear Programming
OPEX	OPerational EXpenditure
PEMEL	Proton Exchange Membrane Electrolysis
PPA	Power Purchase Agreement
PSA	Pressure Swing Adsorption/Adsorber
PV	PhotoVoltaic
RE	Renewable Energy
RTE	Réseau de Transport d'Electricité (Fr)
SMR	Steam Methane Reforming/Reformer
TRL	Technology Readiness Level
TURPE	Tarif d'utilisation du Réseau Public d'Electricité (Fr)

Introduction - Résumé

Pour tenter de maintenir le réchauffement climatique en dessous des 2°C, nous devons faire la transition d'un système basé sur les énergies fossiles vers un système neutre en émission de gaz à effet de serre. Une étape importante pour la réalisation de cet objectif est la décarbonation du secteur industriel pour lequel les émissions directes de CO₂ mondiales s'élèvent à 8,4 Gt en 2020. L'hydrogène a été identifié comme un composant intéressant dans la transition énergétique, particulièrement dans les secteurs du raffinage des produits pétroliers et de la chimie de base où il est aujourd'hui déjà largement utilisé. Des usages dans d'autres secteurs sont également envisagés pour le futur. Les piles à combustibles, capables de convertir l'hydrogène en électricité, offrent de nombreuses solutions dans les secteurs des transports, du stockage inter-saisonnier d'électricité ou de la chaleur industrielle. Par ailleurs, les moteurs à combustion interne d'hydrogène pourraient devenir une alternative aux énergies fossiles traditionnelles.

Cependant, l'hydrogène n'est pas naturellement disponible en grande quantité à notre connaissance, il est donc nécessaire de le produire à partir d'autres ressources énergétiques. Aujourd'hui, l'hydrogène est produit sur site à partir de ressources fossiles avec des procédés fortement émetteurs de gaz à effet de serre. Questionner le contenu carbone de la production d'hydrogène est essentiel pour son intégration dans un système énergétique décarbonné.

Les stratégies pour la production d'hydrogène bas carbone impliquent le plus souvent une production basée sur l'électrolyse, un procédé permettant la conversion chimique de l'eau en hydrogène et oxygène en utilisant une grande quantité d'électricité, le plus souvent d'origine renouvelable. D'autres procédés bas carbone innovants comme la pyrolyse de la biomasse ou le craquage du méthane sont également à l'étude. Une autre piste prometteuse est l'utilisation de procédés conventionnels de production tel que le reformage du méthane (SMR) associé à des unités de capture du CO₂.

De plus, les infrastructures de stockage, transport et distribution n'existent pas encore. Il y a donc de nombreux défis à relever pour utiliser l'hydrogène à grande échelle pour décarboner le système. La diversité des méthodes de production et des défis logistiques souligne la complexité du déploiement de l'hydrogène et des couplages sectoriels, qui nécessitent une planification minutieuse adaptée à des territoires spécifiques et à des contextes énergétiques en constante évolution. Cette planification doit être en mesure d'anticiper les évolutions des facteurs clés tels que le prix de l'électricité et les développements technologiques à venir. La croissance de la demande d'hydrogène dans les différents secteurs doit elle aussi être correctement modélisée et anticipée par les décideurs et les investisseurs.

Des outils robustes permettant de comparer les options et d'évaluer l'impact de la transition énergétique sur différents territoires sont indispensables à une prise de décision éclairée. Les modèles décrits dans la littérature peuvent être classés en trois catégories : les modèles d'analyse opérationnelle, utilisés pour évaluer les performances d'un système énergétique, les modèles d'optimisation des coûts de production et les modèles d'optimisation de la planification des investissements. Les deux dernières catégories de modèle sont particulièrement intéressantes pour étudier l'évolution des systèmes énergétiques multi-énergies, cependant, du fait de l'important temps de calcul que cela implique, il y a peu de cas avec des modèles intégrés combinant les avantages deux catégories.

La revue de littérature révèle une lacune importante dans la compréhension de la transition des systèmes énergétiques actuels vers des systèmes futurs optimisés, en particulier au niveau territorial où les plans de transition sont mis en œuvre. Les plans de transition énergétique existants manquent souvent de bases scientifiques et reposent sur des objectifs arbitraires. Cette thèse vise à combler ces lacunes en développant des outils et des méthodologies d'aide à la décision pour planifier le déploiement de la chaîne d'approvisionnement en hydrogène au sein des territoires. Contrairement aux approches actuelles qui adoptent des perspectives globales, la méthodologie proposée prend en compte la demande locale, les contraintes et les incertitudes, en adaptant les échelles temporelles aux besoins de planification et d'exploitation du système énergétique.

En outre, l'étude met en évidence l'absence de prise en compte des incertitudes liées à l'évolution de la demande, au bouquet énergétique et aux marchés de l'énergie dans la littérature existante. Pour y remédier, une analyse de sensibilité dans le cadre de scénarios cohérents est proposée, ce qui nécessite une méthodologie souple et adaptable. La thèse se concentre sur l'étude des groupements industriels portuaires en tant que territoires clés pour le déploiement de l'hydrogène en raison des synergies potentielles et des opportunités de commerce international.

Les principales questions de recherche visent à déterminer le rôle de l'hydrogène dans la transition énergétique, à identifier les configurations optimales de la chaîne d'approvisionnement, à évaluer les trajectoires d'investissement et à comprendre l'impact des caractéristiques du territoire sur les stratégies de déploiement. L'objectif final est de fournir aux décideurs un outil de planification pour améliorer le déploiement des chaînes d'approvisionnement en hydrogène et faciliter la transition énergétique à l'échelle territoriale.

Parmi les défis à relever pour atteindre ces objectifs, citons la grande diversité des technologies de l'hydrogène, l'intégration d'échelles temporelles et spatiales multiples et la gestion de vastes ensembles de données nécessaires à la modélisation à l'échelle du territoire. Ces défis soulignent la nécessité d'études préliminaires détaillées et d'efforts de collecte de données pour garantir une représentation précise des facteurs spécifiques au territoire et optimiser le déploiement des écosystèmes de l'hydrogène.

Chapter 1

Introduction

1.1 Context

One of the biggest challenges of the century is to successfully transition from a fossil fuel-based energy system to a carbon-neutral one to keep global warming below 2°C [5]. Worldwide, actors in both the public and private sectors committed themselves to reduce their greenhouse gas (GHG) emissions and achieve net zero emissions by 2050 [5, 6]. A key step towards that goal is to decarbonise the industry sector, whose direct CO₂ emissions amounted to 8.4 Gt in 2020 worldwide [7].

Dihydrogen, more commonly called hydrogen, is considered an interesting energy carrier to help decarbonise these sectors. According to the International Energy Agency (IEA), [8] its development is essential to achieve a carbon neutral economy. Hydrogen has been used in the energy and industrial sectors since the end of the 18th century [9] and today it is mainly used to produce ammonia-based fertilizers (27% of total consumption) and to desulfurise oil in refineries (33% of total consumption) [10]. In the future, hydrogen could also be used as an energy carrier, especially due to the development of fuel cells and hydrogen-fueled combustion engines or turbines. Fuel cells are electrochemical devices that can convert hydrogen and oxygen into electricity [11], and hydrogen combustion engines are thermal engines that use hydrogen instead of a fossil resource such as oil or gas [12]. Fuel cells can be used in numerous applications, both stationary and remote, such as transportation, seasonal electricity storage, and industrial heating, to name a few.

Few natural reserves of hydrogen have been identified and are yet to be characterised [13–15]. To date, natural hydrogen is not exploited, so hydrogen has to be produced from another energetic resource. Today, hydrogen is primarily produced on site from fossil resources, essentially natural gas and coal [10]. However, current hydrogen production processes are responsible for a significant amount of GHG [16]. As an example, steam methane reforming (SMR), which is used to produce 59% of hydrogen worldwide, emits around 10 kgCO₂/kgH₂ [17]. El-Emam *et al.* found that even “low-carbon” hydrogen production means emissions range from 1 kgCO₂/kgH₂ to 7.5 kgCO₂/kgH₂ [18]. Consequently, developing low-carbon production pathways for both existing and future uses of hydrogen is a requirement for its use in any decarbonisation effort. Moreover, the infrastructure needed to store, transport, and distribute hydrogen is still limited today and needs to be extended.

When we think of low carbon hydrogen production, water electrolysis [19] immediately comes to mind, as many governments plan its large-scale deployment[20]. Indeed, if the electricity used to power electrolysis is low carbon, then the carbon intensity of the produced hydrogen can be low as well. But many other technologies can also be considered: conventional production pathways, such as SMR, coupled with carbon capture utilisation and storage (CCUS) [21], or more innovative technologies like biomass pyrolysis , methane cracking and thermochemical cycles [16]. Whatever the process, hydrogen production depends on other resources, such as natural gas or electricity. Therefore, the deployment of hydrogen implies sector couplings that can be difficult to manage for hydrogen planning.

We see that the ways to produce hydrogen, but also to transport it and store it are diverse. A challenging question is to define what supply chain is pertinent regarding a specific territory or a specific time. Different territories can have different geographical characteristics and different social and economic constraints. What may be interesting for a territory at some point is not necessarily universal and the question needs to be answered individually. Moreover, the rate of deployment of electrolysis and renewable energies need to be considered because it is technically impossible to build them overnight [22]. That is why the planning of the deployment of all the infrastructure for the production, storage, transportation, distribution, and usage of low carbon hydrogen is complex.

Moreover, the energetic context is expected to change in the next 30 years to achieve zero net emission. Thus, it is difficult for decision makers and investors to anticipate the evolution of the many factors related to hydrogen deployment such as electricity and gas prices, electricity availability, the cost of hydrogen technologies, the increase of hydrogen demand, etc. In this context, they will need tools to compare their different options and understand the impact of the evolution of key factors of the energy transition on their territory.

1.2 Hydrogen and energy transition

Many countries believe that hydrogen is essential for the energy transition in the energetic and economic context previously presented [23]. The European strategy of July 2020 plan the deployment of 40 GW of electrolysis to produce 10 Mt per year of low-carbon hydrogen in 2030 [24]. In France, with the national strategy for the development of low carbon hydrogen, 7 b€ will be invested before 2028 to decarbonise the industry and the mobility sectors. For the industry sector, the objective is to produce 20% to 40% of the hydrogen used with low-carbon production means. These international and national plans are made at the aggregated scale. To put them into practice, more studies are needed at the territory scale.

However, hydrogen is not a miracle solution that will replace fossil fuels. Its deployment must be understood in relation to the evolution of the energetic context. In this context, electricity is particularly important because it is the main energy vector considered to produce low-carbon hydrogen, especially if we consider the deployment of electrolysis. If we use electricity to produce hydrogen, then the carbon content and price of hydrogen are directly linked to the carbon content and price of electricity. Moreover, hydrogen is in competition with electricity for many uses, such as mobility and industrial heat production. As the efficiency of electrolysis cannot reach 100%,

producing hydrogen with electricity itself produced from natural gas or coal will not have a positive impact on reducing GHG emissions. To produce competitive low-carbon hydrogen, it is essential to develop low-carbon electricity production means with low marginal costs.

It is also important to note that existing power production capacities are already used to supply the current electricity demand. Moreover, this demand is expected to grow in the near future because of the possible massive electrification of the transport, industry and building sectors. If we take France as an example, electricity consumption is expected to increase from 470 TWh / year in 2020 to 630 TWh / year in 2050, according to the French transportation system operator: Réseau de Transport d'Électricité (RTE). In RTE's study entitled "Futurs énergétiques 2050" [4], hydrogen produced by electrolysis accounts for 30 TWh/yr of electricity consumption. Thus, new electricity production capacities are needed and their deployment has to be done according to network constraints and renewables variability constraints. In this regard, hydrogen could be interesting as long-term electricity storage and help renewables development.

1.3 Technico-economic analysis of hydrogen supply chain: production, storage and transportation

Like electricity, hydrogen is only an energy vector, an intermediate between a primary resource and a final energy. The following scheme 1.1 presents a non-exhaustive list of production processes and final uses, as well as hydrogen storage en transport infrastructure. The figures in this section are mainly based on the work of Parkinson *et al.* [16] who compared hydrogen production technologies with a life cycle analysis approach, and the IEA's report "The Future of Hydrogen", published in 2019 [10].

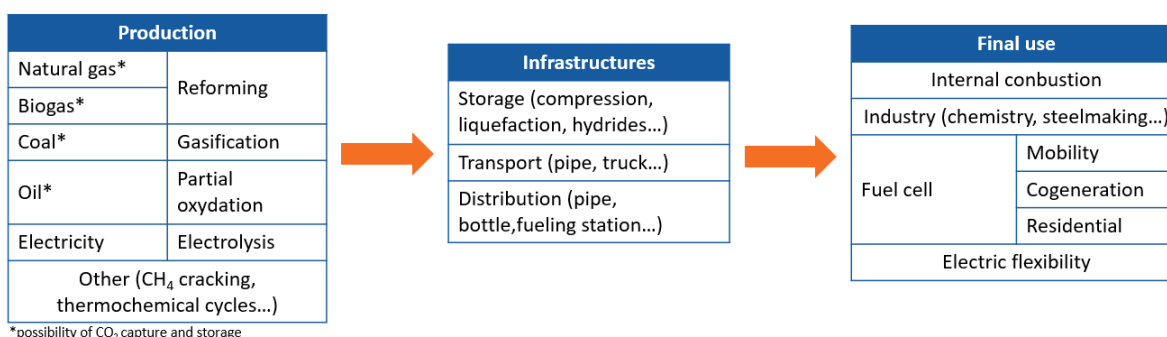


Figure 1.1: Hydrogen value chain

1.3.1 Hydrogen production technologies

According to the IEA's technical report, 59% of worldwide hydrogen is produced with dedicated production means, while 41% comes from industry as a by-product of others processes (chlorine production, steel industry, etc.). In the end, 76% is produced from natural gas, 22% from coal, 0.4% from crude oil and less than 2% from electricity [10]. The main hydrogen production technologies are:

Steam methane reforming (SMR)

Steam methane reforming consists of the chemical reaction of methane with water vapor (650-1000°C, 5-40 bar) with the overall reaction: $CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2$. The efficiency of the process is greater than 70% and the cost of hydrogen production is between 0.84 € / kgH₂ and 1.29 € / kgH₂. The cost directly depends on feedstock gas price and thus depends on the location of the plant. CO₂ emissions range from 10 kgCO₂/kgH₂ to 17 kgCO₂/kgH₂ [10, 16]. CO₂ emissions comes from two different sources: the combustion of natural gas to provide the needed heat and the chemical reaction itself [3].

Gasification of coal

In this process, the coal powder is oxidised with air or pure oxygen at high temperature and high pressure (800-1300°C, 30-70 bar). It produces a mixture of gases called syngas consisting of hydrogen, carbon monoxide, methane, carbon dioxide, and other impurities. To get hydrogen, the different gases have to be separated. The overall chemical reaction is as follows: $CH_{0.8} + 0.6O_2 + 0.7H_2O \rightarrow CO_2 + H_2$. This process has a lower efficiency compared to SMR (around 55%), and is highly CO₂ emitting: between 14.7 kgCO₂/kgH₂ and 26 kgCO₂/kgH₂ if the coal mine is underground and even more if the coal mine is open-air (between 16 kgCO₂/kgH₂ and 31 kgCO₂/kgH₂). However, production costs remain low: 0.8 € / kgH₂ to 1.54 € / kgH₂ [10, 16].

Gasification of biomass

This process is similar to the gasification of coal; however, biomass is more difficult to gasify, and other hydrocarbons are created. Classical temperature and pressure conditions are 500-1400°C and 1-33 bar. This process is rarely used to produce hydrogen, but the CO₂ emitted is biogenic (it was previously captured in the atmosphere when the biomass grew). Production costs range from 1.2 € / kg to 2.5 € / kg and emissions between 0.3 kgCO₂/kgH₂ and 8.6 kgCO₂/kgH₂ [10, 16]

Carbon capture (CCUS)

The three production routes already presented emit directly CO₂. It is possible to capture with CCUS units. Capture rates and costs depend on the technology considered. For natural gas reforming, capture rates range between 50% and 90% with a CO₂ capture and storage costs between 47.5 €/tCO₂ and 71.3 €/tCO₂ [3]. Regarding coal gasification, the capture rates are slightly better (85% to 92%) and the costs are lower: from 35.3 €/tCO₂ to 63 €/tCO₂ [16].

Electrolysis

Electrolysis consists of dissociation of water with and electrical current. It is possible to electrolyse pure water with the reaction $2H_2O \rightarrow 2H_2 + O_2$ or brine (salted water) with the reaction $2NaCl + 2H_2O \rightarrow Cl_2 + H_2 + NaOH$. Electrolysis of brine is usually used to produce chlorine with pure hydrogen as a by-product. Costs and environmental impacts are mainly related to electricity production. In the literature, electrolysis of pure water costs between 3.8 € / kgH₂ and 12.2 € / kgH₂,

which is more expensive than the other processes. CO₂ emissions range between 0.5 kgCO₂/kgH₂ and 2.5 kgCO₂/kgH₂. These values also vary depending on the operation of the electrolyser (load factor) [10].

Methane pyrolysis

Hydrocarbon pyrolysis or cracking consists of the separation of carbon atoms and hydrogen atoms with high temperature and hypoxic atmosphere. This process has the advantage of not creating carbon oxides (CO and CO₂). The chemical reaction is as follows: $CH_4 \leftrightarrow C + 2H_2$. As electrolysis is based on water splitting, cracking is based on methane splitting, however, the enthalpy of reaction is four times higher for electrolysis compared to cracking ($\Delta H^\circ_{CH_4} = 5,25 \text{ kWh/kgH}_2$ et $\Delta H^\circ_{H_2O} = 19,88 \text{ kWh/kgH}_2$). This process is interesting because there are no direct emissions; moreover, carbon black which is a by-product of the reaction has a high economic value. Production costs vary between 1.1 € / kgH₂ and 1.5 €/kgH₂ and emissions between 4.2 kgCO₂/kgH₂ and 9.1 kgCO₂/kgH₂ [16, 25].

Other

Other processes have been under research, for example thermochemical cycles or water photolysis. In these processes, water is split into hydrogen and oxygen like electrolysis. For thermochemical cycles, some reaction intermediates are formed successively, resulting in the decrease in the energy of activation. There are hundreds of cycles but the more promising one are sulfure-iode cycle (900°C) which produces sulfure dioxide SO₂, or copper-chlorine cycle (500°C) which produces chloridric acid (HCl). The reactant used to form reaction intermediates (diiodine, sulfuric acid and copper chloride) stays intact along the process. Photolysis consists of using solar radiation to dissociate the water molecule. These processes are still in the research phase so it is difficult to obtain techno-economic information about them, they won't be included further away in this work.

Table 1.1 summarises the costs and CO₂ emissions of the different hydrogen production routes presented.

1.3.2 Hydrogen storage technologies

Hydrogen density is really low (0.089 kg/Nm³). To efficiently store hydrogen, it has to be compressed or cooled. Moreover, hydrogen is really light, that's why there are risks of leakage. The higher the pressure, the higher the leakage risks. This lightness can be responsible for fugitive emissions if not controlled [26]. Abe *et al.* [27] reviewed storage technologies. Unless otherwise specified, all figures in this paragraph comes from this paper.

Compression

The more common and simplest form to store hydrogen is compression, usually to 200 bar (14.9 kg/m³) for fully metallic reservoirs, and between 350 bar and 700 bar (respectively 25.6 kg/m³ and 42.9 m³) for mobility applications (metal and carbon fiber reservoirs). Furthermore, hydrogen could be stored in underground formations such as salt caverns. These caverns can be newly leached

1.3. TECHNICO-ECONOMIC ANALYSIS OF HYDROGEN SUPPLY CHAIN: PRODUCTION, STORAGE AND TRANSPORTATION

Table 1.1: Hydrogen production technologies costs and CO₂ emissions

Technology	Production cost (€/kgCO ₂)		CO ₂ emissions (kgCO ₂ /kgH ₂)	
	lower bound	upper bound	lower bound	upper bound
SMR	0.84	1.29	10	17
SMR + CCUS	1.6	1.9	3	9.1
Coal	0.8	1.54	14.7	31
Coal + CCUS	1.8	2.2	1.1	10.4
Biomass	1.2	2.5	0.3	8.6
Biomass + CCUS	2.6	3	-11.7	-17.5
CH ₄ pyrolysis	1.1	1.5	4.2	9.1
Electrolysis + RE	3.8	12.2	0.5	2.5
S/I cycle	1.2	2.2	0.4	2.2
Cu/Cl cycle	1.2	2.2	0.7	1.8

or reused after storing fossil fuels. Salt caverns are impermeable to hydrogen, which limit losses in case of seasonal storage. Specific compression energy ranging from 2.7 to 5.8 kWh/kgH₂ depending on the type of compression [28] to attain 900 bar.

Liquefaction

Another physical form to store hydrogen is liquid hydrogen. Liquid hydrogen has a density of 71 kg/m³ at 20 K (-253.15°C), its boiling point temperature at 1 atm. LHV efficiency of liquefaction is around 70% because of cooling (10 kWh/kgH₂) [10]. Moreover, tanks need to be isolated to avoid heat losses and evaporation (boil-off).

Chemical storage

Hydrogen is transformed in another molecule with chemical properties more adapted to storage. The chemical reaction must be reversible to get the hydrogen back. Ammonia (NH₃) and liquid organic hydrogen carrier (LOHC) are examples of this technique. The formed chemical compound can be used as it is, or it has to be reconverted in hydrogen degrading again the total efficiency of the storage. LHV efficiency of ammonia production range from 82% to 93% (from 5 to 12 kWh/kgH₂) and for LOHC it drops to 60% [10]. Sequential chemical transformations lower again the total efficiency of the system (64% à 82% round trip LHV efficiency for ammonia) [10].

Others

Other storage forms are under study, for example “solid” storage. By solid, we talk about physisorption or chemisorption. Physisorption is the adsorption of a molecule (here hydrogen) on a solid surface without any modification of its composition. The surfaces, often carbon based, can have different forms (nanotubes, fibers, zeolites...). On the other hand, chemisorption consists of the reaction of hydrogen with a solid to form a chemical complex (typically a metal hydride). In

both cases a thermal stimulation is needed to get the hydrogen back by reversing the adsorption or the complex formation. These methods allow a high hydrogen density but are heavy (between 13 and 70 kg/kgH₂ [27]).

1.3.3 Transportation of hydrogen

According to the IEA [10], 85% of the hydrogen consumed in the world is produced on site and require no transportation. It is only possible when using small SMR units, but in a more centralised production scheme allowing economies of scale, more transportation infrastructure might be needed.

Trucks/trains

Trucks are the main transportation mean for gaseous and liquid hydrogen for small distances (\leq 300km). Gaseous hydrogen is stored in trailers containing up to 1 100 kg of hydrogen at 500 bar. For liquid hydrogen, cryogenic tanks are fixed on trailers. One trailer can transport up to 4 000 kg of liquid hydrogen [10]. In areas where the infrastructure exists, it is possible to put the trailers on trains, which significantly decreases the carbon footprint [29].

Pipelines

For large volume and long distances, hydrogen pipelines seem to be the more competitive solution. As of today, 5 000 km of pure hydrogen pipelines have been built in the world by private companies. They are used to transport hydrogen from industrial production sites to consumption sites (chemical plants or refineries). According to the IEA report [10], pipeline transportation cost is around 1.6 €/kgH₂ for 2 500 km. over 2 500 km, it seems more interesting to convert hydrogen into ammonia because ammonia pipelines are less expensive. European national gas companies (France, Spain, Denmark, Belgium, Netherlands, Czech Republic, Germany, Italy and Sweden) are discussing about a European hydrogen network called “the hydrogen backbone” [30]. This network would be developed using 75% of retrofitted natural gas existing pipelines.

Ships

For long distances across the sea, hydrogen transportation by ship is considered. Ship transportation imply either hydrogen liquefaction, either hydrogen conversion into ammonia, methanol or LOCH. Boats aiming to transport pure liquid hydrogen are under study but according to the IEA [10], the price is doubled compare to ammonia transportation.

Injection in existing natural gas network

According to studies [10, 30], up to 6% of hydrogen could be mixed with natural gas without any modification of the network. Up to 10% could be injected with minors modification of the existing network. The main problem to increase this rate are the downstream connected technologies which are not adapted to burning hydrogen.

1.4 Energy system modelling literature

Thanks to energy system modelling and optimisation, we can have some answers to these different questions. Mathematical models can help representing an energy system and foresee its evolution under different constraints. Different modelling approaches can be used. Hosseini and al. [31] classified multi-vector energy network models in three categories: operational analysis models, optimal dispatch models (also called production costs models) and optimal planning models (also called capacity expansion models).

1.4.1 Operational analysis models

Operational analysis models include detailed modelling of energy flows and balance that allow to calculate the state parameters (for electricity networks: voltage magnitude and phase angle for example) of a given energy system. They are helpful to understand the physical operability of the system and to evaluate its performance. As these models are not planning models, we won't discuss them any further [31].

1.4.2 Optimal dispatch models

Optimal dispatch models are widely used to determine the optimal operation of a given energy network under constraints in order to satisfy an energy demand [31]. They can include more or less detailed modelling of energy flows, the temporal resolution usually goes from a few minutes to a few hours and the temporal horizon rarely goes above one year. Thanks to the small temporal horizon, they can have more than 30 different spatial nodes. Most of them are Mixed Integer Linear Programming models, or MILP, [29, 32–39], but some are based on genetic algorithms [40–42] or stochastic modelling [43]. In this category, we can think about the ANTARES model developed by the French operator RTE [44, 45] to simulate the operation of the electrical and gas networks interconnected with neighbouring countries. Almansoori and Shah [32] started working on this type of model very early and their model inspired a lot of studies. At first, the objective was to give a snapshot of the operation of the hydrogen supply chain needed for meet a hydrogen demand for mobility in UK. They later improved it to consider greenhouse gases emission and changed the case of study to Germany [29]. Kharel *et al.* [33], Dawood *et al.* [34], Zhang *et al.* [40], Rezk *et al.* [41] and Li *et al.* [46] all investigated hybrid battery/hydrogen electricity storage in a one node model. The first two studies present a MILP formulation while focusing on the place of hydrogen storage in a highly renewable energy mix. The last two studies use a different formulation (genetic algorithms and mixed formulation involving predictive control and TOPSIS methods) and focus on storage operation strategies. Zhang *et al.* [43] and Tlili *et al.* [35] also investigated the potential of hydrogen to offset renewable energy variability. The first study uses a stochastic model to consider uncertainties of renewable production and the second one a MILP model and focus on the importance of networks interconnections. All the papers mentioned above describe models where the only final energy form is electricity. This mean that the purpose of hydrogen is to be reconverted in electricity with a fuel cell or a gas turbine. Samsatli *et al.* [36], Woo *et al.* [37], Colbertaldo *et al.* [38] and Pan *et al.* [39] worked with MILP models including more than one final

energy in order to design the optimal low carbon hydrogen supply chain to provide a given demand (often in the transportation sector). Gabrielli *et al.* [47] added the possibility of carbon capture and Li *et al.* [48] integrated the hydrogen fuelling station planning. To answer the same kind of question at the regional scale, Wang *et al.* [42] had a multi-objective and multi-actor approach involving a genetic algorithm and TOPSIS (Technique for Order Preference by Similarity to Ideal Solution) decision aiding methods. They did not only focus on the technical feasibility but also on the social aspect of the problem considering different decision makers with different priorities.

1.4.3 Optimal planning models

Optimal planning models are used to plan future investments under constraints [31]. Usually, the objective function is a cost function that has to be minimised and the temporal horizon can be over 50 years with several operation years (years for which the system operability is verified). Because of the wide temporal horizon, either the temporal resolution is coarse or clustering methods like time slicing are used to decrease the complexity of the problem [49]. Usually, if there are more than one spatial node in the model then clustering methods are used. Like for the optimal operation models, most of the planning models are MILP [50–56], but they can also be based on genetic algorithms [57, 58]. The epitome of these models is TIMES, a generic model developed by IEA-ETSAP to conduct different types of energy analyses [45, 59, 60]. Like optimal dispatch models, they can consider one or several final energy forms. De-León Almaraz *et al.* [57] worked at the regional scale with a genetic algorithm to determine the optimal deployment of the hydrogen supply chain supplying a given hydrogen demand. Their multi-objective multi-periodic model can find the optimal size and localisation for each new infrastructure across 21 spatial nodes. Later they repeated the simulation at the national scale and compared the results of the two studies [58]. In a similar way, André *et al.* [50] used a MILP model with a heuristic approach to compare different hydrogen transportation technologies. Many other papers proposed multi-node and multienergy MILP models considering a hydrogen demand, each having specific features. Almansoori and Shah [51] developed further their first supply chain design model to make it multi-periodic. McPherson *et al.* [52] investigated the role of hydrogen storage considering infrastructure costs uncertainty. Samsatli *et al.* [53] developed one of the most detailed multienergy generic model using time slices. Han *et al.*'s model [54] has the particularity to consider existing infrastructure in the first investment period. This particular detail is rare in the literature and seems important. Talebian *et al.* [55] compared different greenhouse gas emission reduction policies Seo *et al.* on the other hand, [56] focused on the development of hydrogen infrastructure with a centralised storage configuration. Most of these models have a detailed spatial resolution with several nodes, but none of them have a better time resolution than 84 time slices. According to Gonzato *et al.* [49], even with advanced time clustering methods, renewable variability and storage can only be properly represented with at least 128 representative days. An alternative to the computational cost of high spatial and temporal resolution models can be soft linking as presented by Alimou *et al.* [45]. They developed an algorithm to link the optimal dispatch model ANTARES and the optimal planning model TIMES.

1.5 Modelling hydrogen demand and its evolution

As we could see in the previous section, the majority of optimisation models found in the literature are *demand driven*, which means that the demand is an exogenous parameter responsible for the evolution of the variables. Therefore, it may have a significant impact on the results. It is necessary to model the demand and its potential evolution with particular care.

Today, almost all of the produced hydrogen is used for industrial purpose. The refinery sector is the biggest consumer with 33% of the total produced hydrogen. Ammonia (NH_3) production take the second place with 27% of the global consumption. Ammonia is mainly used as a chemical feedstock in the production of fertilizers. Both of these uses require hydrogen with a high degree of purity. It is also the case for the industrial chemistry sector (around 3% of the consumption). Other sectors, such as industrial heating (23%), methanol production (10%) or direct reduction of iron (3%) are more flexible with the purity. As for the transportation sector, it only represents 0.01% of the current hydrogen consumption [10].

1.5.1 Hydrogen for industrial uses

1.5.2 Oil refining

In the oil refining sector, hydrogen is mainly used to remove the sulfur from the crude oil in the process to make fuels [61]. Many different operations compose the refining process, two of them consume and one produces hydrogen. First, crude oil is distilled: the different fractions composing it are separated thanks to different boiling points. The fractions with high energetic value (propane, butane, methane, gasoline and diesel fuel) go through hydrotreatment, where hydrogen is used to form sulfur hydroxide (H_2S). The heavier fractions go through hydrocracking (hydrogen-consumer step) and catalytic reforming (hydrogen-producer step) where they are decomposed in smaller molecules with higher energetic value. In the end, net hydrogen needs are around $5.5 \text{ kgH}_2/\text{t}$ (one tonne of crude oil is equivalent to 7.6 barrels). Hydrogen needs depend on the demand in fossils fuel that is expected to go down in the future, and the regulation about sulfur quantity that is allowed in fuels [10]. Moreover, the demand of oil-based plastics may increase. Therefore, it is not easy to predict the evolution of hydrogen demand in this sector.

Chemical industry

Hydrogen is a basic component of industrial chemistry. Among the main uses, we can point out ammonia (NH_3) synthesis with the Haber-Bosh process and methanol (CH_3OH) synthesis. Ammonia synthesis requires the reaction of hydrogen (H_2) and nitrogen (N_2) in a reactor maintained at 450°C and 300 bar, following the chemical reaction $\text{N}_2 + 3 \text{H}_2 \longrightarrow 2 \text{NH}_3$ [62]. Hydrogen needs for ammonia production are $177.5 \text{ kgH}_2/\text{tNH}_3$. Concerning methanol, it is produced from synthesis gas (CO , H_2 and CO_2) following the reactions $\text{CO} + 2 \text{H}_2 \longrightarrow \text{CH}_3\text{OH}$ and $\text{CO}_2 + 3 \text{H}_2 \longrightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}$. Hydrogen needs for methanol production are $13.7 \text{ kgH}_2/\text{tCH}_3\text{OH}$. Industrial demand for ammonia and methanol can be considered stable in the future, but these two components can be considered in heavy transportation sector, especially maritime transportation [10].

Steel industry

Today, the widespread blast-furnace basic oxygen furnace (BF-BOF) process produces hydrogen-containing syngas in the coke oven or in the blast furnace steps. Hydrogen, which is a reducing agent of iron, is thus directly produced during the process. The hydrogen surplus (mixed with other gases) is around 6.1 kgH₂/t of steel [63]. The produced syngas is usually burned onsite in order to produce electricity and heat. The current process process emits high CO₂ amounts as it uses coke as the iron reducing agent. It is possible to inject hydrogen directly in the blast furnace to reduce the quantity of coke used. According to Yilmaz *et al.* [64], the optimal hydrogen quantity to inject would be 27.5 kgH₂/t of steel. Another solution to decrease GHG emission in the steel industry is the direct reduction of iron (DRI). This technology uses syngas (CO and H₂) or methane as the iron reducing agent in an electric arc furnace (EAF). In that case, the electricity consumption amounts to 440 kWh_{el}/t of steel. For this last process, hydrogen needs reach 50 kgH₂/t of steel [63, 65, 66]. It is also possible to inject CH₄ in EAF as iron reducing agent.

Mobility and transportation

As of today, hydrogen demand for the mobility almost doesn't exist [10]. In the literature, many papers only consider mobility for the hydrogen demand. Colbertaldo *et al.* [38] present three scenarios for Italy, with 50% of the individual vehicles fleet replaced by fuel cell electric vehicles (FCEV) or battery electric vehicles (BEV) by 2050. Almansoori and Betancourt-Torcat [29] studied individual mobility in Germany and they assume a penetration rate of 10% by 2030 for FCEVs. For De-León Almaraz *et al.* [57, 58, 67], they considered captive fleet of light commercial vehicles or buses. They assume a penetration rate of 25% in 2050.

Electricity network flexibility

Another use considered for hydrogen is to help balancing the electricity network, in line with the increasing role that renewables are expected to play in the future. To compensate for the seasonal variability of renewable electricity production, electricity can be stored as hydrogen. This storage can take place at two timescales: at the scale of the day/week to compensate for renewables variability and at the seasonal scale to compensate for the thermosensibility of the electricity demand and the seasonality of the photovoltaic (PV) solar production. Some studies only considered the use of electrolysis when there is a surplus of electricity (meaning that its price is close to zero). For example, Kavadias *et al.* [68] try to reach self-sufficiency with a highly renewable mix in an autonomous network. They manage to store 71% of the fatal electricity as hydrogen in a mix with 13% of renewables. Wang *et al.* [42] approach is multienergy (electricity, hydrogen and biomass). They also compare electrical storage and hydrogen storage in a system without any interconnection. With their multi-actor perspective, it is interesting to note that their algorithm chose hydrogen storage only for the "maximin solution" which is not the optimised solution but where all actors have a good satisfactory score (even when the sum of all the scores is not the highest). Finally, Tlili *et al.* [69] evaluated producing hydrogen only with renewable electricity surplus in 2035 (according to the "Ampère" scenario of RTE [4]). They showed that if interconnection with neighbouring

countries is considered, the surplus quantity goes down from 7.9 TWh to 1.4 TWh, meaning that interconnections shouldn't be overlooked. In the interconnected case, the hydrogen quantity that can be produced is very low.

1.6 Synthesis of the state-of-the-art

This literature review leads us to several observations:

- There are a lot of different ways to produce hydrogen (around 10 processes presented here, among the most common ones). One of the challenges is to choose the optimal process considering the territory specific features and resources availability.
- Hydrogen storage and transportation infrastructures also have to be adapted to the territory specificities regarding volumes, transportation distance and the final use of the hydrogen.
- The majority of the models found in literature are deterministic and driven by an exogenous hydrogen demand. It means that the estimation of hydrogen demand is a key part of the study. Uncertainties regarding the hydrogen demand evolution are often overlooked or superficial.
- The demand of hydrogen for industrial uses are neglected in the modelling literature, although it is the main hydrogen use today and is expected to remain in the future.
- The modelling literature at local scale is poor. It means that some aspects inherent to the use of hydrogen and its supply chain are likely to be unavailable at a coarser spatial level.
- We note that timeslicing is widely used for integrated modelling (planning as well as operation) to tackle computational cost challenges.
- Finally, we note the importance of interconnections in renewable energy (RE) management. One must keep in mind that they shouldn't be neglected.

1.7 Problem definition and objectives

According to the literature review, the biggest gap in the literature is that only few works have studied the transition path between the existing energy system and what could be an optimised system in a distant future. This aspect is especially important at the scale of a territory where transition plans are put into practice. Energy transition plans often lack scientific bases and objectives can be arbitrary. In this regard, the first objective of this thesis is to develop decision-aiding tools and methodologies to help decision makers to plan hydrogen supply chain deployment at the scale of a territory.

Moreover, models and studies found in literature usually look at the development of an optimised hydrogen supply chain with a temporally and spatially aggregated approach for long term hydrogen deployment. It means that quantities related to renewables electricity production, energy storage and resource prices are averaged. In our methodology, we will seek to develop a tool able to take into account local demand and constraints, considering the existing assets of the territory. The

temporal scales should be adapted to the planning of energy systems (typically 30 years) and its operation (typically with a hourly resolution).

Another aspect that is overlooked in literature is the uncertainties regarding demand evolution, energy mix evolution and energy markets evolution. To take this aspect into account, we will make sensitivity analysis varying parameters and constraints in coherent scenarios. To do so, the developed methodology needs to be flexible and adaptable.

Finally, the last objective is to study a key territory regarding the deployment of hydrogen. Industrial port clusters are interesting territories because a lot of potential hydrogen producers and consumers are regrouped in the same area, allowing for synergies between industries. Moreover, in a more international view of hydrogen, ports are exchange hubs, allowing for an eventual international trade of hydrogen.

Thus, the main questions that we want to answer are:

- What is the place of hydrogen in the energy transition of a given territory, especially in the industrial sector? In other words, how can the hydrogen demand evolve to support the energy transition and the reduction of GHG emissions?
- What would be the optimal supply chain needed to satisfy this hydrogen demand, considering economical, environmental, social, political, geopolitical and technological constraints?
- What would be an optimal investment trajectory given different scenarios and considering the role of existing assets?
- What are the key characteristics of a territory that have an impact on the deployment strategy of a hydrogen ecosystem?

The objective is to provide a planning tool to help the deployment of hydrogen supply chain, allowing decision makers to have a better understanding of how hydrogen can enhance energy transition at the scale of their territory.

1.8 Challenges

To answer these questions, challenges arise. One of the biggest challenge when talking about hydrogen is the diversity of technologies. As we mentioned before, there are plenty of production means and hydrogen uses are very diverse. Optimising the deployment of hydrogen implies energy coupling and sector coupling that can be difficult to apprehend. As an example, to produce hydrogen by electrolysis with renewable electricity, we have to take into account the development of renewable electricity plants and electricity network constraints. All these aspects have to be modelled. Moreover, for each technology, different levels can be achieved in modelling from the “black box” model (simple link between offer and demand) to the “white box” model where the process is modelled in details. The level of detail should depend on the objective of the study. A compromise has to be found between a realistic representation and the complexity.

Another challenge when considering the development of energy systems is the multiple time and spatial scales involved. For spatial scales, three level can be defined: the international/national level

which is interesting to obtain general aggregated figures and main flows, the regional level which is interesting for locating the infrastructures and finally the local cluster level used to optimise the operation of the system. For temporal scales, three can also be defined: the short term to optimise the operation of what is already existing, the medium term to plan today's investments and the long term to plan future investments. Other time scales have to be considered to account for annual variability (policy evolution), seasonal variability (RE variability, electricity heat sensitivity, H₂ storage) and hourly variability (RE storage, RE variability).

Finally, a last challenge would be the large amount of data needed to run the model at the scale of the territory, for instance the weather data to determine the availability of renewables capacities, the techno-economic parameters for each technologies and their evolution over time, the resources prices and their evolution over time and so on. Moreover, the particularities of the studied territory such as local network constraints, existing infrastructures and local renewable potential must be taken into account. It means that detailed preliminary studies are required.

Méthodologie - Résumé

Ce chapitre présente la méthodologie et les outils de modélisation utilisés dans le cadre de la thèse. la méthodologie adoptée comporte trois étapes :

- Tout d'abord, l'attention est portée sur la modélisation de la demande d'hydrogène, en tenant compte des incertitudes dans les hypothèses clés telles que le niveau de préparation technologique (TRL) et les dépenses d'investissement (CAPEX). Des scénarios contrastés sont élaborés pour représenter les différents changements possibles dans les contextes technico-économiques et politiques.
- Ensuite, ces scénarios sont utilisés pour définir le contexte technico-économique général, en intégrant des facteurs tels que les prix de l'électricité et du gaz, et l'évolution de la teneur en carbone. Cette étape s'effectue à une échelle spatiale supérieure à celle de la zone modélisée, comme la modélisation d'une région à l'intérieur d'un pays.
- Enfin, l'évolution de l'écosystème local de l'hydrogène est optimisée à l'aide d'un modèle d'optimisation intégré et flexible, en tenant compte d'éléments tels que les données météorologiques et les contraintes techniques du réseau spécifiques à la zone locale. Le processus d'optimisation permet d'obtenir la trajectoire d'investissement optimale pour les actifs de production, le fonctionnement horaire du système, les émissions de CO₂ et les coûts annuels.

Le modèle développé pour cette étude est un modèle de planification des investissements multi-ressources. Les modèles d'expansion de la capacité visent à identifier la voie d'investissement la moins coûteuse pour une combinaison d'actifs, en tenant compte de facteurs tels que les nouvelles politiques, les avancées technologiques et l'évolution des prix des combustibles au fil du temps. Contrairement aux modèles de la littérature, ce modèle maintient une résolution horaire afin d'optimiser le fonctionnement du système pour chaque période, ce qui permet une compréhension plus précise du stockage et des flux d'électricité renouvelable.

Le modèle intègre quatre ressources énergétiques : le gaz naturel, le biométhane, l'hydrogène et l'électricité, chacune étant convertible et stockable grâce à diverses technologies. Une caractéristique innovante que nous avons implémentée est la prise en compte des technologies existantes qui évoluent sous différentes formes entre les périodes d'investissement, comme l'ajout d'une unité de capture du carbone à un SMR conventionnel existant. En outre, les technologies peuvent être mises hors service prématurément si elles ne sont plus nécessaires, ce qui permet d'intégrer l'infrastructure existante dans la stratégie de transition.

Les résultats du modèle d'optimisation dépendent fortement des données d'entrée en raison du nombre important de paramètres et du large éventail d'incertitudes. Pour y remédier, l'étude construit différents scénarios à partir de l'espace des solutions, en visant un ensemble diversifié de résultats plutôt qu'en testant de manière exhaustive toutes les combinaisons possibles. Chaque scénario combine des paramètres clés dans des limites inférieures et supérieures définies, tirées de références bibliographiques.

La construction de scénarios présente des difficultés car les paramètres sont interconnectés. Par exemple, le prix de l'hydrogène issu de l'électrolyse dépend des prix de l'électricité, qui peuvent à leur tour être influencés par les prix du gaz. Pour assurer la cohérence des données, sont construites des séries temporelles de prix pour l'importation de ressources, en se concentrant particulièrement sur les prix de l'électricité, qui ont un impact significatif sur les trajectoires d'investissement.

Nous faisons l'hypothèse que les technologies basées sur les combustibles fossiles ont atteint leur maturité et que leurs dépenses d'investissement (CAPEX) sont stables, tandis que les coûts des énergies renouvelables et des batteries devraient diminuer au fil du temps en raison des économies d'échelle, des progrès techniques et des effets d'apprentissage. Le CAPEX des électrolyseurs, un paramètre crucial, est sujet à une grande incertitude. La théorie de la courbe d'apprentissage est utilisée pour estimer la réduction des coûts des technologies en développement sur la base de l'expérience de production cumulée.

Chapter 2

Methods and tools

This chapter is dedicated to the presentation of the methodology and the modelling tools that were used to conduct the work in this thesis. In the first section 2.1, the different steps of the methodology are presented. The next section 2.2 is dedicated to introducing the most general form of the developed optimisation model. Finally, some elements regarding the most significant input parameters are given in section 2.3.1.

2.1 The three-step methodology

To achieve the objectives presented in the previous chapter, we decided to develop a tool able to simulate the optimal evolution of an hydrogen ecosystem over time, given the evolution of the hydrogen demand and the techno-economic and political contexts. To do this, we used energy system optimisation, which can help representing an energy system and foreseeing its evolution under different constraints. The main part of the modelling effort is the development of a multienergy capacity expansion model. Our methodology consists in three steps.

Firstly, we pay particular attention to the modelling of the hydrogen demand for the considered area. Bhattacharyya *et al.* [70] pointed out that capacity expansion planning is highly sensitive to boundary conditions and key assumptions. However, in the case of hydrogen development planning, there are a lot of uncertainties about the key assumptions, for instance the CAPEX for low technology readiness level (TRL) technologies. Indeed, there are multiple pathways to reach a net zero emissions energy system and it is not possible to predict accurately how the energy landscape will evolve. In order to address that challenge, we chose to build contrasted scenarios representing different possible changes of the techno-economic and politic contexts.

Then, we use these scenarios to define the general techno-economic context in which is included the area we want to model. At this step, the spatial scale of the general context should be larger than the area we seek to model, for instance a country in order to model a region. This step includes the modelling of electricity hourly prices and carbon content or gas hourly prices and their evolution. An underlying hypothesis is that the choices made at local scale do not impact the larger scale. For the studied cases in this thesis, we work at the scale of the country for the general context. During this second step, we use a production cost optimisation model to obtain hourly some of the hourly

time series needed as boundary conditions for the last step. More details about the calculation of these time series are given in section 2.3.1.

Finally, we optimise the local hydrogen ecosystem evolution using a capacity expansion model. When needed, for example for technologies CAPEX or national policies, we use the same hypotheses as for step two, to ensure the consistency of the data. However, inputs such as weather data or technical network constraints are given for the local area. Thanks to this optimisation, we are able to obtain the optimal investment trajectory for the different production assets, the optimal hourly operation of the system, the hourly CO₂ emission of the system and the annual costs of the system.

Figure 2.1 shows the different steps of the methodology.

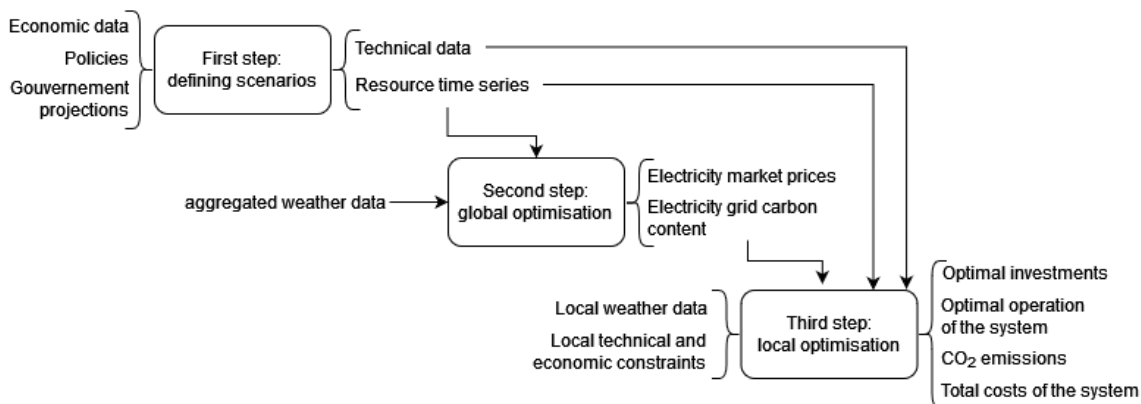


Figure 2.1: Presentation of the three-step methodology.

2.2 Generic model

Our model is an in-house, multi-resource, capacity expansion planning model inspired by the one presented by Samsatli *et al.* [53]. Capacity expansion models are used to find the least-cost investment trajectory of a mix of assets taking into consideration factors such as new policies, technological advancement and changing fuel prices over time. The model of Samsatli *et al.* is an integrated model, meaning that it also optimises the operation of each asset that is invested in. Unlike these authors, we maintained an hourly resolution to optimise the operation of the system for each period in order to have a more precise understanding of storage and renewable electricity flows. We consider different four energy resources: natural gas, biomethane, hydrogen and electricity. A resource can be converted into another resource by a conversion technology and can be stored thanks to a storage technology.

Another feature we added is the possibility for existing technologies to evolve into another form between two investment periods. For example, it is possible to add a carbon capture unit to an existing conventional SMR. Technologies can also be decommissioned before the end of their lifespan if they are not needed anymore. This allows us to take into account the existing infrastructure of the studied area and gain a better understanding of the transition strategy. The graphic representation of the energy system given in Figure 2.2 illustrates how the energy flows are organised between the different technologies.

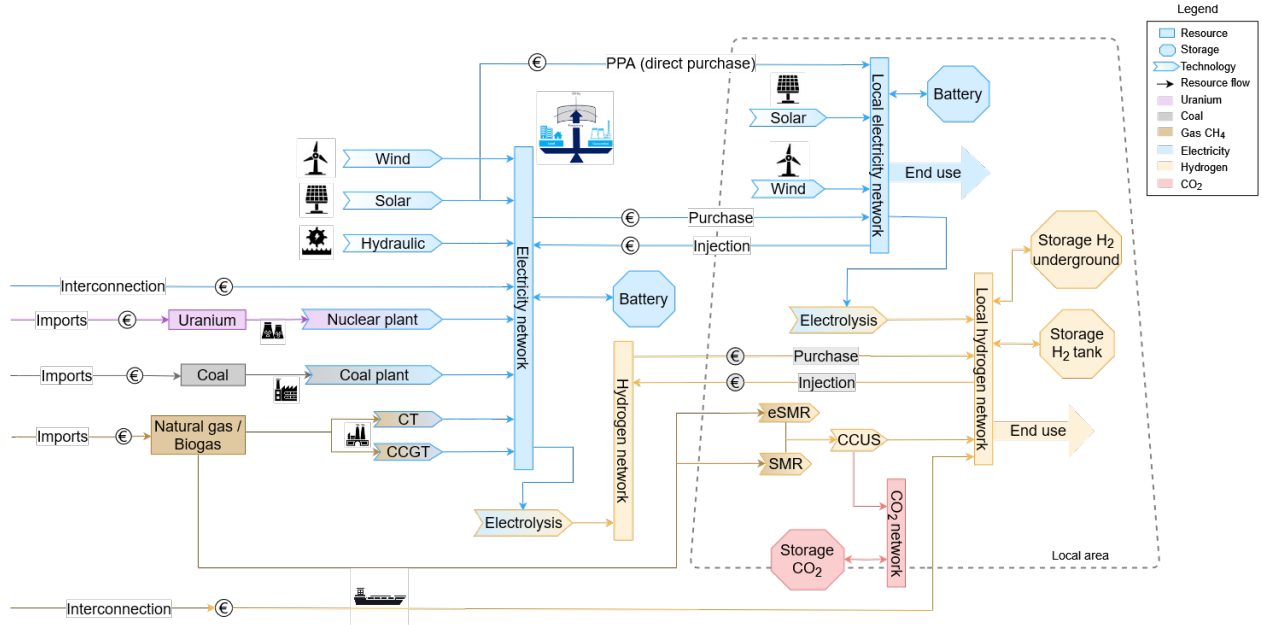


Figure 2.2: Structure of the modelled energy system.

It is formulated as a simple linear optimisation model where the objective is to minimise the total costs of the system under constraints. The general form of the problem can be set as follows :

$$\min_x c^T x$$

$$\begin{cases} Ax \leq b \\ x \in \mathbb{R}^n \end{cases}$$

where $x = (x_1, \dots, x_n)$ are the decision variables (variables decision makers can control), $c = (c_1, \dots, c_n)$ are the associated costs, A is the matrix of constraints and $b = (b_1, \dots, b_n)$ the constraints values.

2.2.1 Sets

The number of sets is the dimension of the problem. A set is an ensemble of elements of the model with the same characteristics. All variables of the model are indexed by one or several sets.

Time scales and spatial scales

In this integrated model, we consider two different sets for the timescales : the planning periods (set y) and the operation time steps (set t). The planning period is used to optimise the investments in new capacities between two operation years of the planning dy . This period should reflect the timescale of decision makers (usually five years for private companies). However, for tractability issues a ten years period is often chosen. The operation time step dt is used to optimise the operation of the invested capacities. To be able to capture renewables variability, this operation time step should be smaller than a day (usually one hour). Figure 2.3 shows how are organised the two time scales.

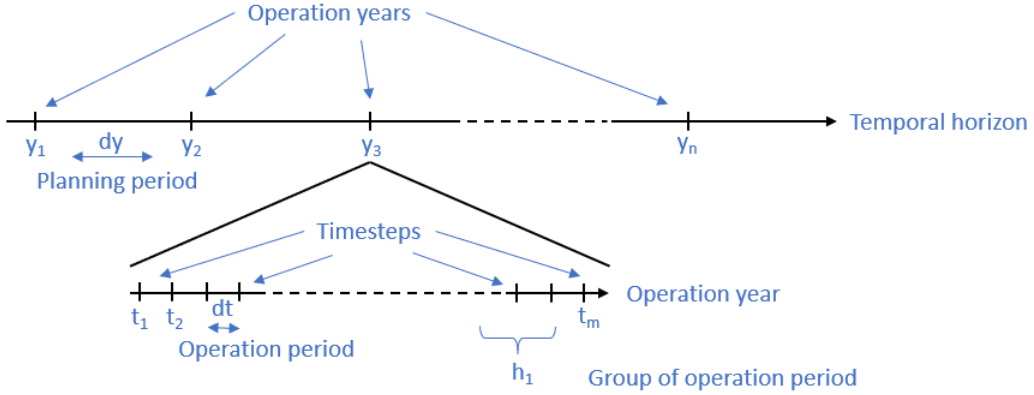


Figure 2.3: Nested time scales

Technologies and resources

In this model, we consider different conversion technologies c that can convert a resource r into another resource r' . During the conversion process, other resources can be consumed or produced. For example, the e-SMR technology converts methane to hydrogen consuming electricity. We also consider storage technologies s , which store one resource but can consume other resources in the process. For example, storing hydrogen consumes electricity for the compression or the liquefaction.

Each conversion technology is detailed with economic parameters (CAPEX, OPEX, economic lifetime), and with technical parameters (conversion factors, minimum/maximum capacity, ramp constraints, CO₂ emissions, minimum/maximum power and dissipation for storage technologies). Resources can be imported from outside the represented territory by paying import costs. Imports are limited by the capacity of the connection, which is also a decision variable. If not competitive enough, a technology can be decommissioned before the end of its lifetime. In that case, the annualised capital cost continues to be paid but the operation and maintenance costs are not eligible anymore. All capacities used during a period should be invested in during the previous investment period. For instance, to determine the techno-economic data, these investments are considered to take place at the middle of the considered period.

2.2.2 Objective function

The objective is to minimise the total cost of the system. The objective function is defined as the sum of different system costs: investment costs that are assumed to be paid in the middle of the investment period, fixed and variable operation costs for each technology, that are assumed to be paid during the operation year, import costs including network costs for each resource and carbon costs, if any carbon tax is applied. All technology costs are annualised regarding a discount factor τ and the lifespan of the technology. To simplify, the discount rate is assumed to be equal to the weighted average capital cost (WACC). The investment cost is assumed to be the mean cost over the period and all costs are annualised to the median year of the period. The objective function is

written as:

$$\min_{P, \bar{P}, I, S, C, \bar{C}, PS} \sum_{n,y} \left[\phi_y^2 \text{OPE}_{n,y} + \sum_{z=1}^y \phi_y^2 \text{CAP}_{n,z,y} + \sum_t \phi_y^2 \text{VAR}_{n,y,t} \right] \quad (2.1)$$

where:

$$\text{OPE}_{n,y} = \sum_c \omega_{y,c} \bar{P}_{n,y,c}^{tot} + \sum_s \omega_{y,s} C_{n,y,s}^{tot} \quad \forall n, y \quad (2.2)$$

is the sum of fixed operation costs for year y and node n ,

$$\text{CAP}_{n,z,y} = \sum_c \beta_{z,c} (\bar{P}_{n,z,c}^{inv} - \bar{P}_{n,z,y,c}^{del}) \phi_{z,c}^1 + \sum_s \left(\beta_{z,s} (C_{n,z,s}^{inv} - C_{n,z,s}^{del}) + \sigma_{z,s} (\bar{C}_{n,z,s}^{inv} - \bar{C}_{n,z,s}^{del}) \right) \phi_{z,s}^1 \quad \forall n, z, y \quad (2.3)$$

are the annualised and actualised fixed investment costs for year z , and:

$$\text{VAR}_{n,y,t} = \sum_r (\gamma_{n,y,r} I_{n,y,t,r} + t_{n,y,r}^{net}) + \sum_c (t_y^{\text{CO}_2} e_{y,t,c}^{\text{CO}_2} + \lambda_{y,c}) P_{n,y,t,c} dt \quad \forall n, y, t \quad (2.4)$$

is the sum of variable importation costs, networks costs and CO₂ emissions costs at time t for year y in node n .

The term:

$$t_{n,y,r}^{net} = \begin{cases} \sum_{t,h} \left[\theta_{h,t} I_{n,y,t,r} + (\text{PS}_{n,y,h} - \text{PS}_{n,y,h-1}) \psi_h \right] & \text{if } r = \text{elec} \\ 0 & \text{if } r \neq \text{elec} \end{cases} \quad \forall n, y \quad (2.5)$$

corresponds to the electricity network cost, and the economic factors:

$$\phi_{y,c}^1 = \frac{\tau}{(1+\tau)(1-(1+\tau)^{-l_{y,c}})} \quad \forall y, c \quad (2.6)$$

$$\phi_y^2 = (1+\tau)^{-(y+\frac{dy}{2}-y_0)} \quad \forall y \quad (2.7)$$

accounts for the investment costs annualisation and actualisation factor (ϕ^1) and the operation costs actualisation factor (ϕ^2). A discount rate of 4% is considered for all investments and actualisation. According to the IEA [71], this number adequately represents the level of risk investing in revenues supported projects for utility scale renewables in Europe.

2.2.3 Decision variables

Decision variables change under constraints to reach the optimum. The number of decision variables is the number of degrees of freedom of the optimisation. They represent real factors over which decision-makers have control. We can separate them in two categories: the ones related to investment decisions (new installed capacities or capacities removed from the system for instance), and the ones related to operation decisions at each time step (such as instant power of each capacity of the system, quantity of energy stored, taken out of storage or imported). The decision variables of this model are presented in Table 2.1.

Table 2.1: List of decision variables.

$\bar{P}_{n,y,c}^{inv/dem/del}$	Installed/decommissioned/retired capacities for conversion technology c
$\bar{C}_{n,y,s}^{inv/dem/del}$	Installed/decommissioned/retired energy capacities for storage technology s
$C_{n,y,s}^{inv/dem/del}$	Maximum rate of storage of s installed/decommissioned/retired
$PS_{n,y,h}$	Power of the connection to the electricity grid for time slot h
$\bar{P}_{n,y,c_1,c_2}^{trans}$	Transformed capacities from conversion technology c_1 to conversion technology c_2
$P_{n,y,t,c}$	Instant power for conversion technology c at time step t
$S_{n,y,t,r,s}^{in/out}$	Quantity of energy stored/taken out of storage at time step t
$I_{n,y,t,r}$	Import of resource r at time step t

2.2.4 Conversion technologies capacity constraints

Investment constraints

The instant power of a given conversion technology $P_{n,y,t,c}$ should remain lower than the available installed capacity $a_{n,y,t,c}\bar{P}_{n,y,c}^{tot}$:

$$P_{n,y,t,c} \leq a_{n,y,t,c}\bar{P}_{n,y,c}^{tot} \quad \forall n, y, t, c \quad (2.8)$$

The invested capacity $P_{n,y,c}^{inv}$ is bounded by the minimum $p_{n,y,c}^{min}$ and the maximum $p_{n,y,c}^{max}$ allowed each year by the decision maker. This constraint could be related to the limited space of the local area for instance.

$$\bar{p}_{n,y,c}^{min} \leq \bar{P}_{n,y,c}^{inv} \leq \bar{p}_{n,y,c}^{max} \quad \forall n, y, c \quad (2.9)$$

A contribution of this model is the possibility for conversion technologies to evolve from one planning period to another, for instance CCS can be added to SMR. Thus, for each period y , the total installed capacity $\bar{P}_{n,y,c}^{tot}$ is defined as the total installed capacity at the previous period $y - dy$, plus the new capacities that were installed or converted, minus the capacities that were removed from the system during period y :

$$\bar{P}_{n,y,c}^{tot} = \bar{P}_{n,y-dy,c}^{tot} + \bar{P}_{n,y,c}^{inv} - \bar{P}_{n,y,c}^{del} - \sum_{z=1}^{y-dy} \bar{P}_{n,z,y,c}^{dem} + \sum_{c_1} \bar{P}_{n,y,c_1,c}^{trans} - \sum_{c_2} \bar{P}_{n,y,c,c_2}^{trans} \quad \forall n, y, t, c \quad (2.10)$$

with the total capacity of conversion technology c_1 being transformed to other conversions technologies at year y $\sum_{c_2} \bar{P}_{n,y,c_1,c_2}^{trans}$ remaining lower than the total installed capacity of c_1 in that same year:

$$\sum_{c_2} \bar{P}_{n,y,c_1,c_2}^{trans} \leq \bar{P}_{n,y,c_1}^{tot} \quad \forall n, y, c \quad (2.11)$$

The capacity of conversion technology c_1 being transformed to the conversion technology c_2 is equal to zero if this transformation is not allowed:

$$\bar{P}_{n,y,c_1,c_2}^{trans} = 0 \quad \text{if } q_{c_1,c_2} = 0 \quad \forall n, y, c \quad (2.12)$$

Decommissioning constraints

In this model, we let the possibility of decommissioning all or part of the total installed capacity before the end of its economic lifetime to save the operation costs. If a capacity is decommissioned before the end of its lifetime, the annualised capital cost continues to be paid but the operation and maintenance costs are no longer eligible. The decommissioning constraint can be written as follow:

$$\begin{cases} \sum_{z=1}^y \bar{P}_{n,yi,z,c}^{dem} = \bar{P}_{n,yi,c}^{inv} & \text{if } yi = yr_{n,y,c}^{inv} \\ \bar{P}_{n,yi,y,c}^{dem} = 0 & \text{if } yi > y \\ \sum_{z=1}^y \bar{P}_{n,yi,z,c}^{dem} \leq \bar{P}_{n,yi,c}^{inv} & \text{else} \end{cases} \quad \forall n, yi, y, c \quad (2.13)$$

where yi is the year when the technology was invested in and $yr_{n,y,c}^{inv}$ the year the technology had to be invested in to arrive at the end of its lifespan during the considered investment period y .

If the installed capacity comes to the end of its lifespan, then it is deleted:

$$\begin{cases} \bar{P}_{n,yi,y,c}^{del} = \bar{P}_{n,yi,c}^{inv} & \text{if } yi \leq yr_{n,y,c}^{inv} \\ \bar{P}_{n,yi,y,c}^{del} = 0 & \text{if } yi > yr_{n,y,c}^{inv} \end{cases} \quad \forall n, yi, y, c \quad (2.14)$$

2.2.5 Storage constraints

Most of the resources of the model can be stored if the right storage technology s is present. For all time steps t , the input rate of storage $S_{n,y,t,s}^{in/out}$ is bounded by the total invested power capacity $\bar{C}_{n,y,s}^{tot}$:

$$0 \leq S_{n,y,t,s}^{in/out} \leq \bar{C}_{n,y,s}^{tot} \quad \forall n, y, t, s \quad (2.15)$$

The total amount of energy in storage $S_{n,y,t,s}$ should remain lower than the total invested energy capacity $C_{n,y,s}^{tot}$:

$$0 \leq S_{n,y,t,s} \leq C_{n,y,s}^{tot} \quad \forall n, y, t, s \quad (2.16)$$

The total energy and power storage capacities at period y are defined as the total capacities at the previous period $y - dy$ plus what was invested in, minus what was removed from the system:

$$\bar{C}_{n,y,s}^{tot} = \bar{C}_{n,y-dy,s}^{tot} + \bar{C}_{n,y,s}^{inv} - \bar{C}_{n,y,s}^{del} \quad \forall n, y, s \quad (2.17)$$

$$C_{n,y,s}^{tot} = C_{n,y-dy,s}^{tot} + C_{n,y,s}^{inv} - C_{n,y,s}^{del} \quad \forall n, y, s \quad (2.18)$$

Invested power and energy capacities are bounded by the minimum and the maximum allowed values:

$$\bar{c}_{n,y,s}^{min} \leq \bar{C}_{n,y,s}^{inv} \leq \bar{c}_{n,y,s}^{max} \quad \forall n, y, s \quad (2.19)$$

$$c_{n,y,s}^{min} \leq C_{n,y,s}^{inv} \leq c_{n,y,s}^{max} \quad \forall n, y, s \quad (2.20)$$

The total amount of energy in the storage at each time step $S_{n,y,t,s}$ is defined as the total amount of energy in the storage at the previous time step plus the quantity that is added in the storage minus the quantity that is taken out of the storage and the dissipation $S_{n,y,t-dt,s}(1 - \delta_{r,s})$:

$$\begin{cases} S_{n,y,t,s} = S_{n,y,t-dt,s}(1 - \delta_{r,s}) + S_{n,y,t,r,s}^{in} \eta_{r,s}^{in} - \frac{S_{n,y,t,r,s}^{out}}{\eta_{r,s}^{out}} & \text{if } r = res_{y,s} \\ S_{n,y,t,r,s}^{cons} = S_{n,y,t,res_{y,s},s}^{in} \eta_{r,s}^{in} + \frac{S_{n,y,t,res_{y,s},s}^{out}}{\eta_{r,s}^{out}} & \text{if } r \neq res_{n,y,s} \end{cases} \quad (2.21)$$

Note that $S_{n,y,t,r,s}^{in}$ and $S_{n,y,t,r,s}^{out}$ are the quantities from the grid point of view. The lower part of equation 2.21 represents the consumption of resource r when storing resource $res_{n,y,s}$ in s . In that case, η^{out} and η^{in} are equal to the consumption of r while using the storage. For example, when storing compressed hydrogen, electricity is needed for the compression.

2.2.6 Supply/demand constraint

The supply/demand equilibrium is verified for each resource at each time step:

$$d_{n,y,t,r} = \sum_c k_{r,c} P_{n,y,t,c} + I_{n,y,t,r} + \sum_s (S_{n,y,t,r,s}^{out} - S_{n,y,t,r,s}^{in} - S_{n,y,t,r,s}^{cons}) \quad \forall n, y, t, r \quad (2.22)$$

where $d_{n,y,t,r}$ is the given demand for the considered area, $k_{r,c} P_{n,y,t,c}$ is the quantity of resource produced or consumed by the different capacities of the system (the resource r is produced by the conversion technology c when the conversion factor $k_{r,c}$ is positive, otherwise, it is consumed), $I_{n,y,t,r}$ is the imported quantity of resource r and $(S_{n,y,t,r,s}^{out} - S_{n,y,t,r,s}^{in} - S_{n,y,t,r,s}^{cons})$ is the quantity of resource r coming from/going into/consumed by the storage capacity s . Resources can be imported from outside the local area by paying the corresponding importation costs.

2.2.7 Other constraints

Some additional constraints can be added to model the local economic, geographical, social and political context. For instance, the volume of biomethane that can be used for hydrogen production is limited by the potential of the area and by competition with other uses. An annual constraint on this volume can be added. Similarly, a constraint on the annual amount of emitted CO₂ can be added in order to model an enforced regulation policy.

2.2.8 Computational tools

The optimisation model was implemented in python using the open source pyomo library. For all the calculations, the commercial solver mosek was used and we also verified the possibility of using the open source solver HiGHS. By default, the interior-point algorithm is used in mosek.

With mosek solver, the reference scenario (only one node) is calculated in 4 minutes and 43 seconds using a CORE i7 processor. The model contains 2,734,532 constraints and 2,804,404 continuous variables (no integer variable). This is leading to 6,930,139 non-zeros values.

The model described in this section is open source and can be found online on the following repository: <https://github.com/Anaelle-Mines/SPHYDERS>. All the data needed to build the different scenarios that will be presented in the following chapters and run the calculations are also available online: <https://zenodo.org/records/10965222>.

2.3 Techno-economic parameters

The results of the presented optimisation model are highly dependent on input data. Given the significant number of parameters and the large range of the uncertainties, we chose to construct

different scenarios from the solution space. Instead of exhaustively testing all the possible combinations, we seek the right combination of parameters in order to obtain contrasted results. That allows us to know which technology mix is expected to emerge in a given context [72]. For each key parameter, we define a reference value taken from the literature, setting a lower and an upper bound, and we construct the scenarios with a combination of these parameters.

The major difficulty in the construction of the scenarios is that parameters are coupled. For example, the hydrogen price produced via electrolysis strongly depends on the electricity price which itself can depend on other resource prices such as gas. Moreover, we have to be aware that for some parameters, choosing a value implies an underlying hypothesis. For instance, assuming that a technology price will decrease may require that this technology is massively adopted. In this section, we will present how we ensure the consistency of the data for each scenario.

2.3.1 Construction of time series for resource import prices

Electricity

One of our main concerns when using the model presented in section 2.2 is to provide hourly electricity prices as they have a significant impact on the investment trajectory of hydrogen production assets, especially on electrolysis. Ruhnau *et al.* [73] showed that the deployment of electrolysis also has an impact on electricity market prices as it brings more flexibility into the energy system. Further, as the share of renewables in the electricity mix is likely to increase, the electricity market prices will be subject to more variability, which we need to model.

Our modelling of the energy system allowed us to identify that electricity prices mainly depend on four factors: the evolution of the electricity production mix (especially the share of renewables), the CAPEX of the production technologies, the operation decisions of the electricity network and the prices of primary resources. To link all of these parameters in a coherent way and generate electricity price series, we adapted the optimisation model presented in section 2.2 to build a production cost model. Production costs models are used to get the optimal operation of a given system. The main difference with capacity expansion models is that capacities are not optimised. In practice, we developed an integrated model with both, the optimisation of investments and the optimisation of the operation. Then, to adapt our model, we modified the parameters to fix the production technologies capacities. In our production cost model, interconnections with neighbouring countries are modelled as a dispatchable generator with a fixed marginal production cost.

To run the calculation, load factor time series for each technology are needed, especially for non-dispatchable renewable production means. When confronted with the challenge of choosing realistic meteorological time series, we decided to base each reference year on the real data of 2019. The weather data for this year is available to download from the website Renewables.ninja [74] where datasets are formatted to provide wind and solar time series. The datasets are taken from the following papers: Grams *et al.* [75], Fattori *et al.* [76], Pfenninger *et al.* [77] and Staffell *et al.* [78]. By taking only one meteorological year, we neglect the effects of climate change and do not investigate the behaviour of the system under extreme climate conditions. To ensure coherence with the local optimisation in the next step, the same year is used. In further work, it would be

interesting to tackle this challenge with a more robust approach.

With this method, we are able to obtain the hourly “grid” electricity prices associated with the selected scenario. With this optimal power dispatch simulation, we are also able to obtain the associated hourly carbon content of the electricity produced, which is a useful input for the next step. Here, we assume that local electrolysers are price takers, i.e. they do not influence national grid power prices. However, the deployment of electrolysis at the national scale is taken into account into the estimation of grid prices.

Cannibalisation of renewables

During the process of developing this methodology, we faced the problem of “cannibalisation of renewables”. In the current system, the market electricity price is given by the marginal cost of the last production plant called to supply the demand. The problem with highly renewable systems is that the marginal cost of renewables is close to zero, so that the market price of electricity becomes really low. This situation is problematic because it means that renewable power plant operators would be in deficit. In fact, these operators will probably sell most of their production directly via power purchase agreement (PPA) at a previously negotiated price covering the cost of the assets. In the end, we added interconnections with neighbouring countries as a flexibility mean with a fixed cost. That way, the excess production of renewables can be valorised and the “cannibalisation” problem is partially solved. Future work should include a better modelling of this phenomena.

Prices of other resources

Without any references saying otherwise, uranium and coal prices are considered the same as today. However, natural gas prices are deeply connected to the geopolitical context and agreement between countries. It may also be related to the weather or the economic context. It is out of the scope of this thesis to predict the future geopolitical context or future crises. An analysis of the French natural gas day-ahead market prices between 2007 and 2019 was done using public data from the French administration (Comission de Régulation de l’Energie) and it showed that gas day-ahead market prices are in the range between 10 €/MWh and 50 €/MWh with a standard deviation around 5 €/MWh during a year. In order to be coherent with meteorological data, we took the prices profile of 2019 (an average of 13.4 €/MWh), but for calculations between 2030 and 2050 we doubled those prices (an average of 26.8 €/MWh) to better represent the actual context. Figure 2.4 shows the gas day ahead market prices for year 2019. We can see well the seasonality of the prices.

For biomethane, the price mainly depends on the CAPEX of the production technologies [79]. For this reason, we considered a fixed price that is likely to decrease, neglecting the seasonality of biomass supply.

We also let the possibility to import zero-carbon hydrogen from outside the territory of interest. It is difficult to evaluate the evolution of the hydrogen price. According to the IEA, it depends on the production technology [80]. To simplify, we take an average importation price including: 4 €/kg for the production, 1.5 €/kg for transportation and 0.5 €/kg for storage and distribution infrastructure, which gives us an average price of 6 €/kg (180 €/MWh) in total.

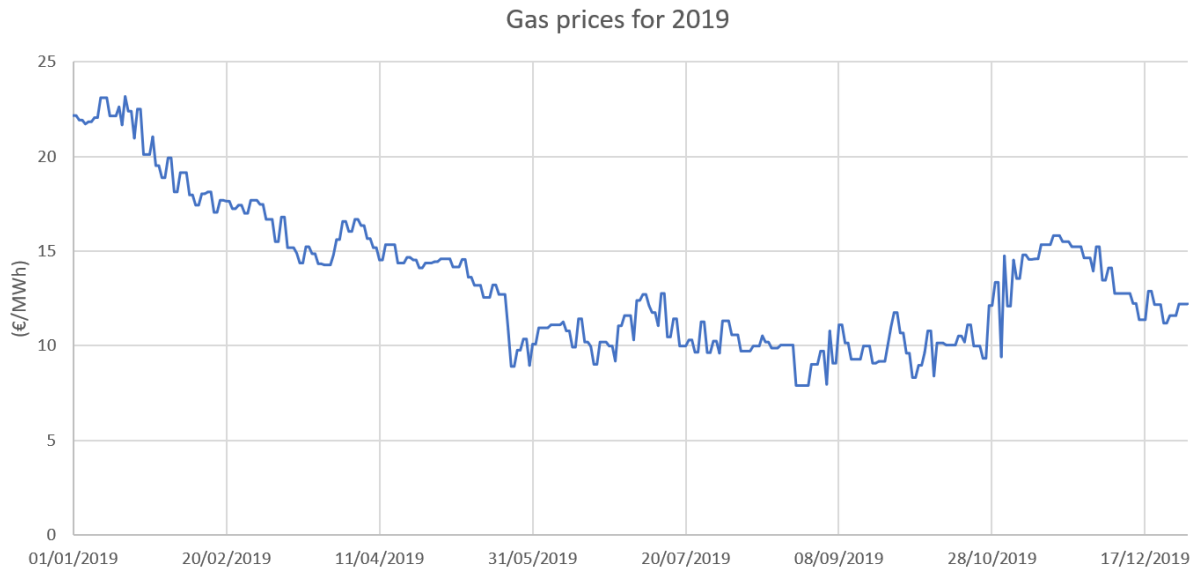


Figure 2.4: Gas day-ahead market prices for year 2019.

2.3.2 Evolution of technologies

Technology prices

We considered that fossil-fuel-based technologies are mature, with high TRL, and have reached stable CAPEX. However, renewables and battery costs are still expected to decrease. This can be due to the economies of scale, technical improvements or learning effects [1, 81]. In 2021, the French transmission system operator RTE conducted a study about the evolution of the electric network for France by 2050, "Futurs énergétiques 2050" [4]. The CAPEX of all electricity production assets are taken from this report.

The CAPEX of electrolyzers is a key parameter with large uncertainties and differences in data from different sources [82]. A common approach to estimate the cost of developing technologies is the learning curve theory introduced by Paul Wright in 1936 [83]. It assumes that accumulative production experience leads to cost reduction, which can be written as:

$$\text{CAPEX}_t = \text{CAPEX}_0 + \left(\frac{X_t}{X_0}\right)^{-\alpha} \quad (2.23)$$

where CAPEX_0 and X_0 are the current CAPEX and cumulative installed capacity of the technology, and X_t the projected cumulative installed capacity. α the learning effect can be described as follows:

$$\text{LR} = 1 - 2^{-\alpha} \quad (2.24)$$

LR is called the learning rate, it represents the obtained cost reduction in percentage whenever the cumulative installed capacity is doubled.

Figure 2.5 shows electrolysis learning curves for learning rates between 10% and 20% calculated using IRENA assumptions [1] ($\text{CAPEX}_{2022} = 750 \text{ \$/kW}_{el}$). According to these curves, electrolyser CAPEX could be between 600 and 800 €/kW_{H₂} in 2030 with a projected world cumulative capacity

of 100 GW, and go down between 200 and 600 €/kW_{H₂} in 2050 depending on the hypothesis concerning cumulative installed capacity. The green line represents the cost projected by the Hydrogen Council in 2030 [2], which is even more optimistic that IRENA projections. According to Jens *et al.* [84], the IAE and RTE based their costs on conservative hypotheses [4, 7, 10, 80] leading to less optimistic cost reductions. Figure 2.6 shows the same learning curves than Figure 2.5 with a zoom on the left part. The purple vertical line shows the IRENA projections and the horizontal lines show the cost projections of the IEA and RTE [4, 10, 80]. They project a cost between 900 and 1000 €/kW_{H₂} in 2030 which correspond to small cumulative installed capacity (between 20 and 30 GW worldwide). In 2050, the IEA and RTE cost projections correspond to the IRENA projection in 2030.

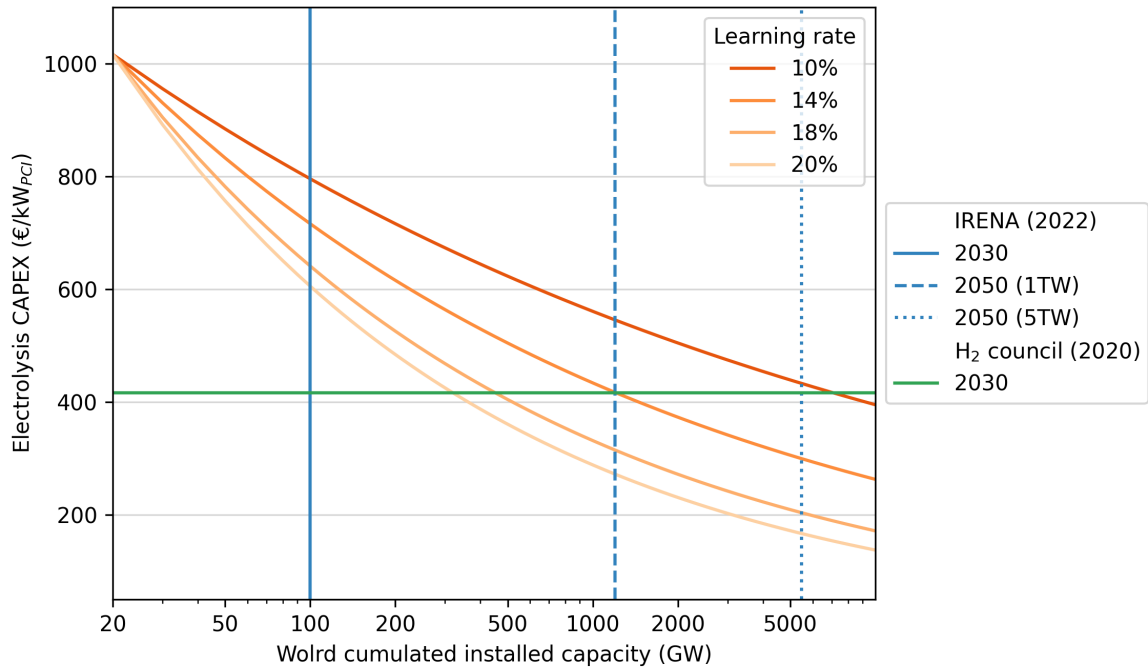


Figure 2.5: Electrolysis learning curves obtained with IRENA assumptions [1] for different learning rates. The blue lines represents the cumulative capacities in 2030 and 2050 projected by the IRENA and the green line the cost projected by the Hydrogen Council [2]

For the rest of the study, apart from the sensitivity analysis on the learning rate, we used a learning rate of 18%, in accordance with IRENA assumptions [1]. It can seem optimistic but Reksten *et al.* (2022) [85] showed a learning rate even higher (between 20% and 25%).

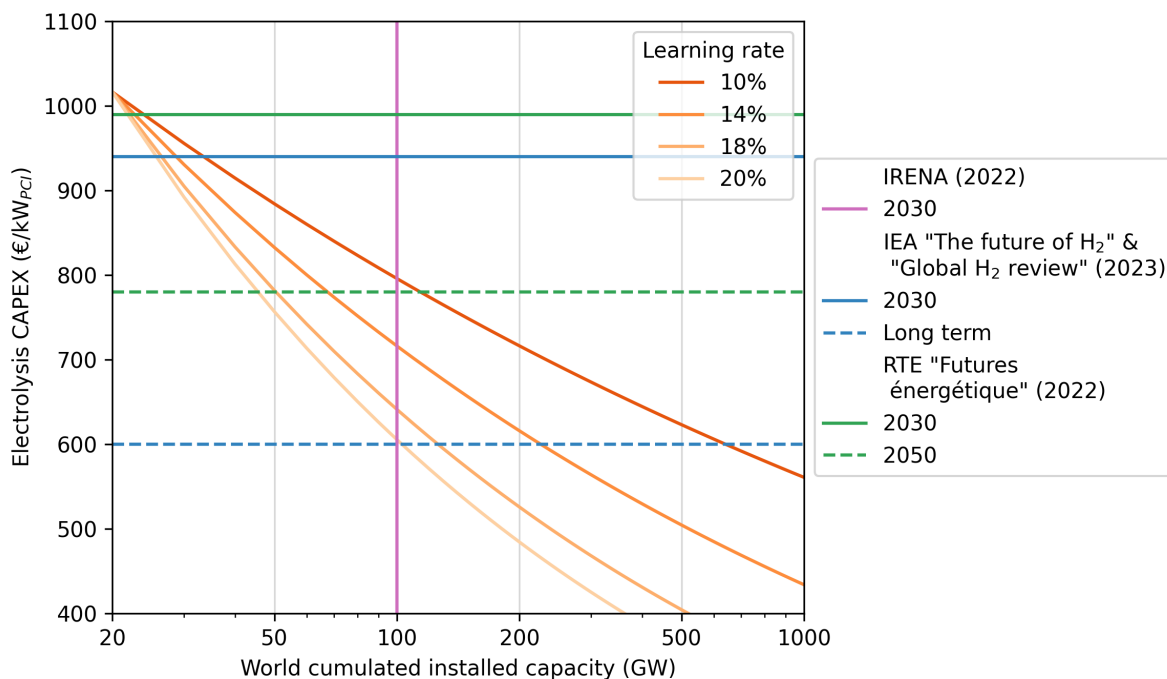


Figure 2.6: Electrolysis learning curves with the IRENA assumptions [1] for different learning rates. The blue lines show the projected costs of the IEA and the green line the projected costs of RTE in 2030 and 2050.

SMR technologies

As mentioned before, some technologies of the model can evolve for one planning period to another without being entirely reinvested. For SMR, it is possible to add CCUS units without having to build a new SMR unit.

Conventional SMR can convert natural gas mostly composed of methane to hydrogen. With a chemical efficiency of 71%, the conventional process consumes 1 mol of natural gas (whose LHV is 12.97 kWh/kg) to produce 2.84 mol of hydrogen (whose LHV 33.3 kWh/kg), for 0.71 mol of CO₂ (44 g/mol). Then the produced gas mixture (H₂ + CO₂ + CH₄ + inerts) is separated using pressure swing adsorption (PSA) process [3]. Moreover, the optimal operation temperature ranges between 800°C and 900°C [86]. To provide the heat, additional natural gas is burned. Burning 1 mol of natural gas produces 1 mol of CO₂, *i.e.* burning 1 MWh of natural gas emits 203.5 kg of CO₂. The tail gas of the PSA, which is mainly composed of unreacted natural gas, CO₂ and some remaining hydrogen, is mixed with fresh natural gas and used as fuel. All the carbon that enter in methane form in the process is converted to CO₂. Figure 2.7 represents the main elements of a conventional SMR process.

In the end, to produce 1 MWh of hydrogen, 1.32 MWh of natural gas are needed and 270 kg of CO₂ are emitted [3, 87]. In this process, CO₂ can be capture in three different places: from the

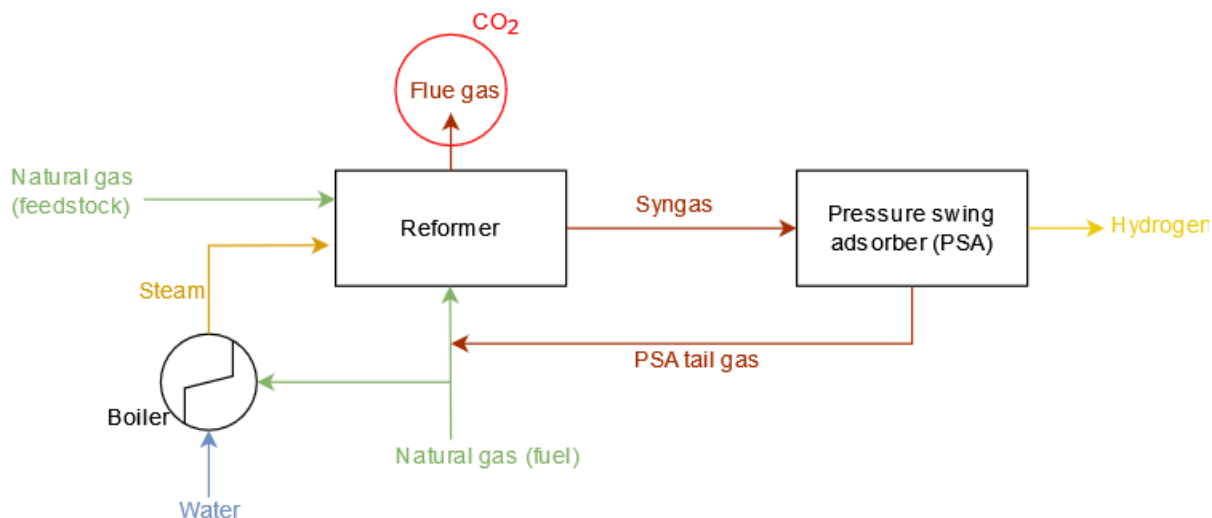


Figure 2.7: Simplified conventional SMR process

syngas between the reactor and the PSA with a capture rate ranging between 54% and 64%, from the PSA tail gas with a capture rate of 52%, or from the flue gas of the reactor with a capture rate of 89% [3, 88]. In the model, only the two last options are considered. With carbon capture, the efficiency of the process decrease. Figure 2.8 shows both options and Table 2.2 recaps the efficiency information for all cases.

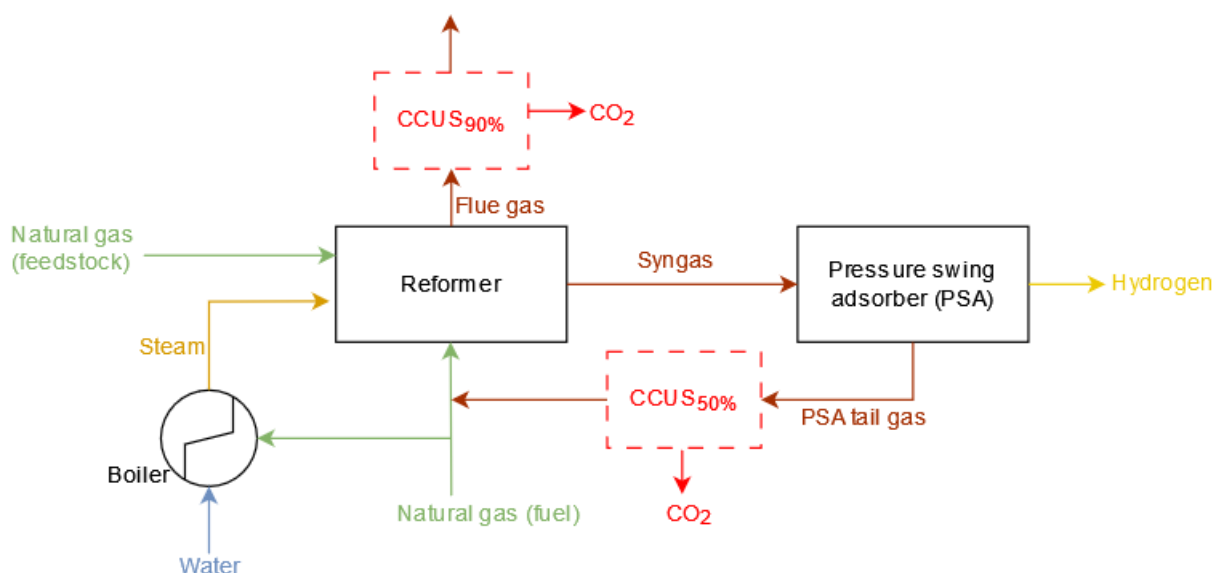
Figure 2.8: Simplified SMR process with possibilities of CO₂ capture.

Table 2.2: Main efficiency parameters for SMR processes [3].

	Units	Conventional (No capture)	PSA tail gas CCUS (50 % CCUS)	PSA + Flue gas CCUS (90 % CCUS)
NG feed	MWh _{CH₄} /MWh _{H₂}	1.133	1.135	1.133
NG fuel	MWh _{CH₄} /MWh _{H₂}	0.187	0.229	0.317
NG total	MWh _{CH₄} /MWh _{H₂}	1.32	1.37	1.45
LHV efficiency	-	76%	73%	69%
CO ₂ emission	kgCO ₂ /MWh _{H₂}	270	130	30
CO ₂ captured	kgCO ₂ /MWh _{H₂}	0	140	240
Capture rate	-	0%	52%	89%

As the hydrogen needs to be separated from CO₂ and N₂ after the reaction, the capture from PSA tail gas is the easiest to implement. In the optimisation, an existing SMR unit can evolve into an SMR+CCUS 50% or into an SMR+CCUS 90%.

Trajectoire optimale de déploiement dans un cluster industriel - Résumé

Nous avons testé notre méthodologie sur un cas d'étude autour du port industriel de Fos-sur-Mer, dans le sud de la France, choisi pour ses conditions favorables au déploiement de l'hydrogène, notamment la forte demande en énergie, l'infrastructure existante pour l'hydrogène, l'adéquation géographique pour le déploiement des énergies renouvelables et la proximité d'un site de stockage géologique potentiel. Fos-sur-Mer est le plus grand port de France et une plaque tournante européenne majeure, traitant historiquement un trafic important de produits dérivés du pétrole, avec trois raffineries de pétrole, des usines de production de méthanol et de chlore, et une aciérie. Un site de stockage géologique d'hydrogène près de Manosque, à une centaine de kilomètres, ajoute à son potentiel.

L'étude vise à évaluer comment l'écosystème de l'hydrogène dans la région peut évoluer pour réduire les émissions de gaz à effet de serre et s'adapter aux changements des demandes d'hydrogène et d'électricité. Elle prévoit une diminution progressive de la demande d'hydrogène des raffineries et souligne l'adoption de technologies d'injection d'hydrogène dans l'industrie sidérurgique. La demande nette d'hydrogène devrait augmenter régulièrement au cours de la période de simulation. En 2020, une partie de la demande d'hydrogène est satisfaite grâce au sous-produit d'une usine de production de chlore voisine, le reste étant fourni par des unités de reformage du méthane à la vapeur sur site. Cela permet d'établir une base de référence pour les émissions de CO₂ liées à la production d'hydrogène.

Le scénario de référence s'étend sur cinquante ans, de 2010 à 2060, divisé en cinq périodes d'investissement et d'exploitation (2010-2020 à 2050-2060). Il intègre les actifs existants et les données historiques pour la période initiale (2010-2020). Quatre technologies de production d'hydrogène sont envisagées : le SMR conventionnel, deux types de SMR avec capture et stockage du carbone (CCUS) et l'électrolyse alcaline. Les options de capture du carbone permettent de capter 50% ou 90% des émissions. Les coûts de distribution de l'hydrogène sont négligés dans ce scénario. L'électricité nécessaire à la production d'hydrogène provient d'énergies renouvelables locales (solaire, éolienne terrestre et offshore) ou du réseau. L'évolution du réseau électrique national suit le scénario N1 75% renouvelable issu du rapport "Futurs Energétiques 2050" de RTE. Les options de stockage comprennent les batteries Li-ion, les réservoirs d'hydrogène comprimé ou les cavités salines souterraines.

La deuxième étape de la méthodologie consiste à optimiser le coût de production pour le sys-

tème électrique français, ce qui permet d'obtenir les prix marché de l'électricité, donnée d'entrée indispensable pour l'optimisation de la planification des capacités de production d'hydrogène. La monotone de prix obtenue pour la période 2010-2020 s'alignent étroitement sur les prix réels de 2019, ce qui valide les hypothèses et la méthodologie choisies. L'analyse est étendue à toutes les périodes, en mettant en évidence les variations de la pénétration des énergies renouvelables et des prix de l'électricité.

Les résultats de l'optimisation de la trajectoire d'investissement pour le scénario de référence montrent un développement progressif de l'électrolyse en parallèle du développement de capacités de production d'électricité renouvelable dédiées, soutenu par l'ajout d'unité de capture du carbone sur les SMR conventionnels existants sur le territoire. En dernière période, le mix de production d'hydrogène est proche des 50% de production par électrolyse, le reste étant produit par les SMR avec capture. Les émissions de CO₂ sont réduites de manière significative au fil du temps grâce à ces investissements, les émissions de CO₂ par kilogramme d'hydrogène produit passant de 4 kgCO₂/kgH₂ à 1,38 kgCO₂/kgH₂. L'investissement et le fonctionnement du stockage de l'hydrogène à l'aide de réservoirs d'hydrogène gazeux comprimé sont également examinés, montrant une augmentation de la capacité de stockage au fil des ans pour répondre aux fluctuations de la demande.

L'évolution du coût de l'hydrogène est analysée en tenant compte des coûts de production et des prix de l'électricité. Le coût moyen de production de l'hydrogène varie de 1,5 €/kgH₂ à 2,6 €/kgH₂ sur différentes périodes, sous l'influence de facteurs tels que la taxe carbone, les prix du gaz naturel et les prix de l'électricité. Les résultats soulignent l'importance de l'électrolyse dans la production d'hydrogène à faible teneur en carbone, les systèmes hybrides combinant l'électrolyse et les technologies SMR existantes s'avérant rentables. L'impact des prix de l'électricité sur le déploiement de l'électrolyse est mis en évidence, avec la nécessité de disposer d'énergies renouvelables dédiées pour alimenter efficacement les électrolyseurs. Toutefois, des incertitudes subsistent en ce qui concerne des facteurs tels que les prix du gaz, les prix de l'électricité et les politiques de régulation du carbone, qui pourraient influencer ces résultats à l'avenir.

Chapter 3

Optimal deployment trajectory of an industrial cluster

3.1 Fos-sur-Mer case study

3.1.1 Context

In order to develop, test and validate our methodology, we choose to work on the industrial port of Fos-sur-mer in the south of France. This region combines many factors favourable to the deployment of hydrogen like a high energy demand, an already existing hydrogen ecosystem, a favourable geography for the deployment of renewables such as solar panels and offshore wind turbines and a nearby geological storage site. In this section we will present the context of this cluster and the main hypotheses. Some of them are not inherent to harbours and can be generalised to other basins, but some hypotheses are specific to this particular zone.

The port of Fos-sur-Mer is the biggest port in France and one of the most important in Europe. It is situated on the Mediterranean coast, close to Marseille in the "Région SUD" province. Historically, one of its main activities has been the traffic of oil derived products (non refined oil: 28% of the traffic in 2019, refined oil: 15% of the traffic in 2019, chemicals: 5% of traffic in 2019 [89]). Three oil refineries are located in this area. The largest two represent a production of 16.7 Mt/yr of refined oil [90, 91] and consume around 102.5 kt/yr of hydrogen [61]. Moreover, there are also two methanol production plants (3.5 kt/yr of H₂ consumption) and two chlorine production plants (11.3 kt/yr of H₂ production [92, 93]). In addition, another potential hydrogen consumer is the steelmaking plant ArcelorMittal that produces around 3.7 Mt/yr of steel with two conventional blast furnaces [94].

An interesting site for geological storage of hydrogen is located at 100 km from Fos-sur-mer, near the city of Manosque. This site already hosts seven salt caverns used for seasonal storage of methane operated by the company Storengy, and two salt caverns are being leached for hydrogen storage purposes. For hydrogen, each cavern have a capacity of around 130 GWh at 170 bars (source: personal communication with Storengy employees). In the future, it could be possible to retrofit methane caverns for hydrogen storage.

In this context, we want to determine how the hydrogen ecosystem could evolve in order to:

1. emit less greenhouse gases;
2. adapt to the evolution of hydrogen demand;
3. adapt to the evolution of the electric system.

3.1.2 Demand evolution in the cluster

The evolution of hydrogen demand is considered as follows:

- Methanol: constant consumption for industrial purposes. In this study, we do not consider the use of methanol in other sectors like maritime transportation.
- Refinery: progressive decrease in consumption until -80% in 2040 due to the conversion of the vehicle fleet into fossil-free vehicles [95, 96]. However, we do not consider refining needs for plastic production.
- Steel industry: hydrogen injection in blast furnaces and direct reduction iron (DRI) furnaces are the two technologies being considered to reduce CO₂ emissions in the steel industry. Injecting hydrogen into a conventional blast furnace helps to reduce the quantity of coke used during the iron ore reduction process [64]. The DRI process uses an electric arc furnace (EAF) to directly reduce iron pellets with the reducing agent (typically natural gas or hydrogen) [97]. For our study, we consider one smart carbon furnace in 2030, one smart carbon furnace and two DRI furnace in 2040 and two DRI furnaces in 2050. The demand for newly produced iron is considered steady state as the part of recycled iron in the production is expected to grow. These assumptions were made following discussions with ArcelorMittal in Fos-sur-mer. Note that it is also possible to inject CH₄ in EAF as iron reducing agent. We keep in mind that it would not make sense to produced hydrogen from CH₄ to inject it in an EAF [98].

Based on these assumptions, hydrogen net demand increase from 360 MWh_{LHV}/h (i.e. 94.6 kt/yr) in 2020 to 460 MWh_{LHV}/h (i.e. 121 kt/yr) in 2030, then 590 MWh_{LHV}/h (i.e. 155 kt/yr) in 2040 and finally 755 MWh_{LHV}/h (i.e. 198 kt/yr) in 2050. In this simulation we maintain a base-load consumption. The estimated industrial hydrogen demand evolution is represented in Figure 3.1.

In 2020, 11.3 kt of the 106 kt/yr hydrogen demand are supplied as a by-product from a nearby chlorine production plant, which is transported by pipeline. The rest of the demand is supplied by on-site conventional SMR units. This represents an SMR capacity of 360 MW operating every hour of the year. This will be the starting point of any computation, referred as the first period of the planning from 2010 to 2020. It gives us a reference for hydrogen production CO₂ emissions of 8.7 kgCO₂/kgH₂.

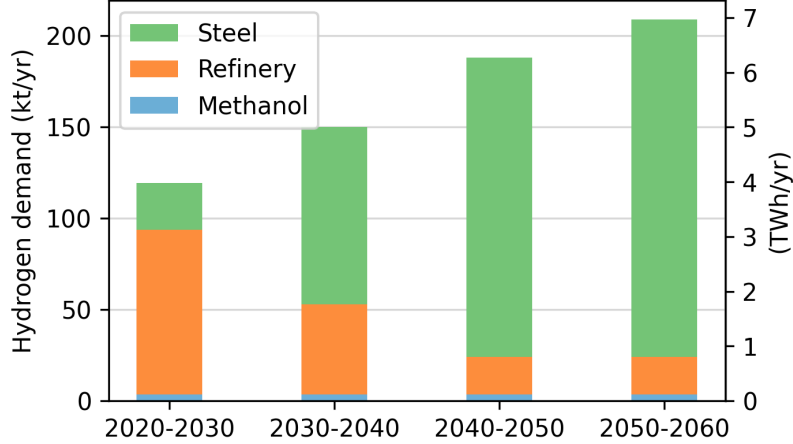


Figure 3.1: Estimated industrial hydrogen demand evolution in Fos-sur-mer cluster between 2020 and 2060.

3.2 Description of the reference scenario

We define a reference scenario that will help us to compare all the variants and identify the parameters with a significant impact. The temporal horizon of this reference study is fifty years, from 2010 to 2060, comprising five periods: 2010-2020, 2020-2030, 2030-2040, 2040-2050 and 2050-2060. The first four periods are investment periods and the last four are operation periods. Note that the first investment period (from 2010 to 2020) is constrained by what we know already happened. It allows us to take into account existing assets and see the evolution with today. Concerning operation, the resolution is one hour (8760 time steps per year).

We consider four different conversion technologies to produce hydrogen: conventional SMR (existing ones or new ones), two types of SMR with carbon capture and storage units (SMR + CCUS), and alkaline electrolysis (AEL). Proton exchange membrane electrolysis was also considered at first but the resolution of the operation is not adequate to compare the two electrolysis technologies. Indeed, the PEMEL technology advantages over AEL are mostly the small footprint, which is not a decision criteria in our modelling, and the better flexibility regarding stop and start cycles [1]. For this last element, the resolution of the operation (one hour) is too coarse to capture any advantage. For carbon capture units, we consider two options: capture from the PSA tail gas stream, which allows the capture of 50% (CCUS 50%) of the total emissions, and capture from the flue gas stream, which allows the capture of 90% of the total emissions (CCUS 90%) [3]. In this reference scenario we consider that hydrogen production means are situated close to the hydrogen consumption site, neglecting hydrogen distribution costs.

We consider that the existing electricity production technologies are used to satisfy the current electricity demand in the area. The additional electricity needed to power the different technologies of the model (electrolysis and carbon capture) comes from two different sources: dedicated local renewables that need to be invested (solar panels, onshore wind turbines or offshore floating wind

turbines) or electricity from the grid (day-ahead market). The national electricity grid evolution is based on the N1 scenario of RTE's "Futurs Energétiques 2050" report, for which renewables penetration reach 75% in 2050 [4]. It is also possible to invest in storage technologies for electricity (Li-ion batteries) and hydrogen (compressed H₂ tanks or underground salt caverns depending on the scenario). Table 3.1 sums up the main technical parameters for these technologies.

Table 3.1: Values of the main technical parameters for the technologies considered.

Technology	LHV efficiency	Lifetime (years)	Ramp up and down (hours)	Variable costs ^a (€/MWh)	CO ₂ emissions ^b (kgCO ₂ /MWh)	Ref.
Alkaline electrolysis	65%	20	<1h	-	-	[1, 99]
Conventional SMR	78%	30	3h30	0.21	-	[81]
SMR + CCUS 50%	75%	30	3h30	7.71	-150	[3]
SMR + CCUS 90%	69%	30	3h30	13.70	-270	[3]
Solar PV	100%	25-30	<1h	-	-	[81]
Onshore wind	100%	25-30	<1h	-	-	[81]
Offshore wind (floating)	100%	20-40	<1h	-	-	[81]
Li-ion battery	92% (in) 92% (out) 92% (hold)	15	-	-	-	[81]
H ₂ tank	98% (in) 100% (out) 100% (hold)	20	-	-	-	[99]
H ₂ salt caverns	98% (in) 100% (out) 100% (hold)	40	-	-	-	[100]

^aincluding catalyst replacement and CO₂ treatment but not including fuel price when the resource exists in the model

^bfor gas based technologies, we consider that all the fossil CH₄ used is turned into CO₂ if not captured (203 kgCO₂/MWhCH₄)

Hydrogen production technologies can be invested without any capacity constraint but local renewables are constrained due to the lack of space. Considering the available space in the area, solar PV and onshore wind development are limited to 300 MW each (calculated based on the space available in the harbour area, in discussion with employees from the "Région SUD"), and floating offshore wind is limited to 1 GW. Maximum capacity invested per investment period is also limited to take into account the pace of deployment: 100 MW/period for solar PV and onshore wind and 500 MW/period for offshore wind. For storage, lithium-ion batteries and compressed hydrogen tanks are considered in the reference scenario.

The reference scenario is built with the economic parameters we found the most realistic in literature. Table 3.2 gives the value of the main parameters. All the other investigated scenarios are built from the reference scenario, changing one parameter at a time to precisely analyse the impact of this parameter.

Table 3.2: Values of the main parameters for the reference scenario.

Parameters		Units	2020	2030	2040	2050	Ref.
			2030	2040	2050	2060	
Part of renewables in grid mix		-	31%	46%	69%	79%	Calc.
Captured CO ₂ treatment price		€/tCO ₂	50	50	50	50	[3]
Biomethane price		€/MWh _{CH₄}	120	110	100	90	[79]
Natural gas average price		€/MWh _{CH₄}	13.5	27	27	27	Calc.
Carbon tax		€/tCO ₂	90	115	140	165	[101]
Electrolysis	CAPEX	€/kW _{H₂}	1,016	641	375	315	[1]
	OPEX	€/kW _{H₂} /yr	15	15	15	15	[4]
Conventional SMR	CAPEX	€/kW _{H₂}	1,300	1,300	1,300	1,300	[81]
	OPEX	€/kW _{H₂} /yr	25	25	25	25	[81]
SMR + CCUS 50%	CAPEX	€/kW _{H₂}	1,850	1,850	1,850	1,850	[3]
	OPEX	€/kW _{H₂} /yr	33	33	33	33	[3]
SMR + CCUS 90%	CAPEX	€/kW _{H₂}	2,350	2,350	2,350	2,350	[3]
	OPEX	€/kW _{H₂} /yr	39	39	39	39	[3]
Solar PV	CAPEX	€/kW _{el}	747	597	517	477	[4]
	OPEX	€/kW _{el} /yr	11	10	9	8	[4]
Onshore wind	CAPEX	€/kW _{el}	1,300	1,200	1,050	900	[4]
	OPEX	€/kW _{el} /yr	40	35	30	25	[4]
Offshore wind (floating)	CAPEX	€/kW _{el}	3,100	2,500	2,200	1,900	[4]
	OPEX	€/kW _{el} /yr	110	80	60	50	[4]
Battery Li-ion	CAPEX	€/kWh _{el}	314	273	203	158	[4]
		€/kW _{el}	220	200	165	165	[4]
	OPEX	€/kW _{el} /yr	11	11	11	11	[4]
Compressed H ₂ tank	CAPEX	€/kWh _{H₂}	5.4	5.4	5.4	5.4	[99]
		€/kW _{H₂}	12.6	12.6	12.6	12.6	[99]
	OPEX	€/kW _{H₂} /yr	2	2	2	2	[99]
H ₂ salt caverns	CAPEX ^a	€/kWh _{H₂}	0.28	0.28	0.28	0.28	[100]
		€/kW _{H₂}	545	545	545	545	[100]
	OPEX	€/kW _{H₂} /yr	2	2	2	2	[100]

^aIncludes H₂ transportation by pipeline from the caverns to consumption site (about 100 km).

3.3 Description of the indicators used

In this section, the indicators used to analyse the results will be described. These indicators will also be used in the next chapters when presenting the different analyses.

3.3.1 Levelised cost of hydrogen

The levelised cost of hydrogen (LCOH) is the average net present cost of hydrogen generation for a production unit over its lifetime. In our case, this cost includes the production and the storage of hydrogen. It represents the total cost of the system per unit of produced hydrogen. It is calculated as follows:

$$\text{LCOH}_c = \frac{\text{sum of costs over lifetime}}{\text{sum of hydrogen energy produced over lifetime}} \quad (3.1)$$

$$= \frac{\sum_{y=y_0}^{l_{y,c}} \left(\sum_z^y \text{CAP}_{z,y,c} + \text{OPE}_{y,c} + \sum_t \text{VAR}_{y,t,c} \right)}{\sum_{y,t}^{l_{y,c}} \frac{\sum_t^{8760} k_{H2,c} P_{y,t,c}}{(1+\tau)^{t_{c,y}}}} \quad (3.2)$$

where $\text{CAP}_{z,y,c}$, $\text{OPE}_{y,c}$, $\text{VAR}_{y,t,c}$ are the CAPEX, OPEX and variables costs annualised over the lifetime as defined in equations (2.2, 2.3, 2.4) for a hydrogen conversion technology c , and $\sum_t^{8760} k_{H2,c} P_{y,t,c}$ the hydrogen produced over the lifetime of the considered technology. Note that this equation is still valid for electricity production means to calculate the levelised costs of electricity (LCOE). For electrolysis, the CAPEX and OPEX relate to electrolysers, and the variable costs include electricity feedstock, electricity network taxes, hydrogen storage, and the carbon tax corresponding to grid electricity carbon content. When electricity is coming from dedicated renewables, the electricity feedstock cost is calculated from the LCOE of the considered renewables and thus, includes the CAPEX and OPEX of the invested technologies. For SMR, CAPEX and OPEX relate to reactors and CCUS units, and the variables costs include gas feedstock (natural gas or biomethane), catalyst replacement, captured CO_2 treatment and the carbon tax corresponding to the emissions of the reactor.

3.3.2 Carbon emissions

The amount of carbon emitted by the system is also a very important decision criteria. In the model, CO_2 emissions are included in the optimisation through the carbon tax. Two indicators can be used to represent CO_2 emissions: the carbon content of hydrogen and the cumulative emissions. The carbon content of hydrogen is defined as the CO_2 emitted per unit of produced hydrogen (3.3), and the cumulative emissions are defined as the total emissions of the system (3.4):

$$\text{Carbon content for } y = \frac{\sum_{t,c} e_{y,t,c}^{\text{CO}_2} \times k_{H2,c} P_{y,t,c}}{\sum_{t,c} k_{H2,c} P_{y,t,c}} \quad c \in \text{H}_2 \text{ production mean} \quad (3.3)$$

$$\text{Cumulative emissions at } y = \sum_z^y \left(\sum_{t,c} e_{z,t,c}^{\text{CO}_2} \times k_{H2,c} P_{z,t,c} \right) \times 10 \quad c \in \text{H}_2 \text{ production mean} \quad (3.4)$$

For the cumulative emissions, the factor 10 corresponds to the duration of the operation period. Note that the carbon content of the electricity used in electrolysis is included in the carbon content of the produced hydrogen.

3.3.3 Installed capacity, produced energy and load factors

Other important indicators are the optimised installed capacity and the optimal operation for each technology of the model. Indeed, the objective of the modelling is to help the planning of the deployment of new technologies. We also want to understand how these technologies can be optimally operated and how resilient the system can be. An interesting indicator is the load factor of a technology, which indicates if the asset is used to its full capacity. The load factor is defined as follows:

$$\text{Load factor at } y = \frac{\sum_t^{8,760} P_{y,t,c}}{\bar{P}_{y,c}^{tot} \times 8,760} \quad \forall c \quad (3.5)$$

3.4 Results for the reference scenario

3.4.1 Production cost model (France scale)

The second step of the methodology involves running the production cost model for the electric system at the scale of France with the chosen hypotheses in order to obtain the input data to run the model for our local area. The data we need are grid electricity prices and the corresponding carbon content. As mentioned before, we based our simulation on the N1 75% renewable scenario from the RTE report [4]. Table 3.3 gives the capacities used to run the operation model.

Table 3.3: France installed capacities for the electric system according to the RTE's N1 scenario (GW) [4].

Period	Coal	Gas	Solar PV	Onshore wind	Offshore wind	Hydro	Historical nuclear	New nuclear	Flex ^a
2020-2030	3.5	9.5	22	25	2.6	26	61	0	0.9
2030-2040	0.5	6	57	40	13	27	51	3	4
2040-2050	0	0.5	99	53	33	29	29	10	12
2050-2060	0	0.5	118	58	45	30	15.5	13	26

^aIncludes hydrogen storage in salt caverns, electrolysers and Li-ion batteries. These values were obtained through optimisation while the others capacities were fixed

Figure 3.2 shows the grid electricity price duration curve for the 2020-2030 period, drawn with the result of the production cost model at the national level. In this representation, electricity prices are ordered by the number of time steps the day-ahead market price have reached them. In today electricity market, production units are sorted by variable production cost. Then, production units are called in this order until [102] the demand is satisfied, and the last production plant needed to meet the demand is called "marginal production plant". With this system, the electricity price often corresponds to the variable cost of the marginal production plant. In the graph, we can see flat parts corresponding to the variable cost of the marginal production plant on the market.

For the 2020-2030 period, we can see that we are close to 2019 real prices, which is our reference year for meteorological data. This result allows us to validate the chosen hypotheses and the methodology. The differences can be explained by the simplified modelling, especially on two points. First, for a technology, all parameters are considered the same for all plants (efficiency, variable costs) when in reality variations exists between the different plants. Second, interconnection with neighbouring countries are modelled with a fixed price and a fixed carbon content. However, our methodology gives a good approximation of the evolution of electricity prices which is necessary for modelling the deployment of electrolysis.

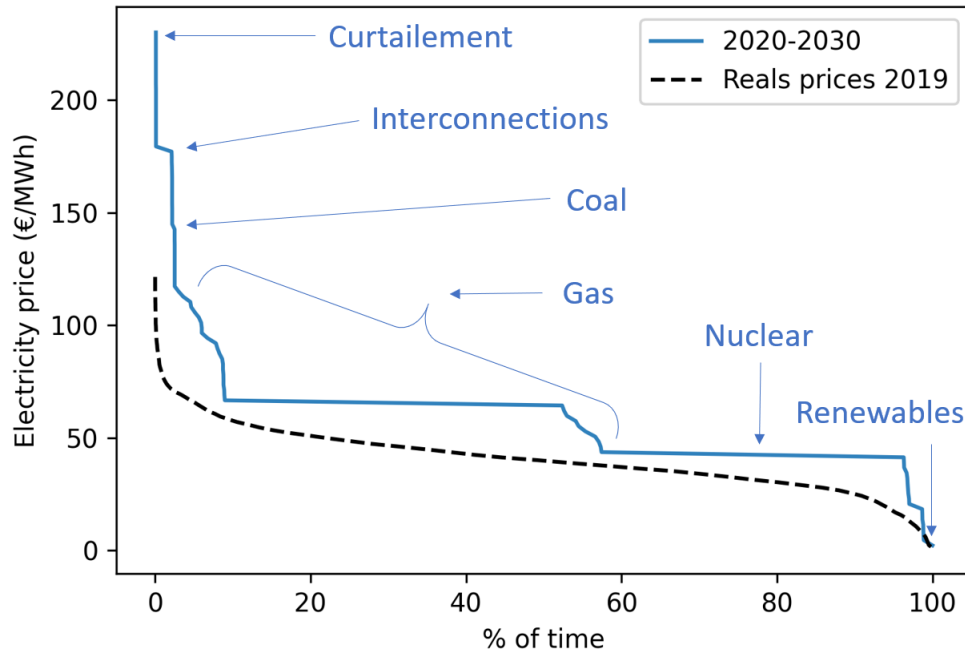


Figure 3.2: Grid electricity price duration curve from simulation for period 2020-2030. The black dotted line represent the observed curve for 2019 (which was taken as a reference for the meteorological data). The annotations show the cost of the marginal production plant.

Figure 3.3 shows the price duration curves for all periods. Between 2020-2030 (in blue) and the three other periods, we can see an important gap of around 100 €/MWh for the highest flat section, corresponding to interconnections. This can be explained by the fixed-price modelling of interconnections as mentioned before. However, we are not interested by this section of the graph because when interconnections are marginal, electricity is too expensive to be used for electrolysis. For these time steps (around half of the time), the grid is already overloaded.

We are much more interested by the the rightmost flat section, corresponding to renewables, where prices are close to zero. We can see that this section is shifting to the left especially for the last two periods. This means that renewables penetration in the market is higher (about 25% of the time for these two years). This results were expected, since we fixed the evolution of electricity production capacities according to RTE 75% renewable scenario (N1) [4].

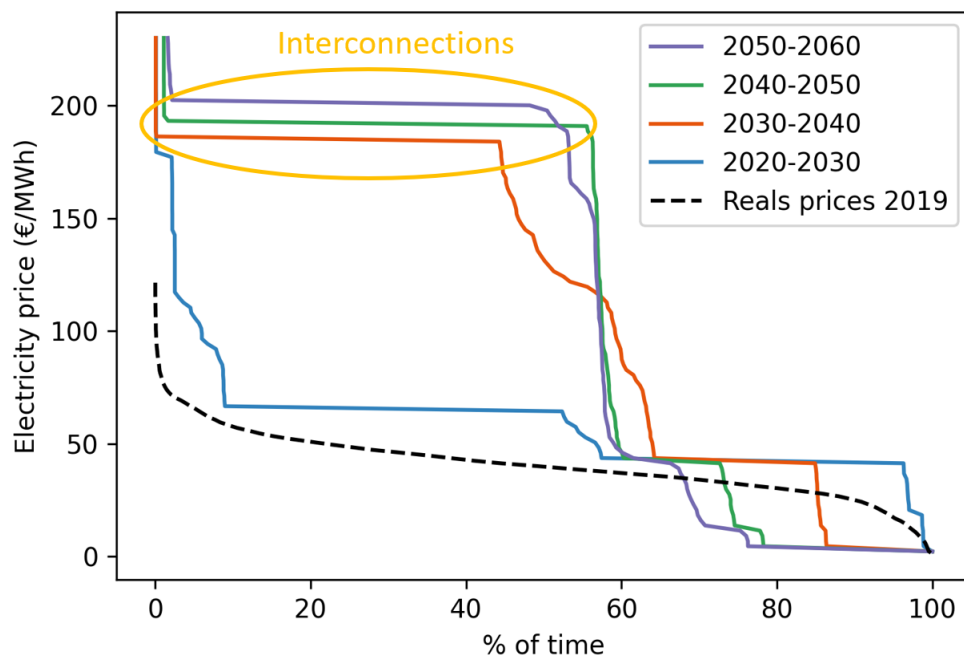


Figure 3.3: Grid electricity price duration curves from simulation for all periods. The black dotted line represent the observed curve for 2019 (which was taken as a reference for the meteorological data).

3.4.2 Capacity expansion model (local scale)

Invested capacities

For the reference scenario, the optimal investments in the different technologies are presented in Figure 3.4. The upper graph shows the investments in hydrogen production technologies, while the lower graph shows the investments in dedicated local renewable electricity production technologies. In the second investment period (2030-2040), the 411 MW_{H_2} from the first period are equipped with CCUS 50% and an additional 114 MW_{H_2} of SMR + CCUS 50% is invested in. In the third period, some new SMR units are invested in for a total of 646 MW_{H_2} ; and for the last period, the existing SMR from the first period come the the end of their life. 365 MW_{H_2} of the initial 411 MW_{H_2} are replaced bringing the total to 600 MW_{H_2} . From the third period only, investments are made in electrolysis and local renewables, reaching 1,343 MW for electrolysis and 318 MW_{H_2} for local renewables (150 MW_{el} , the maximum potential is reached for onshore wind, and 109 MW_{el} for solar).

Operation of the system and CO_2 emissions

Figure 3.5 presents the optimal operation of the system. The bars represent the hydrogen production for each technology and the percentage the share of the demand that is supplied by the considered asset. During the second operation period (2030-2040), all oh the hydrogen is produced with SMR with carbon capture which brings down CO_2 emissions from 4 $\text{kgCO}_2/\text{kgH}_2$ to 4.9

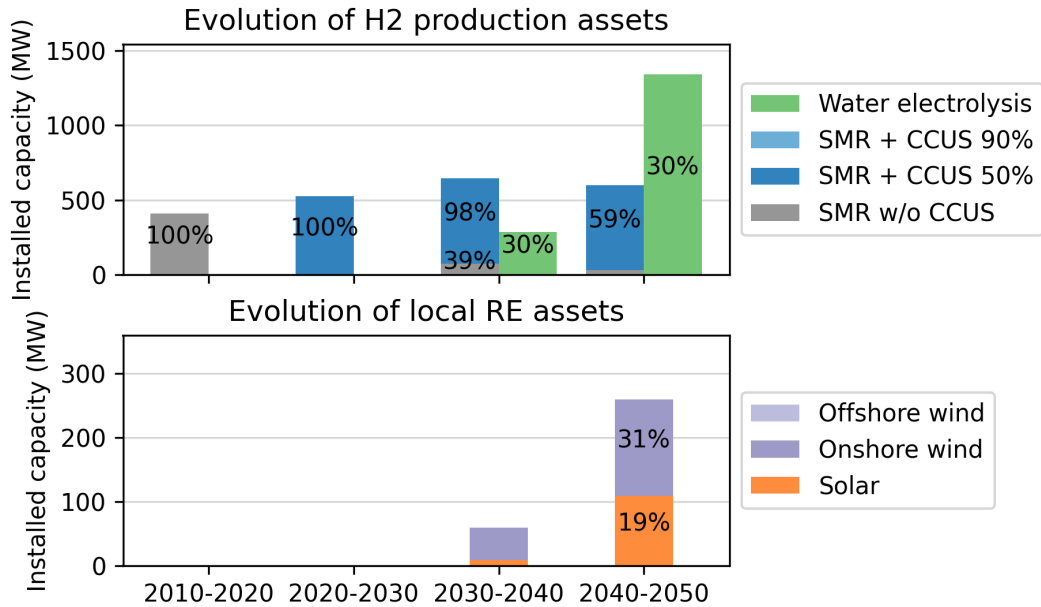


Figure 3.4: Investment trajectory in the hydrogen and electricity production assets for between 2010 and 2050. The percentage on the bars represent the load factor for each technology for the following operation period (if the capacity is over 10 MW).

kgCO₂/kgH₂. In the third and fourth operation periods, electrolysis (green bars) and SMR (grey and blue bars) share the production. During the third period (2040-2050), only 12% is produced by electrolysis and in the last period it grows to more than 50%. The hatched blue bars represent the share of hydrogen that is produced by biomethane reforming (5.2% in the last period) while the lighter green bars represent the proportion of hydrogen that is produced by electrolysis from dedicated local renewable electricity (5.7% in the last period). Note that this reference scenario uses 454 GWh of biomethane in the last period (1.65% of the potential of the "Région SUD" province where Fos-sur-mer is located according to [79]). With the optimised operation profile calculated, the load factor of electrolysis is 30%.

In the last period, CO₂ emissions decrease to 1.38 kgCO₂/kgH₂. For a comparison, the threshold for low carbon hydrogen is set to 3.38 kgCO₂/kgH₂ according to the European taxonomy [23]. The small amount of biomethane used in reforming units helps decreasing carbon emissions. Indeed, apart from fugitive emissions, biomethane emissions are considered as zero. According to [16], hydrogen carbon footprint ranges from 3 to 9 kgCO₂/kgH₂ for SMR with CCS and from 0.5 to 2.5 kgCO₂/kgH₂ for electrolysis depending on the electricity mix. Our results fall into these boundaries. If we were to compare the total emission from 2020 to 2060 in this reference scenario to a "business as usual" case (meaning that all the supply comes from conventional SMR, and the carbon tax not increasing), the avoided emission would be 30 MtCO₂ (653 kt/year for period 2030-2040, 888 kt/year for period 2040-2050 and 1449 kt/year for period 2050-2060). If we compare the avoided emissions to the cost difference between the reference case and the b.a.u case, it represents a cost

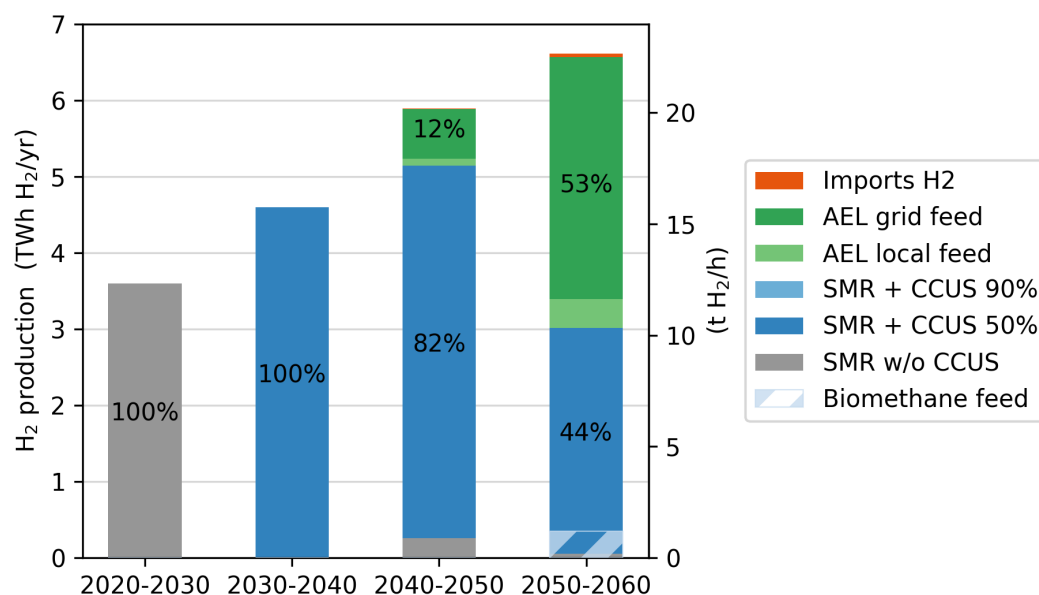


Figure 3.5: Hydrogen production by technology. The percentages on the bars represent the share of the demand that is supplied by the considered technology (if over 10%).

of avoided CO_2 of 73.3 €/tCO_2 . Figure 3.6 shows the evolution of the carbon content of hydrogen (left axis) and the evolution of the cumulative emissions over the horizon (right axis).

Investment and operation of the storage

In this reference scenario, we let the possibility to invest in Li-ion batteries or gaseous compressed hydrogen tanks. In the results, only hydrogen tanks are used. In our case, with a base-load hydrogen demand, batteries are not competitive to store electricity in order to produce hydrogen, as it is much cheaper to store directly store the hydrogen even if it means oversizing the electrolyzers. This is the case as we keep controllable hydrogen production capacity with SMR and as electricity from the grid can be used at any time. In Figure 3.7, we can see the evolution of the inventory for the hydrogen storage over an operation year for the different periods. As the demand is supplied by SMR during the two first operation periods, there is no need for a storage before 2040-2050 period (other than a buffer storage that is included in the cost of the plant). The invested capacity in the third operation period (2040-2050) is 2.6 GWh while the invested power (equal to the maximum flow in/out of the storage) for the same period is 185 MW. For the last period, the invested capacity goes to 32.6 GWh when the invested power rises to 1.1 GW meaning that completely fill the storage would take around 30h. For comparison, the biggest liquid hydrogen storage to date is owned by the NASA at the Kennedy Space Center in Florida and has a capacity of 9 GWh and is 20 m tall [103], and a larger tank of around 13 GWh is under study, which would bring the total capacity to 22 GWh. Compared to this, a capacity of 30 GWh seems quite large. A geological site favourable

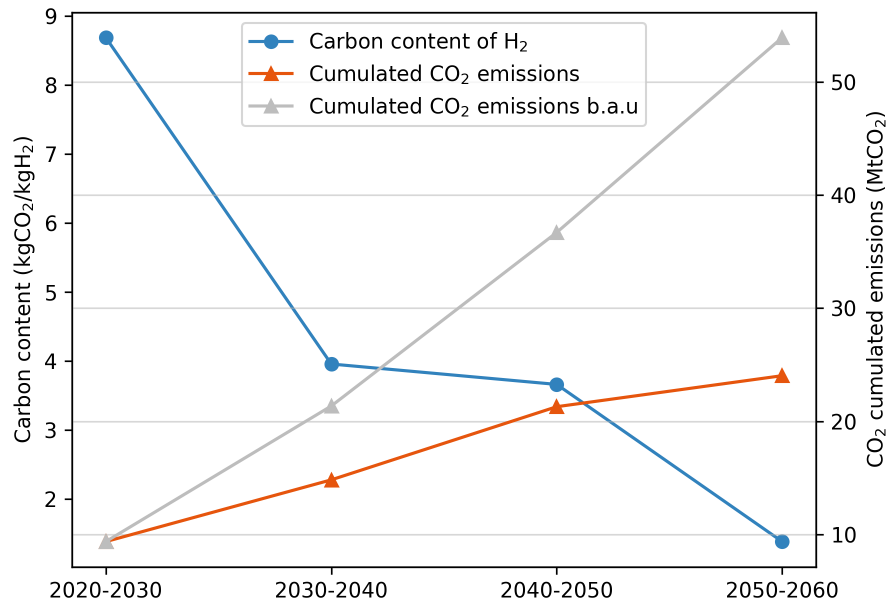


Figure 3.6: Carbon content of hydrogen evolution (left axis and blue line) and cumulative CO₂ emissions (right axis) from 2020 to 2060. In grey, cumulative emissions for a "business as usual" scenario allowing only conventional SMR.

to the development of large hydrogen salt cavern is close to the studied area. This possibility will be presented latter in this work.

In Figure 3.7 we see that hydrogen storage essentially help to mitigate the variability of renewables and electricity grid prices. Thus, it is operated with a high frequency. Note that on this figure, data has been smoothed with a 20 h rolling-average window for better readability. With the raw version, we can see intra-day variability even better (Figure 3.8).

Hydrogen cost

Figure 6.4 details the evolution of the cost structure of each hydrogen production technology. This graph presents the cost of both production and storage, and does not include transportation and distribution of hydrogen. For the reference scenario, the average hydrogen production cost (dotted grey lines) goes from 1.5 €/kgH₂ to 2.3 €/kgH₂ during the first and the second periods, mainly because increases in the carbon tax and natural gas prices. Then, the average production cost increases to 2.4 €/kgH₂ in 2040-2050 and to 2.6 €/kgH₂ in the last period, while the carbon tax continues to increase. The cumulative average price over the horizon is 2.29 €/kgH₂. For SMR, the hydrogen price strongly depends on natural gas, biomethane prices and carbon tax. For electrolysis, the price depends on electricity prices.

Table 3.4 sums up the electricity average price from the grid and local dedicated renewables (third and fourth period only). The average grid price almost doubles from the first operation

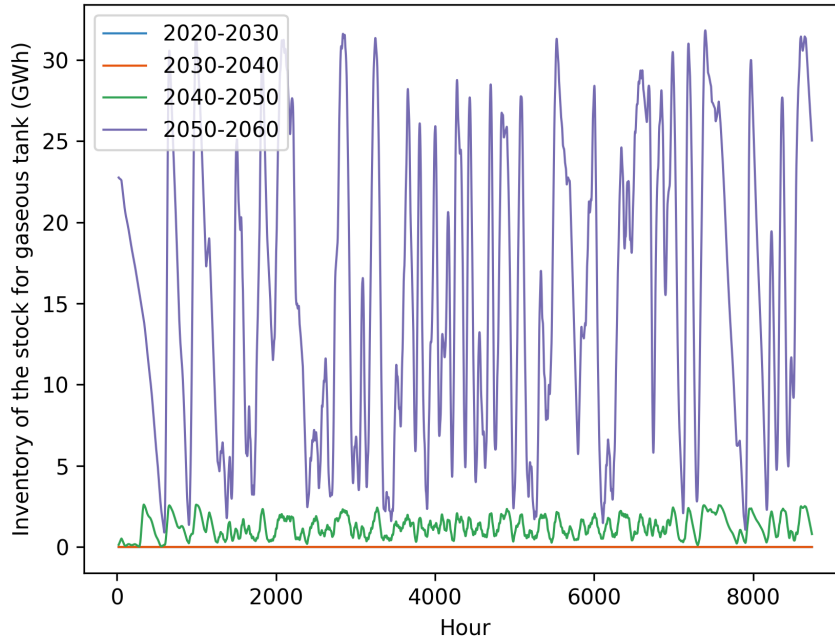


Figure 3.7: Stock inventory for gaseous storage in tank (data has been smoothed with a 20 h rolling-average window).

period to the second, due to the increase of gas price. Indeed, the electricity price is often following the gas price as gas turbines are peak production means. For the last two periods, electricity costs in average around 143 €/MWh, which is really expensive to feed electrolysers. According to the IEA, hydrogen produced from electrolysis with a load factor over 2.000 hours feeded with electricity at 87 €/MWh costs around 4.5 €/kgH₂ (CAPEX equal to 390 €/MWh_{el}) [10]. However, in our scenario, the cost of hydrogen produced by electrolysis remains around 2 €/kgH₂. First, as we mentioned above, 10% of the electricity is coming from dedicated renewables with an average price of 45.4 €/MWh in the third period and 38.2 €/MWh in the fourth period. Then, if we look at the number of hours for which the grid electricity price is below these values, we attain 40% in the second period and 33% in the last period. As we previously analysed, with a high share of renewables in the mix, electricity is more expensive on average but there are also more time steps with low electricity prices.

It is also worth to mention that network taxes play a big part in the final hydrogen cost. Indeed, they represents more than 80% of the grid electricity costs (from the electrolyser point of view) and around 60% of the total electricity costs including electricity coming from local renewables.

Once again, these results are comparable to the ones found in literature. In 2019, Parkinson *et al.* [16] found that SMR production price ranges from 0.9 to 2 €/kgH₂ without considering carbon tax, and electrolysis production cost ranges from 4.1 to 13.4 €/kgH₂. These results are supported by a recent study of [8]. In their projection, the IEA found ranges of 1 to 5 €/kgH₂ for renewable electrolysis production and of 2 to 6 €/kgH₂ for nuclear electrolysis production in 2050. In Figure

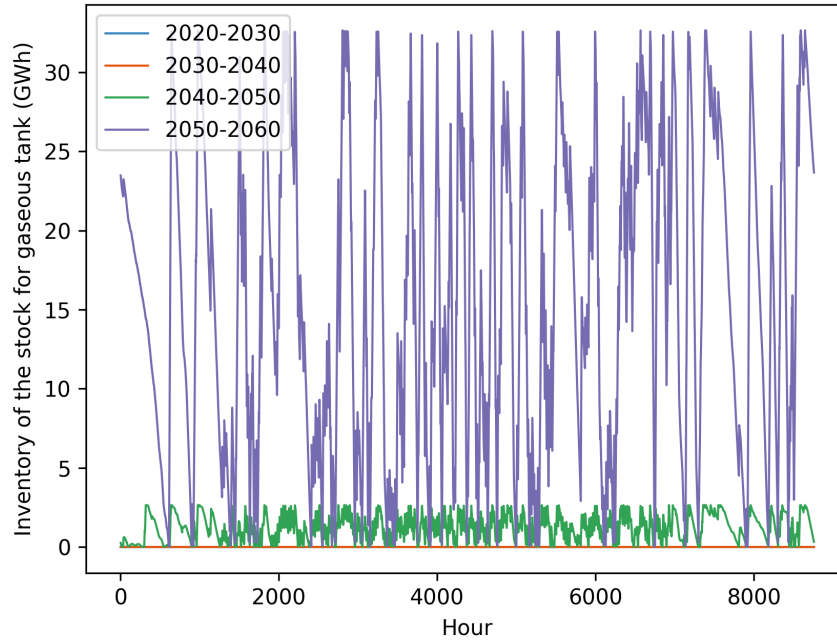


Figure 3.8: Stock inventory for gaseous storage in tank.

Year	2020-2030	2030-2040	2040-2050	2050-2060
Average price grid (€/MWh)	58.5	114.6	144.3	142.3
Local renewable average price (€/MWh)	-	-	45.4	38.2
Number of hour grid < local RE (h)	-	-	3,525	2,902
Average price of used grid electricity ^a	-	-	16.3	15.8

^aIncluding network taxes

Table 3.4: Electricity prices for the reference scenario.

6.4, we see that in our reference scenario, the cost of hydrogen produced by electrolysis remains around 2 €/kgH₂ from the third period (2030-2040) thanks to the hybridisation with existing SMR capacities. The latter play the role of peak production mean to compensate the variability of renewables. We can see it well in Figure 3.10, which represents the weekly hydrogen production by technology during the last period. This point will be developed later in this work.

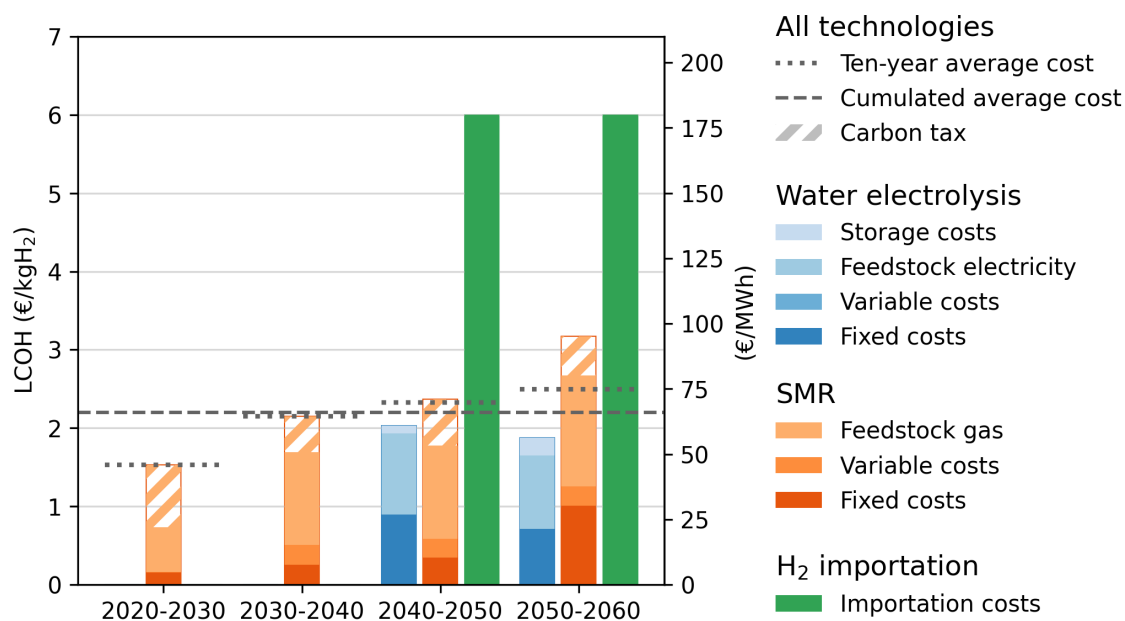


Figure 3.9: Levelised cost of hydrogen production and storage (LCOH) for alkaline electrolysis and steam methane reforming technologies, and for importations between 2020 and 2060.

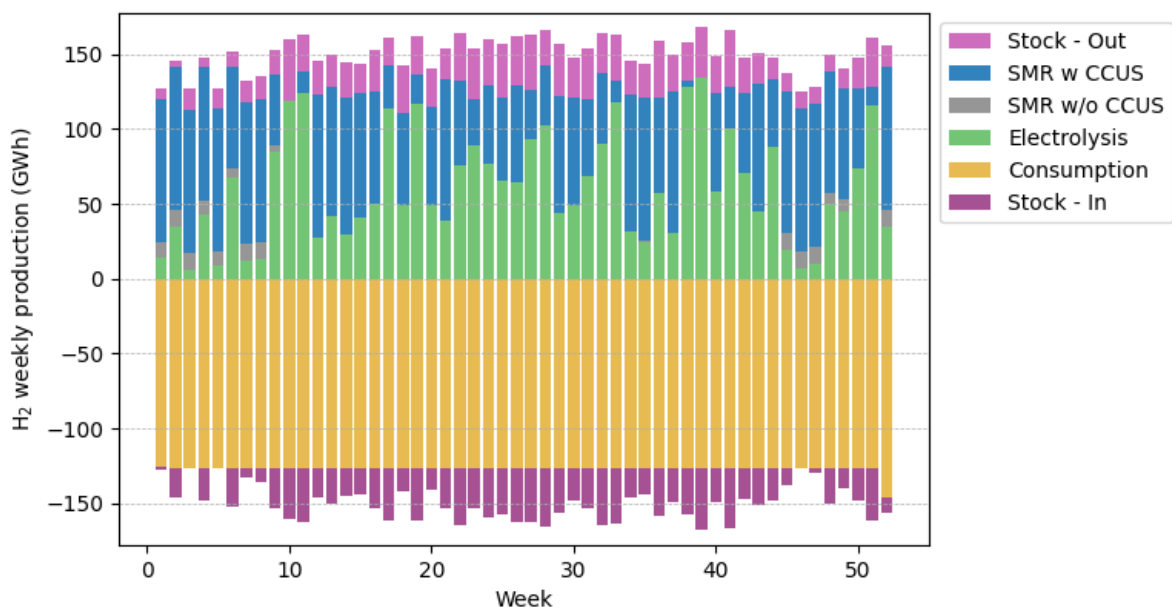


Figure 3.10: Weekly hydrogen production by technology for the 2050-2060 operation period.

3.5 Conclusion

The results for the reference scenario show that under the considered techno-economic context, electrolysis is expected to play a major role in low-carbon hydrogen production, but existing SMR will be useful in the transition to decrease the overall production costs for two reasons. First, CCUS could be a key option to decarbonise hydrogen production on the short term, with SMR bringing flexibility to the system, playing the role of peak production mean. The electrolysis load factor is at the lower competitiveness limit compared to values found in the literature (30% compared to 30%-70% in [10]). We can conclude that hybrid systems with both electrolysis and SMR are less expensive than systems with either technology alone.

We established the decisive impact of electricity prices on electrolysis deployment. By linking the evolution of grid electricity prices at national scale with electrolysis operation at local scale, we found that running electrolyzers with grid electricity is not competitive for most of the time step of the year. In the last period, capacities invested in local renewables reach the upper bound of the limited renewable potential, except for floating offshore wind. The optimal deployment trajectory involves building dedicated renewables to power electrolyzers, although in constrained territories, space might be a limiting factor. This shows that depending on the territory, space for renewable electricity production might be the limiting factor to electrolysis development.

We need to keep in mind that we were able to obtain these results by making numerous assumptions. Nevertheless, there are strong uncertainties about how will evolve several crucial factors, such as gas prices, electricity prices, CAPEX for different production and storage units or carbon regulation policy. Quantifying those uncertainties is not an easy task. In the following chapters, we will look more in details into these three issues.

Analyses de sensibilités et robustesse du système - Résumé

Ce chapitre se concentre sur l'identification des paramètres significatifs ayant un impact sur le déploiement de l'hydrogène en reprenant l'étude de cas industriel présentée précédemment, et sur l'analyse des facteurs clés impliqués. Ces paramètres comprennent le coût moyen pondéré du capital, le prix du gaz naturel, le prix du traitement du CO₂ capturé, le prix du biométhane, le taux d'apprentissage pour les dépenses en capital liées à l'électrolyse, la présence d'un vaste stockage souterrain, le potentiel renouvelable et les coûts d'importation de l'hydrogène.

L'étude prend la forme d'analyses de sensibilité successives pour comprendre comment la variation de ces paramètres affecte les coûts et les conditions favorisant les infrastructures d'hydrogène vertes ou bleues. Ce chapitre souligne que les visions incertaines de l'avenir peuvent influencer les résultats réels et met l'accent sur la nécessité d'évaluer la robustesse des différents scénarios.

Une procédure d'analyse de la robustesse en deux étapes est également proposée. Tout d'abord, l'optimisation est effectuée sur la base de scénarios anticipés afin d'obtenir un déploiement technologique optimale. Ensuite, l'optimisation est réexécutée à capacités fixées mais avec des hypothèses de scénarios alternatifs pour comprendre comment le système peut fonctionner de manière optimale dans différentes conditions futures. Diverses paires de scénarios sont analysées pour évaluer les réponses et la robustesse du système.

Les résultats montrent que le coût moyen pondéré du capital influe sur les décisions d'investissement, favorisant les technologies dont les coûts d'exploitation sont plus faibles, comme l'électrolyse et le captage du carbone, avec des systèmes de garantie des revenus qui contribuent à la sécurité des investissements, à l'instar des énergies renouvelables. Les unités existantes de reformage du méthane à la vapeur (SMR) jouent un rôle crucial dans la transition, en restant compétitives malgré les prix élevés du gaz naturel, du biométhane et du traitement du CO₂. La compétitivité des SMR peut être renforcée par le captage du carbone et l'intégration du biométhane, ce qui pourrait conduire à des émissions de CO₂ négatives.

L'analyse souligne également qu'en plus des prix de l'électricité qui limitent la compétitivité de l'électrolyse, les dépenses d'investissement de l'électrolyseur sont un facteur important, ce qui pose des problèmes pour la viabilité de l'électrolyse. Le déploiement optimal implique l'utilisation d'énergies renouvelables dédiées à l'électrolyse, en tenant compte des limites posées par le potentiel local d'énergies renouvelables, ce qui nécessite une certaine flexibilité du système. Cette flexibilité peut provenir de moyens de production d'hydrogène contrôlables comme le SMR, d'un stockage

souterrain important comme des cavités salines, ou d'importations rentables d'hydrogène à faible teneur en carbone, en fonction du contexte et de la compétitivité des prix.

Dans un second temps, la robustesse des différents scénarios est analysée. L'étude montre que la présence d'un important stockage d'hydrogène rend le système plus rentable et plus résilient grâce à une plus grande flexibilité. Les scénarios impliquant un gaz naturel cher ou une interdiction des SMR à partir de 2040 sont les plus coûteux, ce qui souligne la nécessité d'anticiper ces scénarios. Le scénario d'importation d'hydrogène, bien que potentiellement rentable, comporte des risques si la prévision des prix d'importation échouent. Une comparaison matricielle des différences de coût entre les scénarios est mise en place pour indiquer leur robustesse ou leur caractère risqué. Les scénarios avec un gaz naturel cher ou une interdiction des SMR sont robustes (impacts moins coûteux), tandis que le scénario d'importation d'hydrogène est plus risqué (impacts plus coûteux). Les approches prudentes en matière de CAPEX pour les énergies renouvelables et l'électrolyse n'ont généralement pas d'impact significatif sur les coûts de l'hydrogène, sauf dans des cas comme l'interdiction du SMR à partir de 2040. Dans l'ensemble, l'étude recommande d'envisager des scénarios pessimistes pour assurer la robustesse du système, en soulignant les risques associés à des hypothèses optimistes telles que l'importation d'hydrogène bon marché.

Chapter 4

Sensitivity analyses and robustness of the system

In this chapter, we seek to point out different parameters that have a significant impact on hydrogen deployment for the previously presented industrial harbour case study and discuss the key factors involved. First, we were interested in the weighted average capital cost (equal to the discount rate), which has an impact on every cost in the model. Then we analyse the impact of parameters on SMR operation: the natural gas price, the captured CO₂ treatment price and the biomethane price. Finally, we analyse three parameters that impact more the electrolysis deployment: the learning rate (LR) for the electrolysis CAPEX, the presence of large underground storage close to the hydrogen production site, and the renewable potential of the local area. We also examine the impact of cheaper hydrogen prices for importation from outside of the region of interest.

Some of these key parameters are relative to long-term macroeconomic evolution and are unknown today. This is the case, for example, of the natural gas price. Others can be affected by state support or a more global industrial strategy. They cannot be predicted easily or treated endogenously in our model. This is the reason why we propose a sensitivity analysis to show how they change the results, such as the cost, but also to determine the conditions that are favourable to the deployment of green or blue hydrogen infrastructures.

Describing the behaviour of our model when varying a few key parameters obviously emphasises that the vision we have of the uncertain future can shape the future itself. Therefore, it is important to evaluate in return whether a particular vision of the future, with the associated decisions on the hydrogen supply chain, is robust to uncertainties. This is why we propose a robustness analysis in the second part of this chapter. To do so, we propose a two-step procedure that allows one to evaluate the robustness of a scenario built on a future "A", fully described by the set of techno-economic assumptions used as input, with respect to another future "B". We first run the whole optimisation with the anticipated scenario "A" and obtain the optimal trajectory of capacities for the different technologies. In the second step, we run the optimisation a second time with fixed capacities corresponding to the results of the first optimisation and with assumptions from the future "B". That way, we are able to see how our system "A" with non-optimal capacities can be operated to answer the demand to the best of its ability within the condition future "B". We

propose several analyses with different pairs of futures "A" and "B".

4.1 Sensitivity analyses

4.1.1 Weighted average cost of capital (WACC)

Table 4.1: Synthesis of the scenarios for the WACC analysis.

Scenario name	WACC (%)
Reference	4%
WACC= x %	$x \in [2\%, 11\%]$

The weighted average cost of capital (WACC) model the relation between the value of 1€ in the year n and 1€ a year later. It is a key parameter in analysis of plury-annual investment whose value can be justified differently depending on the context. It can integrate different elements, such as the risk of investments in new assets or the expected rate of return on investment. When it is high, short-term returns are preferred, and this often leads to a solution with low capital cost and higher operational cost. A value of 4% is common for a decision on a public project with low risk, while 8% or more would reflect a private project with medium risk.

In this analysis, we take ten different values for the WAAC, from 2% to 11%. Figure 4.1 represents the contribution of each asset to the hydrogen demand in the planning horizon. We can see that for a high WACC, investments in new capacities are kept to a minimum. Above 8%, CCUS units are not used, and more than 80% of the total demand is supplied by conventional SMR. With a high WACC, it is more advantageous to pay the carbon tax and importation costs annually than to invest in more expensive low-carbon technologies (electrolysis or CCUS). On the contrary, with a low WACC, investments in expensive technologies are more interesting. For WACC lower than 4%, electrolysis and the dedicated renewables associated with it are well developed, reaching a share of 60% of the demand for the 2% scenario. Between 4% and 6%, the preferred technology is SMR + CCUS 50% for which the cost is well balanced between the CAPEX and the marginal costs.

If we look at the average LCOH, blue line in Figure 4.2, we see that it increases linearly with the WACC, between 2.1 €/kgH₂ in the most favourable case (WACC = 2%) and 3€/kgH₂. The average carbon content (orange line) also increases with WACC, but is not linear. A maximum of 7 kgCO₂/kgH₂ is reached for the 9% case. For the scenarios 10% and 11%, this content decreases slightly due to low-carbon hydrogen imports reaching 0.2 TWh (green line). Biomethane imports (purple line) reach a maximum for WACC = 6%, but stay below 0.15 TWh in total for the planning horizon. We note a turning point around WACC = 8% after which the mix does not change significantly.

We note that CO₂ emissions are more sensible to the WACC variation than the LCOH. Emissions are almost doubling while the LCOH is growing less than 50%. This indicates that a low capital cost is necessary to help reducing carbon emissions. this can be an argument to encourage public policies to subsidise electrolysis and renewable energy development.

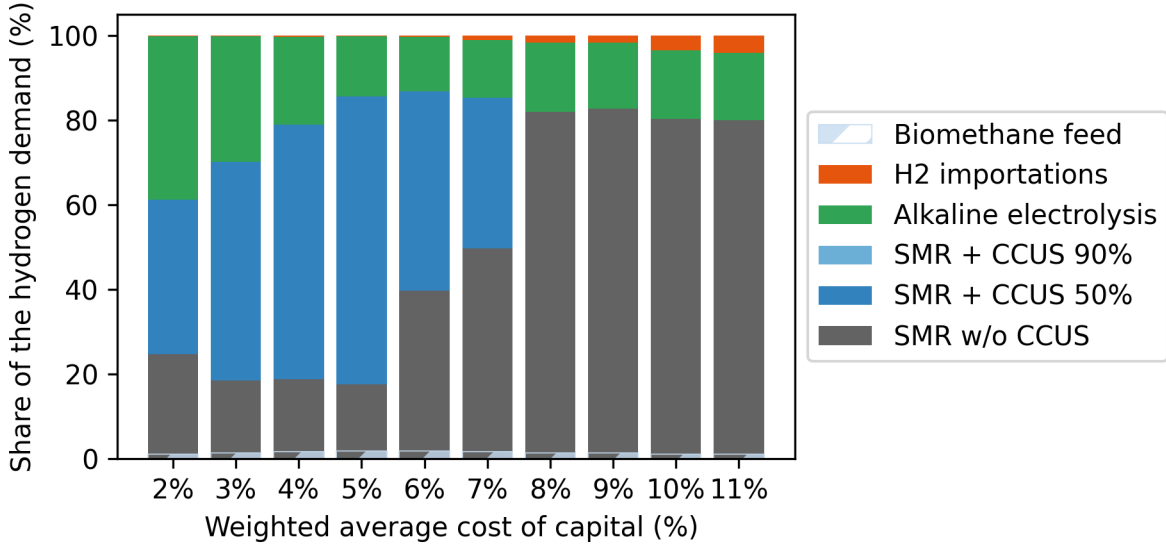


Figure 4.1: Contribution of the assets to the hydrogen supply for the horizon period for different values of the WACC.

4.1.2 Electrolysis CAPEX learning rate

Today’s cost of an electrolyser is relatively high (i.e. larger than 1500 €/kW), whether it is alkaline or PEM technology. PEM has a lower TRL than alkaline. If alkaline can be considered as an old technology, it has never reached the scale of development that is foreseen for the next few years. It is important to model the associated cost reduction and to analyse the consequence on the results. A low enough CAPEX can favour the development of an electrolyser fed with a low capacity factor dedicated to renewable production.

As explained in Chapter 3, the learning rate indicates the cost reduction that comes with the production experience for relatively new technologies. Here, we focus on alkaline electrolysis, a key technology when we discuss low-carbon hydrogen deployment. In the case of alkaline electrolysis, we cannot really say that the technology is new, but scaling up production can lead to cost reductions [85]. In this sensitivity analysis, the learning rate of electrolysis varies from 10% to 28%, which leads to electrolysis CAPEX varying from 604 to 860 €/kW_{LHV} (930 to 1320 €/kW_{el}) in 2030 and from 146 to 545 €/kW_{LHV} (225 to 840 kW_{el}) in 2050.

Table 4.2: Synthesis of the scenarios for the learning rate sensitivity analysis.

Scenario name	Learning rate (%)	Electrolysis CAPEX (€/kW _{LHV})
Reference	18%	2030: 641, 2040: 375, 2050: 315
LR= x %	$x \in [10\%, 28\%]$	2030: $\in [474, 795]$, 2050: $\in [146, 545]$

The upper graph in Figure 4.3 shows the average LCOH (blue line) and the average carbon content of hydrogen (orange line) for different values of LR for the planning horizon. The LCOH

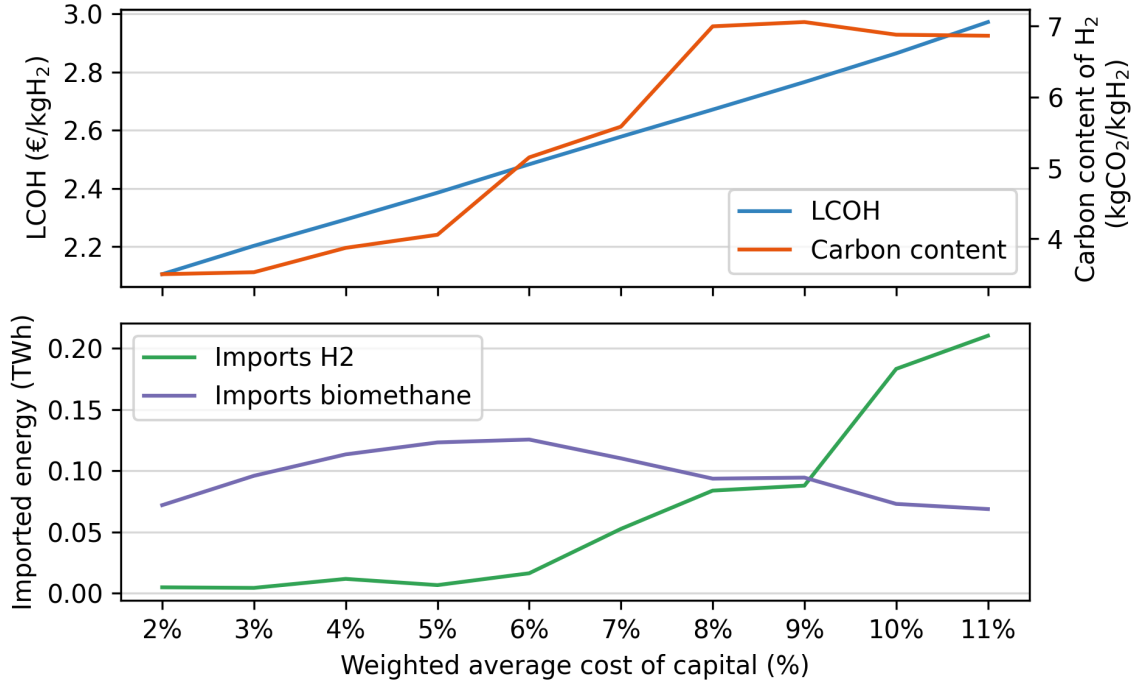


Figure 4.2: Average LCOH and average carbon content of hydrogen, hydrogen imported quantities and biomethane imported quantities for different values of the WACC.

decreases almost linearly (coefficient of determination $R^2 = 0.9983$) from 2.33 to 2.21 €/kgH₂ when the learning rate increases. However, the carbon content decreases from LR = 10% to a minimum of 3.6 kgCO₂/kgH₂ at LR = 22% and then increases slightly again. The lowest emission scenario (LR = 22%) is obtained for an electrolysis cost of 570 €/kW_{LHV} (877 kW_{el}) in 2030, 291 €/kW_{LHV} (448 kW_{el}) in 2040 and 234 €/kW_{LHV} (360 kW_{el}) in 2050 (see the middle graph of Figure 4.3 representing electrolyser CAPEX). It corresponds to an installed electrolysis capacity of 1169 MW in 2040 and 1619 MW in 2050 (lower graph of Figure 4.3). We note that even in the most favourable case (LR = 28%), electrolyzers begin to be installed for the third operating period (2040-2050). In the most favourable case (LR = 10%), they are installed only for the last period.

Figure 4.4 shows the contribution of the different assets to the hydrogen supply of LR that goes from 10% to 28%. The share of electrolysis is logically increasing from around 10% in the case LR = 10% to around 30% in the scenario LR = 28%. The share of conventional SMR is also increasing with LR because it is less interesting to invest in carbon capture if electrolysis is cheaper. Indeed, when the LR is high, the SMR are less used and then it becomes less interesting to invest in carbon capture units. That is why, even if it is close, the lowest emission scenario (LR = 22%) is not the one with the highest electrolysis capacity (LR = 28%). The share of carbon capture, on the other hand, is decreasing with LR. In the case of LR = 10%, it reaches 70% of the production, while it only reaches 40% when LR = 28%. For LR = 10%, 100% of the demand is supplied by SMR with 50% carbon capture for the second and third operating periods (from 2030 to 2050). More generally, we can still conclude that CO₂ emissions are decreasing when the learning rate is

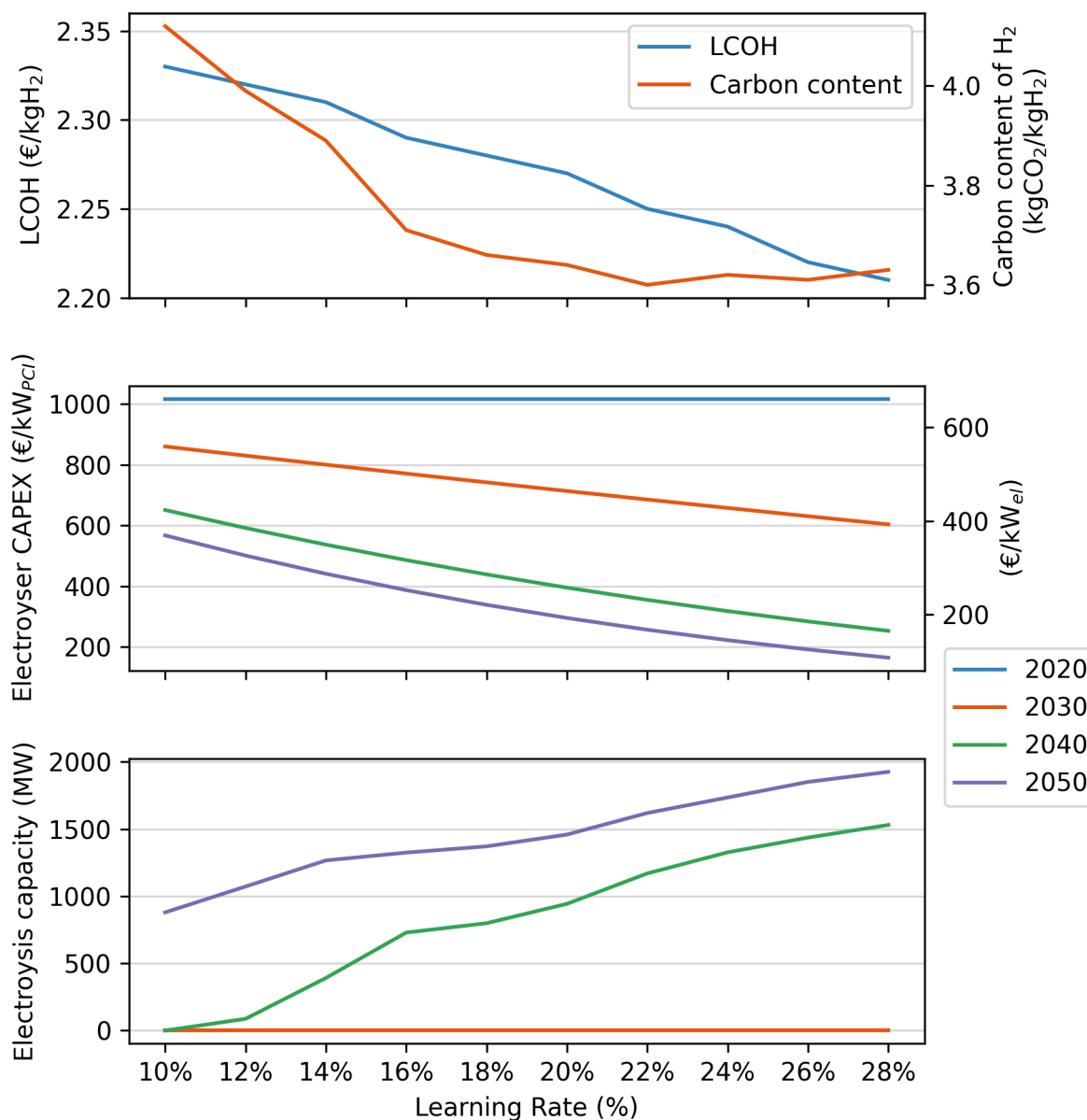


Figure 4.3: Average LCOH and average carbon content of hydrogen, electrolysis CAPEX and electrolysis installed capacities for different learning rates.

increasing.

4.1.3 Natural gas prices

In most cases today, extracting natural gas is possible at very low cost. The price of gaz also reflects the cost of necessary infrastructure for transport and storage, and as gas is not as easy to

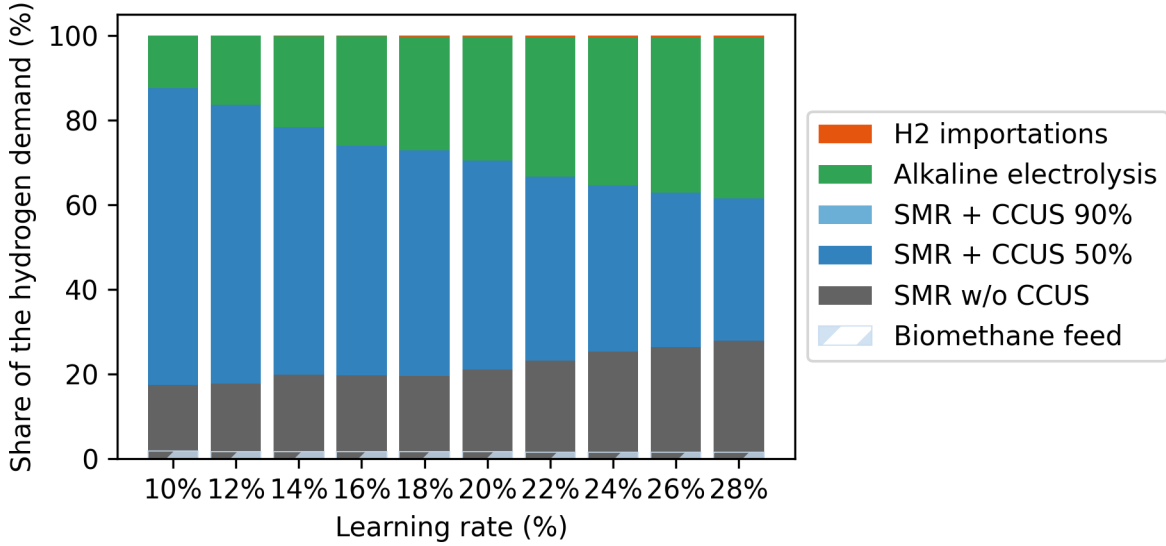


Figure 4.4: Contribution of the assets to the hydrogen supply for the horizon period for different values of LR.

transport world wide as oil, the price can vary depending on the region of the world. However, very strong variation in price can occur when demand is varying too rapidly or in the case of geopolitical conflict. This is what happened recently with the end of the COVID in 2021 and the Ukrainian war that started in February 2022. It is not possible to know what the cost will be of natural gas in the future, but the recent events and observed prices give clear indications of the kind of variations that can occur.

The sensitivity analysis in this section concerns natural gas prices. As a reminder, the prices of natural gas in the reference scenario are calculated from the prices observed during 2019, which is the reference year for meteorological data. Natural gas prices are modelled hourly. The average observed price in 2019 is 13.4 €/MWh, and we kept this value for the first planning period (2020-2030). For the remaining period, in the reference scenario, this price doubles (27 €/MWh on average) until the end of the planning horizon. For the sensitivity analysis, natural gas prices are calculated with a homothety on the price series to keep the price spread consistent with the meteorological data. We increased the average price from 15 €/MWh to 100 €/MWh.

Table 4.3: Synthesis of the scenarios for the natural gas sensitivity analysis.

Scenario name	CH ₄ average price after 2020 (€/MWh)
Reference	27
NG= x €/MWh	$x \in [15, 100]$

The upper graph of Figure 4.5 shows the average LCOH and the average carbon content of hydrogen for different average prices of natural gas for the planning horizon. The average LCOH increases with natural gas prices until it reaches stability around 2.8 €/kgH₂ for NG = 70€/MWh.

The results are similar for all scenarios between $NG = 70\text{€}/\text{MWh}$ and $NG = 100\text{€}/\text{MWh}$. It means that even with expensive natural gas, SMR can still provide a service to the hydrogen supply chain. The share of biomethane used as feedstock also increases with the price of natural gas. It is intuitive that biomethane becomes more competitive when the price of natural gas increases. As a reminder, the price of biomethane decreases from $120\text{€} / \text{MWh}$ in 2020 to $75\text{€}/\text{MWh}$ in 2050. For $NG = 70\text{€} / \text{MWh}$ and above, 100% of the SMR feedstock is biomethane during the last period. For the most expensive scenario, the biomethane share is greater than 87% in the 2030-2040 period and equal to 99% in the 2040-2050 period. However, the total amount of biomethane consumed (4.66 TWh in total and 1.6 TWh in the last period) remains acceptable, as it only represents 5.7% of the potential of the area in the period 2050-2060. Hydrogen imports stay low, reaching a maximum of 213 GWh for the whole planning horizon for the scenario of $NG = 60\text{€} / \text{MWh}$.

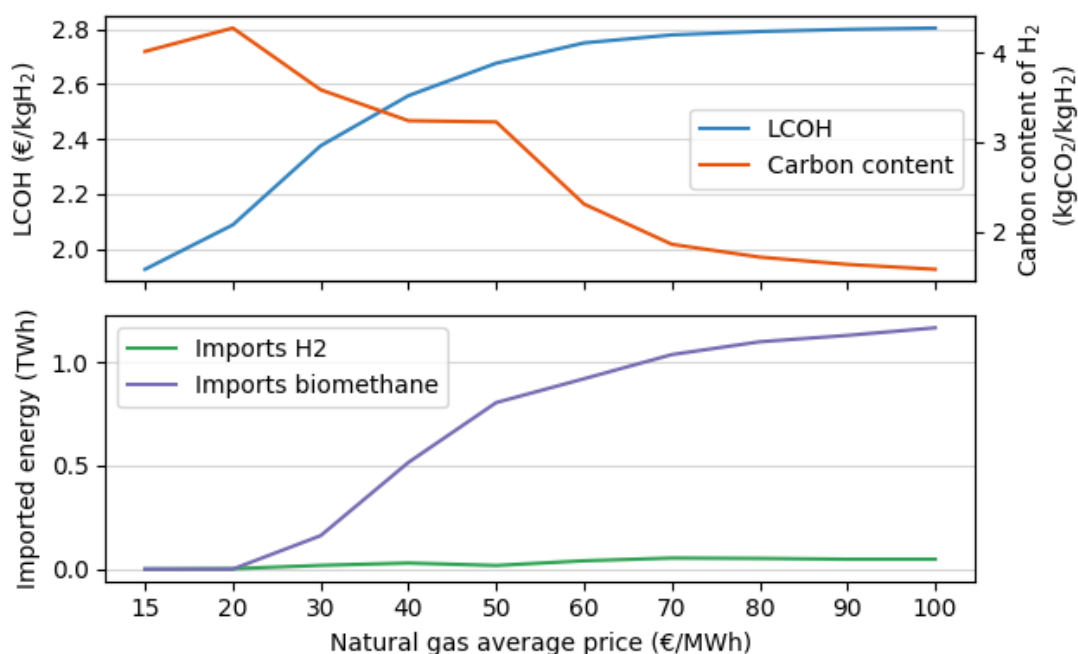


Figure 4.5: Average LCOH and average carbon content of hydrogen, hydrogen imported quantities and biomethane imported quantities for different prices of natural gas.

If we look at the average carbon content, it is going down from 4 to $\text{kgCO}_2/\text{kgH}_2$ 1.6 $\text{kgCO}_2/\text{kgH}_2$ when the price of natural gas increases. These results were expected with the use of electrolysis and biomethane. It decreases more significantly when the average price of natural gas exceeds $50\text{€} / \text{MWh}$ and biomethane replaces CCUS units. If we look at the average carbon content between 2030 and 2060, it falls below the European threshold for low-carbon hydrogen of $3.38\text{ kgCO}_2/\text{kgH}_2$ [23] when the price of natural gas reaches $60\text{€} / \text{MWh}$.

Figure 4.6 represents the contribution of the assets to the supply of hydrogen demand for the horizon period for the different prices of natural gas. It is interesting to note that carbon capture with 90% capture rate is competitive only when the average price of natural gas is below $20\text{€}/\text{MWh}$. As mentioned before, we can see that SMR + CCUS are progressively replaced by electrolysis and

conventional SMR with biomethane feedstock as natural gas prices are increasing. We point out that beyond an average price of 50 €/MWh, the share of electrolysis was capped at around 60% of the total hydrogen production. It corresponds to a share of 81% if we only look at the last operation period.

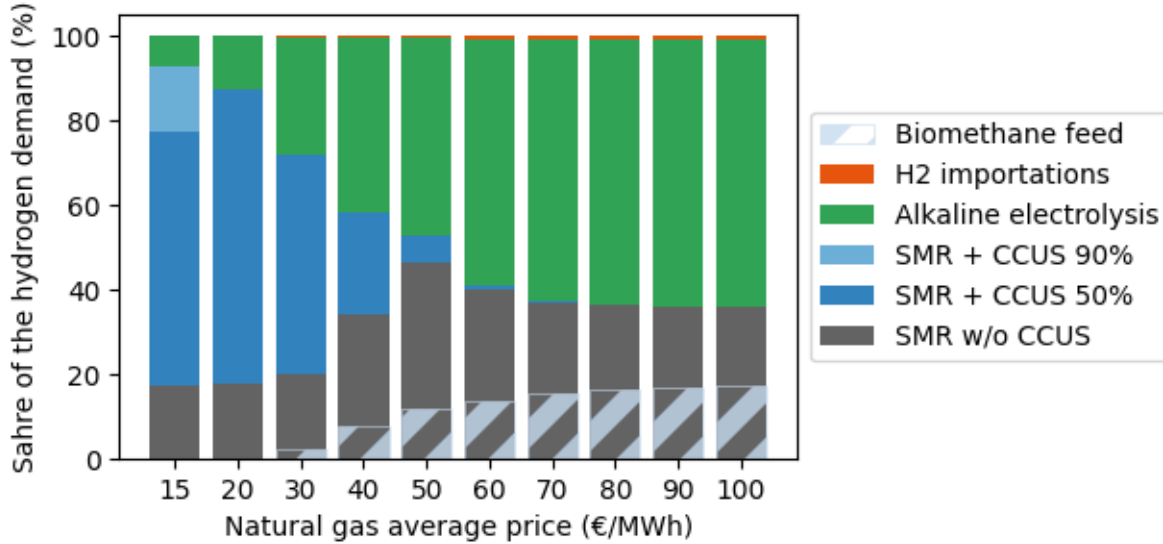


Figure 4.6: Contribution of the assets to the hydrogen supply for the horizon period for different prices of natural gas.

4.1.4 CO₂ treatment price

The CO₂ treatment price refers to transportation and storage costs, with the hypothesis that CO₂ cannot be reused. Our multi-resource model could be modified to consider the reuse of CO₂ and thus endogenise the value of CO₂, but it is out of the scope of this thesis. In the reference scenario we consider a cost of 50 € for each ton of CO₂ captured, based on the analysis of IEA study [3] for the Netherlands. Our case is located on the Mediterranean coastline and the geography is supposed to be less favourable to storage of CO₂. To explore a wide spectrum of prices and test the limits of carbon capture competitiveness, we tested two scenarios with a cost of 10 €/tCO₂ (cheap CO₂ treatment scenario) and 100 €/tCO₂ (expensive CO₂ treatment scenario).

Table 4.4: Synthesis of the scenarios for the CO₂ treatment price sensitivity analysis.

Scenario name	CO ₂ price (€/tCO ₂)
Reference	Treatment: 50 Tax: 65-165
Cheap carbon treatment	Treatment: 10
Expensive carbon treatment	Treatment: 100

Figure 4.7 details hydrogen production by asset for each operation period for the three different

values of the CO₂ treatment prices. We see that the more expensive the CO₂ treatment is, the less CCUS and the more electrolysis is employed. In the case where CO₂ aftertreatment is the least expensive (10 €/tCO₂), SMR with capture is massively used from the second period of the plan (2020-2030) and electrolysis is invested only for the last period. For the most expensive scenario (treatment=100 €/tCO₂), carbon capture is not used at all.

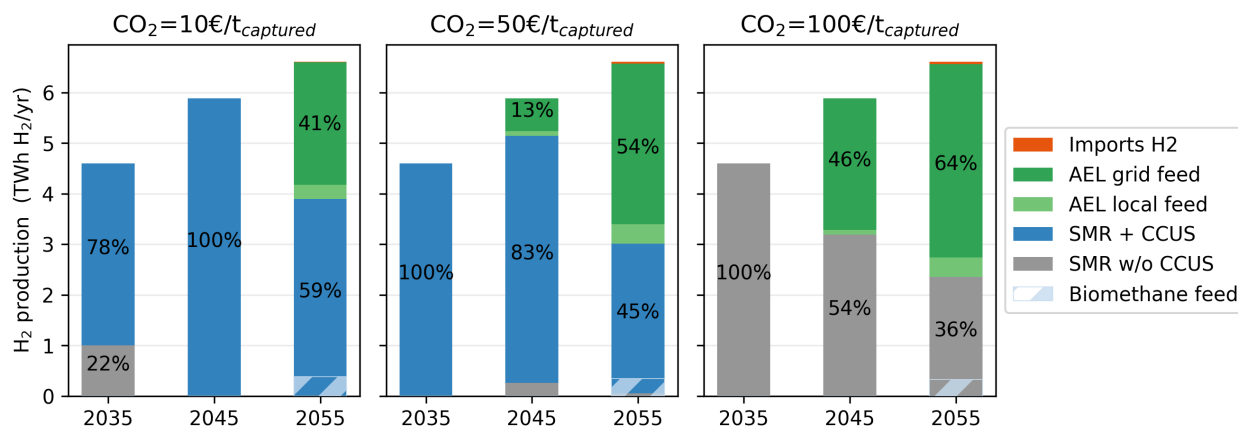


Figure 4.7: Comparison of hydrogen production by technology for different captured CO₂ post-treatment prices. To the left 10€/tCO₂, in the middle the reference scenario with 50€/tCO₂ and to the right 100€/tCO₂

We can also see in Figure 4.8, representing the carbon content of hydrogen for each scenario and for each operation period, that for the reference scenario and the cheaper carbon treatment scenario (blue and orange lines) CO₂ emissions are about 1 kg CO₂/kgH₂ lower than in the expensive case (green line). To conclude, we can say that the carbon capture price does not significantly impact the final hydrogen carbon content and distribution between SMR and electrolysis but changes the trajectory to reach this final mix.

4.1.5 Biomethane prices

Unlike natural gas, biomethane is a local resource whose price is less related to international geopolitical conflicts. The extraction cost is much larger than that of natural gas, around 100€/MWh today in France, but it is expected to decrease in the future. However, it is a very limited resource, and tension on demand could also increase the prices.

For biomethane prices, we compare the reference scenario, in which biomethane prices go down from 120 €/MWh in 2020 to 75 €/MWh in 2050 [79] in increments of 15 €/MWh, with a case where they decrease from 120 to 60 €/MWh in increments of 20 €/MWh (cheap biomethane scenario) and a case where they drop from 120 to 90 €/MWh in increments of 10 €/MWh (expensive biomethane scenario).

Figure 4.9 shows the hydrogen production by technology for the last three operating periods. On the left, the cheap biomethane scenario, in the middle the reference scenario, and on the right, the expensive biomethane scenario. We can see that the biomethane prices do not have a big

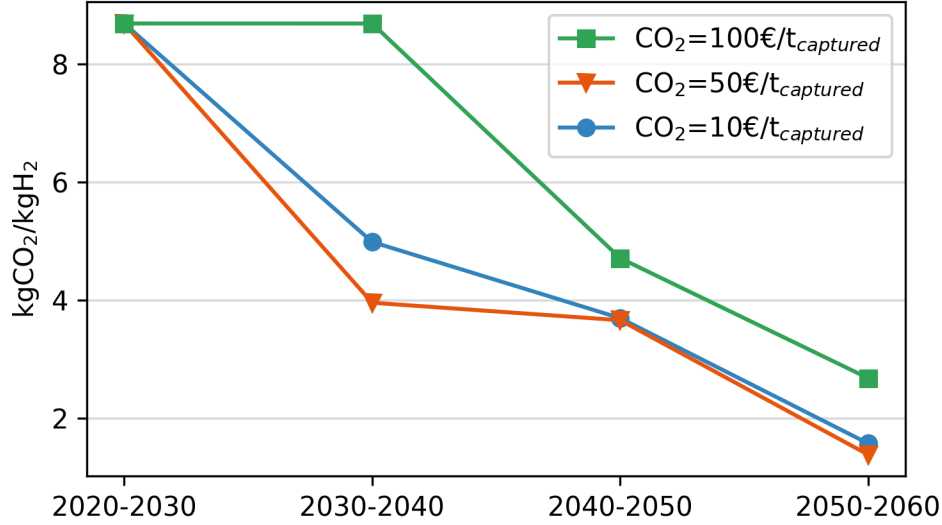


Figure 4.8: Comparison of carbon content for different captured CO₂ post-treatment prices. In blue 10€/tCO₂, in orange the reference scenario with 50€/tCO₂ and in green 100€/tCO₂

Table 4.5: Synthesis of the scenarios for the biomethane price sensitivity analysis. The biomethane prices are in €/MWh

Scenario name	Price in 2030	Price in 2040	Price in 2050
Reference	105	90	75
Cheap biomethane	100	80	60
Expensive biomethane	110	100	90

impact on investment and on the production mix: the share of hydrogen produced by electrolysis is between 50% and 54%.

For the three scenarios, biomethane is used as soon as its price falls below 90 €/MWh. As a reminder, in the reference scenario, 454 GWh of biomethane are used. If biomethane is only 15 €/MWh more expensive (100 €/MWh in 2050), then biomethane is not used and the carbon content of hydrogen is almost unchanged. However, if biomethane is only 15 €/MWh less expensive (60 €/MWh in 2050), then half of the gas used to power the SMR is biomethane (2 TWh or 7.3% of the theoretical potential of the "Région SUD"). In that case, CO₂ emissions were null in the last period.

Hydrogen price is not significantly impacted by biomethane price. Figure 4.10 shows the structure of hydrogen production costs for these three cases during the last operation period. The price of hydrogen is around 3 €/kgH₂ for all scenarios. This result shows that SMR technology is not sensitive to the price of biomethane. With the same invested capacity, it is possible to adapt to the evolution of the biomethane market. When biomethane is expensive, more carbon tax is paid.

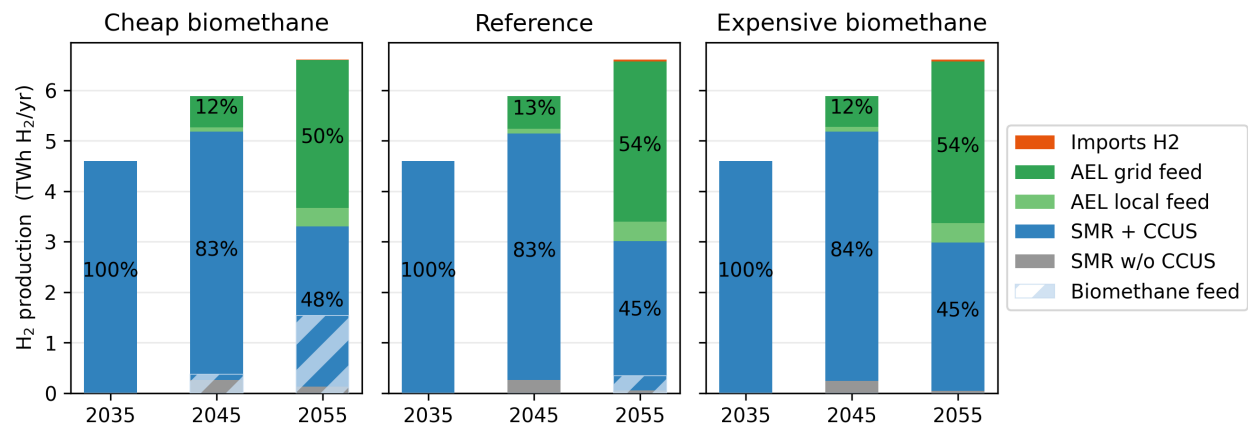


Figure 4.9: Comparison of hydrogen production by technology for different biomethane prices. On the left 60 €/MWh, in the middle the reference scenario with 75 €/MWh and on the right 90 €/MWh. The percentage on the bars represents the share of the demand supplied by the technology (if greater than 10%).

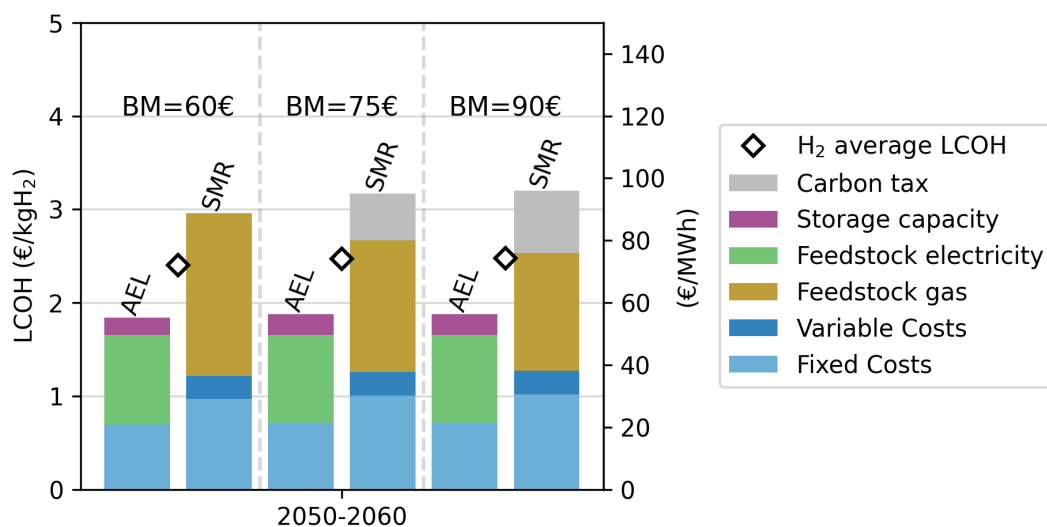


Figure 4.10: Hydrogen cost distribution for the last operation period (2050-2060) for electrolysis and SMR for different prices of biomethane.

However, the cheap biomethane scenario is the only one that allows reducing CO₂ emissions to 0 (compare to 1.8 kgCO₂/kgH₂ and 1.4 kgCO₂/kgH₂ for the other two cases), due to the "negative emissions" coming from the capture of biogenic CO₂. For the expensive biomethane case, the carbon tax represents 10% of the final cost of SMR production (0.3 €/ kgH₂ out of 3.2 €/kgH₂). It is interesting to see that for these three cases, the investment in electrolysis is similar (the difference is around 10%), as is the final production balance between SMR and electrolysis. This analysis shows that the price of biomethane is not a limit to the deployment of electrolysis.

4.1.6 Renewable potential

The development of photovoltaic and wind power production is a key element of the energy transition toward low-carbon economies. Their development next to the electrolyser can be a strong lever toward cost reduction, because it can allow the cost reduction of the grid connection. Additionally, investing today in electricity production associated with electrolysers reduces future risks on electricity prices. Indeed, as already mentioned, these prices could be affected by several important exogenous factors, such as the price of natural gas or the undercapacity of the system. However, the land necessary for their development can be a strong constraint affecting the overall project cost.

In this section, we examine the impact of the renewable potential of the area. We compare the reference scenario with a case where the potential for local renewables is doubled, which could represent stronger political will or better social acceptance of renewables, and a case where the potential is unlimited. This last case allows us to have an idea of how much space is missing to reach the optimum. Latter in this work, we consider the possibility to build the renewable capacities further away, where space is available. In further work, we could also include power purchase agreements to power electrolysers, which would mean unlimited access to renewables capacities, depending on the demand equilibrium.

Table 4.6: Synthesis of all the different scenarios for the renewable potential sensitivity analysis.

Scenario name	RE potential
Reference	Solar: 150 MW Onshore: 150 MW Offshore: 1 GW
Doubled renewable potential	Solar: 300 MW Onshore: 300 MW Offshore: 2 GW
Unlimited renewable potential	No capacity constraint

Figure 4.11 shows the hydrogen production by technology for the different scenarios. We find that the quantity of hydrogen produced by electrolysis is more than doubled when the limit on renewable potential is removed. During the last period, it goes from 3.6 TWh for the reference case to 5.1 TWh for the unlimited case. We can also see that the amount of local renewables in the electricity mix to feed electrolysers increases as the potential for renewables increases. It goes from 11% for the reference scenario to 20% and 66%, respectively, for the doubled case and the unlimited case. We note that even in the last case, some SMR capacity is maintained and a small amount of biomethane is used.

If we look at the costs, we find that for these three scenarios, the hydrogen cost is roughly the same (a difference less than 1%), and the same applies for CO₂ emissions. We find that the unlimited renewables configuration is achieved with 575 MW of onshore wind and 2.2 GW of solar PV for the 2050-2060 period. At the scale of the region this does not seem unreachable, but the space is clearly missing around the Fos-sur-mer direct area.

However, if we look at the electrolysis investments in Figure 4.12, we can see that the electrolysis capacity reached in the last period is roughly the same for all the scenarios analysed. We also note that the load factor in 2050 increases from 30% in the reference scenario to 43% in the unlimited scenario. It means that in the reference case, electrolysis is oversized to compensate for renewables

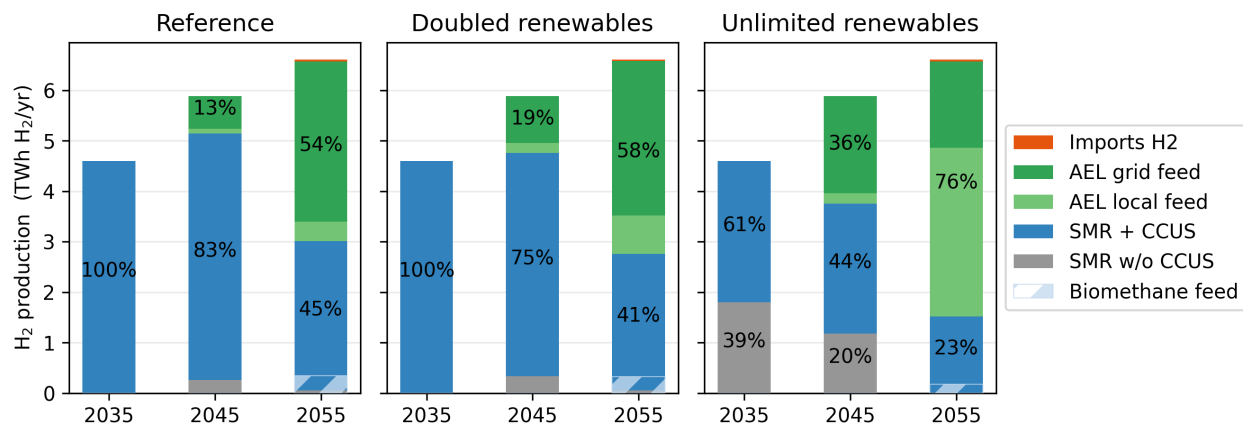


Figure 4.11: Comparison of hydrogen production by technology for different levels of renewable potential. On the left, the reference scenario, in the middle the doubled potential scenario, and on the right the unlimited renewable potential scenario. The percentages on the bars represent the share of hydrogen demand supplied by the technology (if greater than 10%).

variability and volatility of electricity prices. These results show that the less space there is to install dedicated renewables, the more flexibility is needed.

4.1.7 Geological storage

Geological underground storage is an important game changer in the development of the hydrogen value chain. Indeed, it allows to reach very large volumes of energy storage at low cost, and consequently, it offers an affordable seasonal storage capacity. However, this kind of storage can be unreachable for different reasons. If a storage close to production and consumption site is possible, there associated development can be delayed for several reasons, such as technical difficulties, or the competition with other vectors (oil, gas or maybe CO₂ later).

Here, we analyse the impact of the presence of a large underground storage on the deployment of electrolysis. We compare the reference scenario, without geological storage, with two scenarios in which geological storage is possible 100 km away from the consumption site. In the first case, the renewable potential is the same as in the reference scenario, and in the second case, the renewable potential is unlimited. Note that the capacity and power of the geological storage are optimised, as are the capacity and power of the tank storage in the reference scenario.

Figure 4.13 shows the hydrogen production by technology for the three different scenarios. We see that the presence of geological storage increases the share of electrolysis in the production mix. However, if the renewable potential is limited (the two graphs on the left), we see that the share of electrolysis production is kept at 82% in the 2050-2060 period, as it was in the analysis of the sensitivity of our results to the price of natural gas. If this limit is removed, then the electrolysis share is reached by 94% of the production, including 66% of dedicated renewable feedstock, in the last operation period. As was the case for the unlimited renewable potential scenario without geological storage (see section 4.1.6), the local dedicated renewable share for electrolysis in the

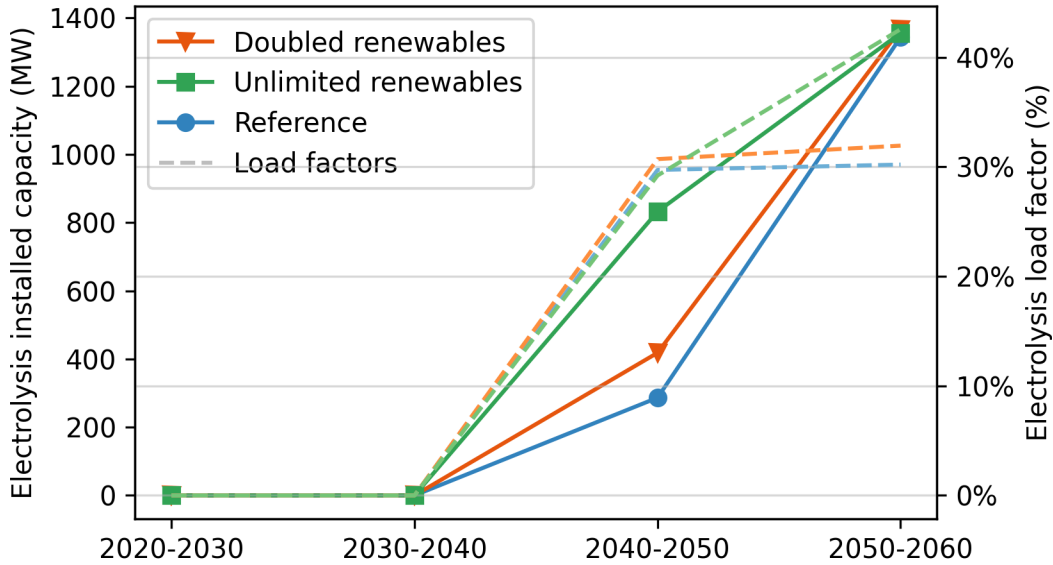


Figure 4.12: Comparison of electrolysis capacity investment trajectory for different renewable potential levels. The dotted lines represent the electrolysis load factors.

Table 4.7: Synthesis of all the different scenarios for the geological storage sensitivity analysis.

Scenario name	RE potential	H ₂ storage
Without geological storage	Solar: 150 MW Onshore: 150 MW Offshore: 1 GW	H ₂ tank
With geological storage	Solar: 150 MW Onshore: 150 MW Offshore: 1 GW	Salt caverns
With geological storage + unlimited renewables	No capacity constraint	Salt caverns

unlimited potential with geological storage scenario reaches around 40%.

Figure 4.14 shows that the presence of large hydrogen storage helps reduce hydrogen production costs. We find that geological storage reduces the average LCOH by 6%, and if the storage is combined with unlimited rechargeable potential, the cost can be reduced by almost 10%. However, the electrolysis is oversized in the geological storage scenario (2 GW for a load factor of 30% in 2050-2060) compared to the unlimited and geological storage scenario (1.7 GW for a load factor of 42% in 2050-2060).

4.1.8 Hydrogen imports

In our modelling work, the hydrogen value chain is considered to be developed locally. However, there are several initiatives to develop large-scale infrastructure that will interconnect hydrogen systems together. This could be through a European hydrogen backbone, seaborne importation of

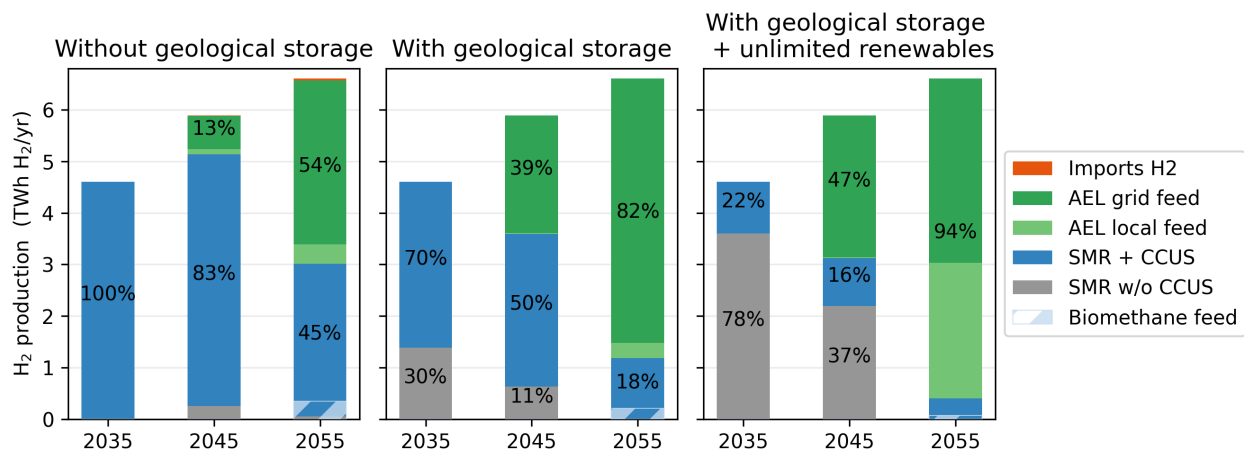


Figure 4.13: Comparison of the hydrogen production by technology for scenarios with and without geological storage. On the left, the reference scenario without geological storage, in the middle, the scenario with geological storage, and on the right, the unlimited renewable potential with geological storage scenario. The percentages on the bars represent the share of hydrogen demand supplied by the technology (if greater than 10%).

liquid hydrogen or, more likely, transport around the world in the form of ammoniac. This means that in the future, a local hydrogen value chain like the one we study will have to face a more global market with hydrogen possibly produced in places with lower electricity costs or eventually hydrogen obtained from natural sources. This possible imports will come with two highly uncertain factors: how cheap and when.

In this section, we analyse the sensibility of our results to the possibility to import low-carbon hydrogen from outside of the territory of interest. The carbon content of the imported hydrogen is considered null as we only consider direct emissions in our model. In the reference scenario, the hydrogen importation price was fixed at 6 €/kgH₂ (180 €/MWh). As already seen in Chapter 2, the hydrogen price is composed as follows: 4 €/kg for production, 1.5 €/kg for transportation and 0.5 €/kg for storage and distribution infrastructure [80].

In the hydrogen import scenario, we consider that this importation price is decreasing from 6 €/kg in 2020 to 2 €/kg in 2050. This could represent the deployment of massive low-carbon hydrogen production in regions with high renewable potential. In the scenario of cheap hydrogen imports, we examine the possibility of importing very cheap low carbon hydrogen at a price of 2 €/kg from 2030. This could represent the development of natural hydrogen resources [14, 15].

Figure 4.15 shows the hydrogen production by technology for the three different described scenarios. The orange bars represent the import contribution. We see that imports play a significant role as soon as the import price falls below 3 €/kg. We also note that with the chosen hypotheses, even in the most optimistic case (hydrogen price at 2 €/kg), it is still interesting to invest in electrolysis for around 30% of the production. These 30% correspond to the moments where grid electricity is cheap, with renewables as marginal production means. In the hydrogen import scenario, the electrolysis LCOH in the last period is 1.8 €/kg and for the cheap hydrogen import scenario, it is 1.7 €/kg. Indeed, the average price for the grid electricity used in these three

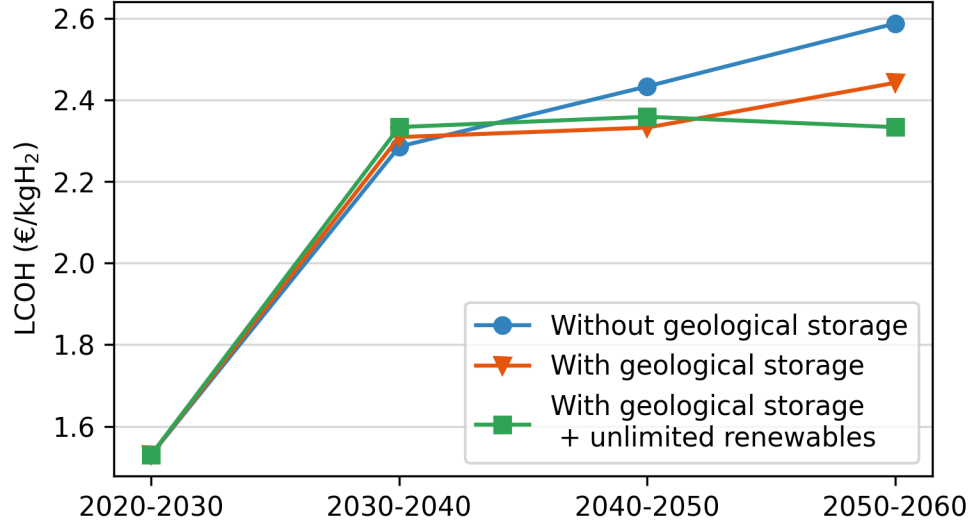


Figure 4.14: Comparison of the average LCOH for scenarios with and without geological storage.

Table 4.8: Synthesis of all the different scenarios for hydrogen importation sensitivity analysis. Hydrogen prices are given in €/kgH₂

Scenario name	H ₂ price in 2030	H ₂ price in 2040	H ₂ price in 2050
Reference	6	6	6
Hydrogen imports	4	3	2
Cheap hydrogen imports	2	2	2

scenarios is between 2.4 and 3 €/MWh in the 2050-2060 period (around 16 €/MWh if grid taxes are included).

4.1.9 Discussion

In the previous sections, we discussed some of the main parameters that impact the development of the hydrogen supply chain on the scale of our territory of interest, an industrial port with a base-load that increases hydrogen demand. First, we looked at the weighted average cost of capital, which is a fundamental parameter regarding the investment in new capacities. We found that increasing its value will disadvantage new technologies with high CAPEX and low OPEX, such as electrolysis and carbon capture. It could be interesting to secure investments by implementing revenue guarantee schemes, as was the case for the deployment of renewables.

We also emphasised the key role that existing steam methane reforming units play in the transition to keep hydrogen competitive. Even with expensive natural gas prices, expensive biomethane prices and expensive CO₂ treatment prices, between 36% and 45% of the demand is still supplied by SMR (with or without carbon capture) in the last operation period. SMR can be improved with

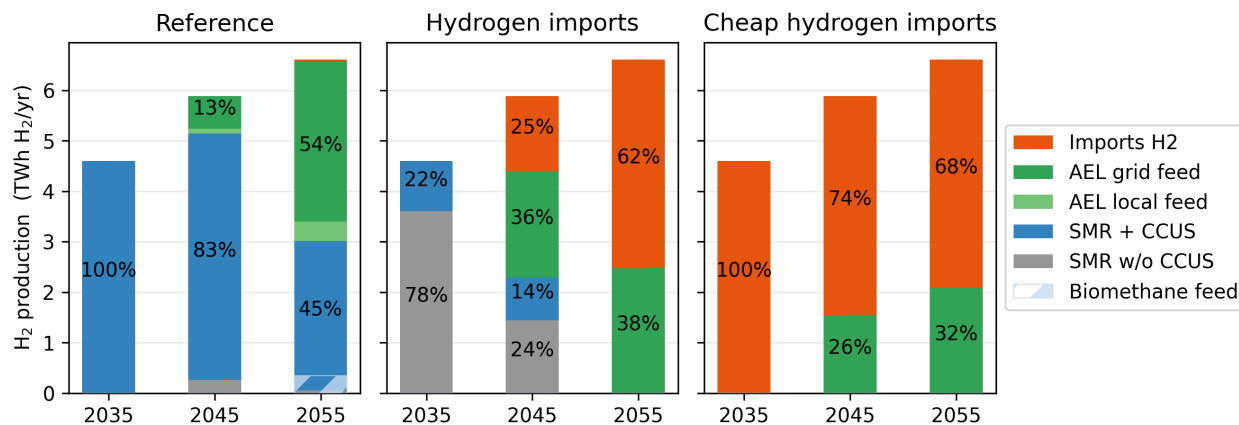


Figure 4.15: Comparison of hydrogen production by technology for different price of hydrogen importation. On the left, the reference scenario with 6 € / kg, in the middle, the hydrogen imports scenario with a progression decreasing from 6 to 2 € / kg, and on the right the cheap hydrogen imports scenario with a price of 2 €/kg. The percentage on the bars represents the share of the demand supplied by the technology (if > 10%).

carbon capture units depending on the context and can be fed with biomethane if the natural gas is expensive. The combination of carbon capture and biomethane can lead to negative emissions production. The limit for CCUS competitiveness is around 50€ per ton of captured CO₂. Biomethane competitiveness is around 90€/MWh, but this limit can decrease if natural gas prices increase.

In Chapter 3, the analysis of the reference scenario led to the hypothesis that electricity prices were a limit to the competitiveness of electrolysis. From this chapter we can add that the CAPEX of electrolysers, which is a parameter with significant uncertainties, can also be a limit to electrolysis competitiveness. When linking the evolution of grid electricity prices at the national scale with electrolysis operations at the local scale, we found that running electrolysers with grid electricity is not competitive for most of the time step of the year. The optimal deployment trajectory involves building dedicated renewables to power electrolysers, although in some territories, renewable power potential might be a limiting factor. We established that the smaller the local renewable power potential, the more flexibility the system will need. In our case, this flexibility can be brought about by controllable hydrogen production means such as SMR, large underground hydrogen storage means such as salt caverns, or cheap low-carbon hydrogen imports.

4.2 Robustness of the different scenarios

In the previous section, we have analysed one by one some of the main parameters impacting the future hydrogen production mix in our territory of interest. However, for each optimisation, we considered that the future is perfectly anticipated, so the system is optimally developed to face an unfavourable situation. In reality, we cannot anticipate what will happen, so we were interested in understanding how a planned energy system can adapt to an unanticipated event. To do so, we define and run eight scenarios, called "Anticipated scenarios", for which the capacities and the operation

are optimised. Then, the eight resulting systems are confronted to eight different scenarios, which we called "Actual scenarios" for which the optimisation is run with fixed capacities. It means that only the operation is optimised, not the investments. When the results of the perfectly anticipated optimisation and the actual scenario optimisation are close, it means that the anticipated scenario is robust to the parameter we varied.

The anticipated scenarios are as follows.

- The reference scenario, described in Chapter 3.
- Cheap biomethane scenario, where the biomethane price is going from 120 €/MWh to 60€/MWh. it could represent less stress on biomethane demand.
- Expensive renewables scenario, where renewables and electrolysis are more expensive than in other scenarios. For renewables, the CAPEX are the "high" hypothesis from RTE's "Futurs énergétiques 2050" report [4], for electrolysis, we still assume a learning rate of 18%, but the world cumulative installed capacities are divided by two (CAPEX going from 1,016 €/kW_{LHV} in 2020 to 300 €/kW_{LHV} in 2050).
- Expensive carbon treatment scenario, where the captures CO₂ price is 100 €/tCO₂.
- Unlimited renewable potential, where the limits on the installed capacities of renewable energies are removed.
- Hydrogen imports, where the price of hydrogen imports decreases from 6 € / kg in 2020 to 2 €/kg in 2050.
- Expensive natural gas, where natural gas prices are multiplied by 5 compared to 2019 for the 2030-2060 period. It could represent a geopolitical crisis like the one we are facing with the war between Ukraine and Russia in 2023.
- Ban on SMR from 2040, where the SMR capacities are forced to 0 from 2040 to 2060. This scenario could represent a political decision to move away from fossil energy. For this scenario alone, the capacities are fixed only for the 2020-2040 period. For the 2040-2060 period, the capacities are optimised (as if a new policy were being applied).

The actual scenarios are the same as the anticipated ones with one exception : the unlimited renewable potential scenario is replaced by the cheap imports scenario where the hydrogen importation price is 2 €/kg from 2030 to 2060.

Figure 4.16 presents the results of this analysis. The two matrices show the average LCOH from 2020 to 2060 for different combinations of anticipated and actual scenarios. The upper matrix shows the results without geological storage, while the lower matrix shows the same analysis with geological storage for all the scenarios. Each row represents an anticipated scenario, which means that the capacities are fixed along the row. Each column represents an actual scenario, meaning that all the parameters except the capacities are fixed for the column. On the diagonal, we can find the perfectly optimised cost for each scenario (except the unlimited renewable X cheap hydrogen import case). The colours represent the value of the LCOH, going from dark blue (below 2 €/kgH₂)

to yellow (3.4 €/kgH₂). With the coloured representation, we can say at first glance that the darker lines and columns are the less expensive scenarios, the most unified lines (same colour all along) are the most robust scenarios, the most diverse lines are the riskiest prediction for the future, and the lighter columns are the least favourable scenarios for hydrogen deployment.

The first result is that the presence of a large geological storage makes the system cheaper and more robust as we can see that the lower matrix is darker and more unified than the upper one. This result was expected since storage brings flexibility to the system. We can also see at first glance two columns and a line that stand out. We see that the expensive natural gas scenario and the ban on SMR from 2040 scenario are the most expensive ones. The two columns on the right of the graph are especially yellow compared to others, meaning that these contexts have a significant impact on hydrogen final cost if we do not anticipate them. The hydrogen import scenario line also draws attention for being especially inconsistent. It means that anticipating the possibility to import cheaper hydrogen in the future is a risky bet because if the prediction does not materialise, then hydrogen production will be much more expensive than anticipated. However, if the prediction comes true (see hydrogen import line with hydrogen imports or cheap hydrogen imports columns), then it becomes the least costly scenario because less new capacities are needed. We can also see, by comparing the two matrix, that the hydrogen import line is the same because there is no investment in geological storage, even if allowed, in the hydrogen import scenario. As a reminder, here we focus only on our territory of interest. If hydrogen exportation to another region was authorised, then geological storage would probably be interesting in the hydrogen import scenario.

To conclude, we can say that anticipating pessimist scenarios like expensive carbon treatment, expensive natural gas, or ban on SMR from 2040, allows to build more costly but more robust energy systems. On the other hand, betting on cheap use of SMR seems to be risky.

Figure 4.17 shows the same results but with a different perspective. We represent the average LCOH difference between the operation optimised only scenario and the corresponding perfectly anticipated scenario (on the diagonal of the matrix except for the unlimited renewable potential scenario). In red are the positive cost differences, meaning that the events of the actual scenarios make hydrogen more expensive, and in green the negative cost differences, meaning that the events of the actual scenarios induce a reduction in the cost of hydrogen production. Here, we can also read that the expensive natural gas scenario and the ban on SMR from 2040 scenario are the most robust ones (white or green), and the hydrogen imports scenario is the most risky one (lot of red). Being conservative about renewable and electrolysis CAPEX (expensive renewable scenario) does not seem to increase significantly hydrogen cost except if SMR are banned from 2040. We note that there is only 1.35 €/kgH₂ difference between the highest average LCOH and the lowest average LCOH for the 64 scenarios of this study.

Figure 4.18 shows the distribution of the LCOH (upper graph), the carbon content of hydrogen (middle graph), and the quantities of imported hydrogen (lower graph) for all the anticipated scenarios for all the operation periods of the planning. The grey bars represent the average over the operation horizon (2020-2060). Note that the 2020-2030 period is the same for all scenarios and is represented by the blue dotted lines.

In these graphs, the shorter the bars, the more robust the scenario is, as events of the actual

4.2. ROBUSTNESS OF THE DIFFERENT SCENARIOS

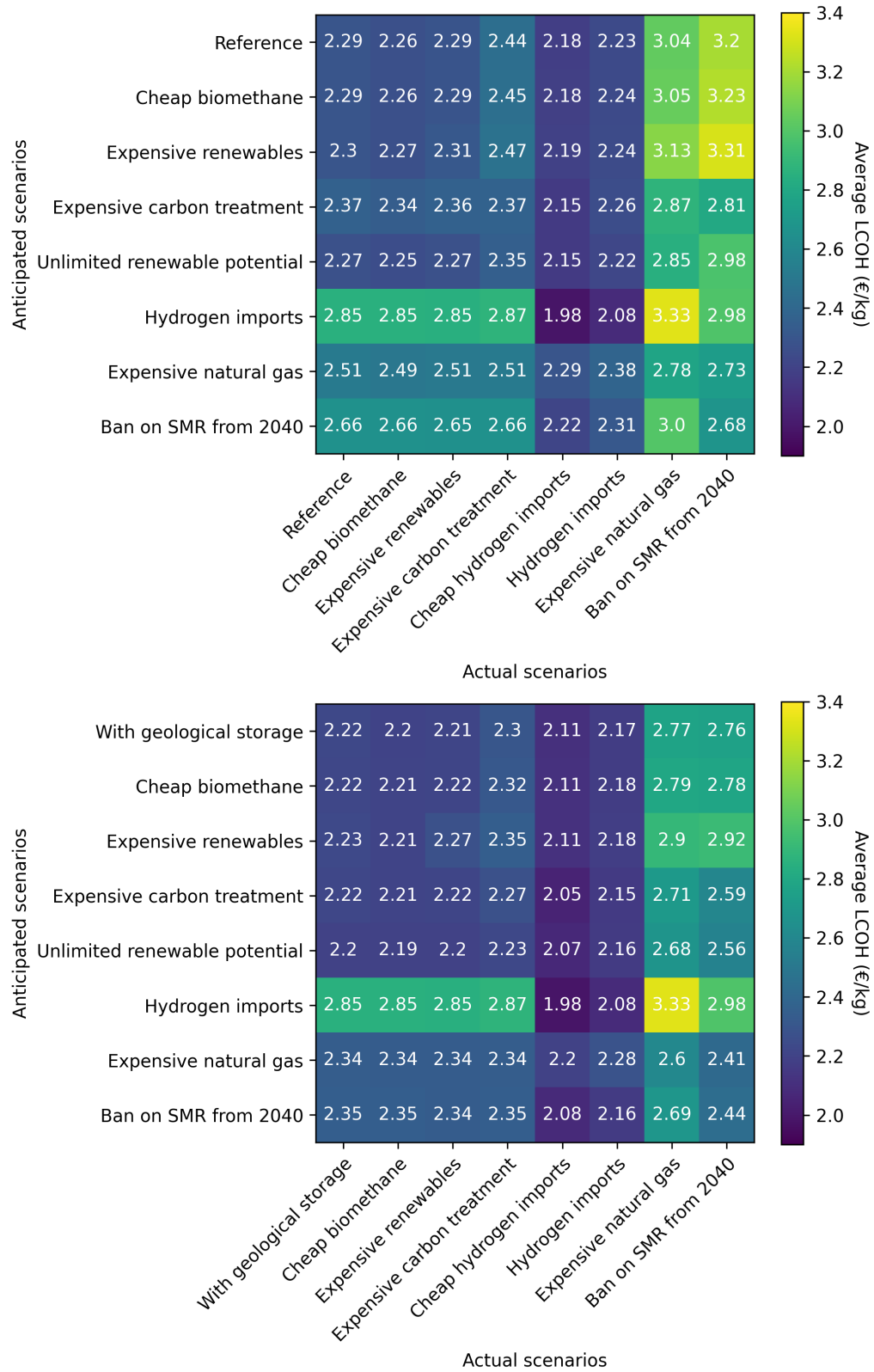


Figure 4.16: Matrix of costs for the robustness analysis. Each case represents the average LCOH of the considered scenario.

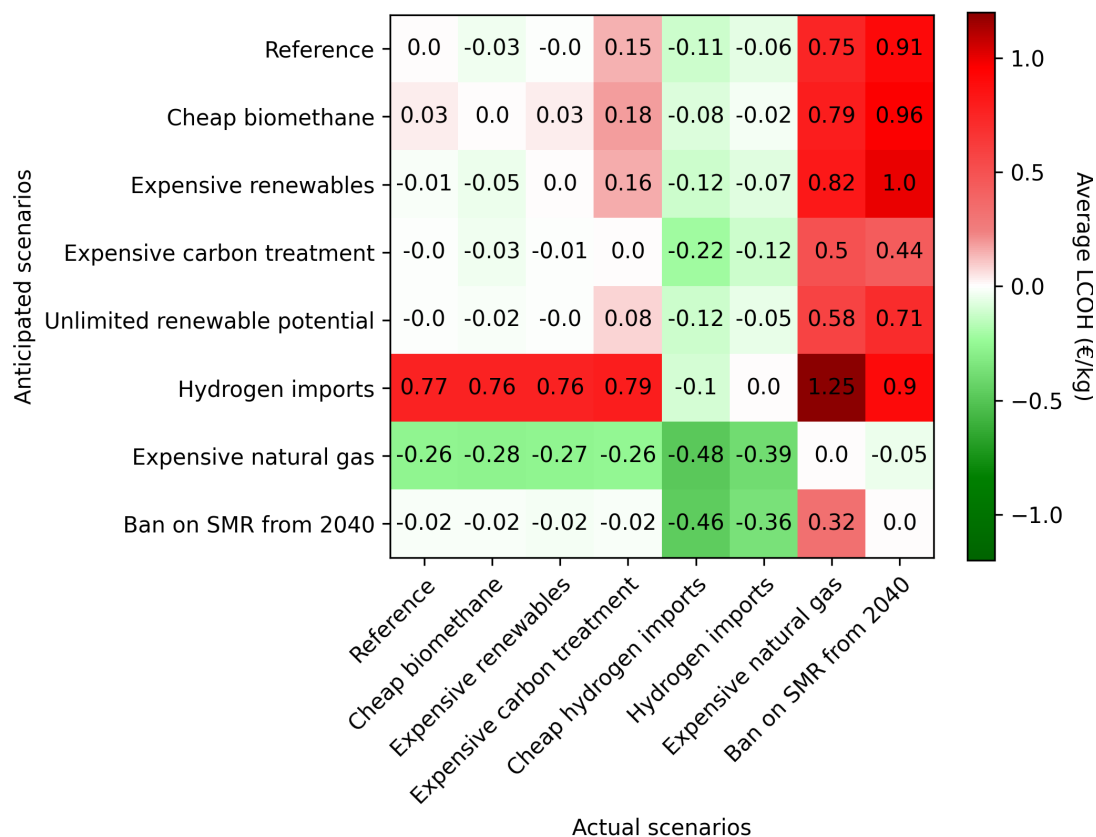


Figure 4.17: Matrix of cost differences between the perfectly optimised scenario and the optimised operation only scenarios. Each case represents the average LCOH difference between the two scenarios.

scenarios do not have a significant impact on the results. If we look at the LCOH (upper graph), the most robust scenarios are the expensive natural gas scenario and the ban on SMR from 2040 scenario. The unlimited renewable scenario is also quite stable both in terms of costs and in terms of carbon emissions (middle graph). The scenario with the largest distribution of carbon emissions is the expensive carbon treatment scenario, whereas it is stable with respect to hydrogen cost. Indeed, in that scenario, no investment in carbon capture is made, so to keep the cost under control, conventional SMR is needed.

Looking at the hydrogen imports graph (lower graph), we can see that except for the hydrogen import scenario, the distribution is similar for all scenarios. The expensive carbon treatment scenario is a bit larger than the others, while the ban on SMR from 2040 is more stable than the others regarding this aspect. For most of the scenarios, we can avoid hydrogen imports in the perfectly anticipated case. We can also note that imports are higher in the last period in the perfectly anticipated hydrogen import scenario than in any other scenarios. It means that in non-optimised scenarios, even with cheap hydrogen (2 €/kg in 2050), the invested capacities are still used.

More generally, the results of this section show that the reference scenario, the cheap biomethane

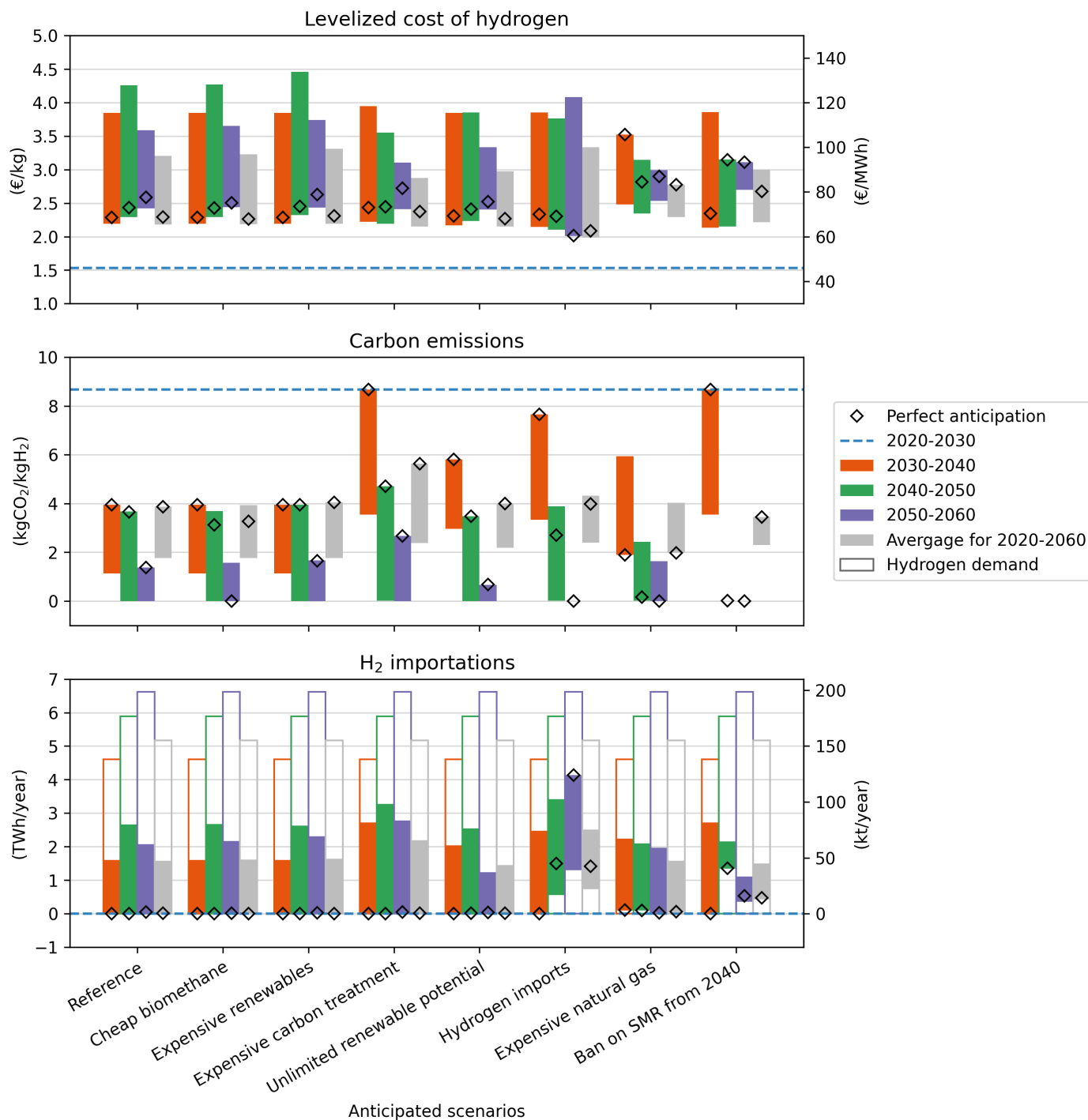


Figure 4.18: Distribution of the LCOH (upper graph), the carbon content of hydrogen (middle graph), and the hydrogen imported quantities (lower graph) for the eight anticipated scenarios. The black diamond shows the value for the perfectly anticipated optimisation.

scenario, the expensive renewable scenario, and the unlimited renewable potential scenario are robust to each other with a deviation of less than 0.18 € / kg for an average LCOH of around 2.3 € / kg (with a deviation of less than 10%). However, the expensive natural gas scenario and the ban on SMR from 2040 scenario include events that can influence the hydrogen price a lot. It is risky not to consider these cases when developing the system.

4.3 Conclusion

In Chapter 2, we propose a methodology to simulate the optimal evolution of investment and operation of a hydrogen production infrastructure. It allows us to analyse the important techno-economic parameters in the evolution of a future hydrogen hub. In Chapter 3, we applied the described methodology to an industrial harbour in south of France, but the results presented are highly dependent on the chosen hypotheses. For this reason, we have performed several sensitivity analyses on critical parameters.

These sensitivity analyses highlighted that even if the results are sensitive to many uncertain parameters, in the end the hydrogen production mix tends to be a combination of electrolysis and SMR. Indeed, the SMR can still be competitive, even under unfavourable conditions (expensive feedstock or higher variable costs). This is especially the case since some conventional SMR are already present in our territory of interest. In light of these results, hybridisation of electrolysis is the optimal solution. With hybridisation, electrolyzers can be competitive with low load factors (around 30%), allowing renewable electricity feedstock (from the grid or directly connected dedicated renewable plants) to be part of the mix.

In a second phase, we also tested the robustness of different scenarios by stressing them with non-anticipated events. It came out that the most pessimistic scenarios in terms of hydrogen cost are the most robust ones. Indeed, the scenarios using less SMR either because the feedstock gas is expensive, either because of public policy are on average more expensive than the others, but they are less disturbed by unanticipated events. We can conclude that scenarios with more electrolysis capacity and dedicated renewable energy tend to be more robust than others. In this study, we did not let the possibility to change the development plan to adapt to the new regulation or to face the crisis. To do so, in further work it could be interesting to implement a rolling-horizon algorithm [104].

Valeur d'hybridation des SMR - Résumé

Ce chapitre examine le rôle crucial du reformage du méthane à la vapeur (SMR) dans la réduction des coûts de l'électrolyse et l'amélioration de la flexibilité du système. Elle introduit le concept de "valeur d'hybridation du SMR" en tant qu'indicateur permettant de quantifier la contribution du SMR au système. Cette valeur reflète les avantages en termes de réduction des coûts et de flexibilité apportés par le SMR lorsqu'il est combiné à l'électrolyse.

L'analyse se penche ensuite sur l'évaluation de cette valeur d'hybridation dans différents scénarios moins favorables au SMR. Ces scénarios incluent des contextes avec un stockage souterrain important, un potentiel renouvelable illimité, une taxe carbone élevée et une matière première gazeuse coûteuse. En outre, les variations de paramètres tels que le coût du post-traitement du CO₂ capturé et les niveaux de taxe carbone sont explorés pour évaluer leur impact sur la valeur d'hybridation du SMR. Un post-traitement du CO₂ moins coûteux et des taxes sur le carbone moins élevées devraient favoriser une valeur d'hybridation plus élevée pour le SMR, tandis que des solutions plus coûteuses réduiraient cette valeur.

la valeur d'hybridation du SMR est définie comme la différence moyenne du coût de l'hydrogène (LCOH) entre un système avec SMR et un système sans SMR, tous autres paramètres égaux par ailleurs. Dans un premier temps, nous comparons les scénarios avec et sans SMR, avec différentes dates d'interdiction du SMR (2030, 2040, 2050) pour représenter les changements politiques en faveur de l'abandon des combustibles fossiles. L'analyse montre que les scénarios interdisant le SMR plus tôt conduisent à des LCOH moyens plus élevés sur l'horizon de planification, soulignant l'impact du SMR sur le coût de la production d'hydrogène.

Une analyse plus poussée compare les valeurs d'hybridation du SMR dans différents scénarios tels qu'un potentiel renouvelable illimité, la disponibilité du stockage géologique, des prix élevés pour le gaz naturel, un biométhane cher, et des variations dans les coûts de traitement du carbone et les taxes sur le carbone. L'étude montre que la valeur d'hybridation du SMR est influencée de manière significative par les prix du gaz naturel, le gaz cher réduisant l'impact du SMR. Les scénarios de biométhane coûteux présentent des valeurs d'hybridation SMR plus élevées.

Le chapitre conclut en soulignant le rôle essentiel du méthane à usage domestique pour maintenir la compétitivité de l'hydrogène et l'importance d'une planification soignée à long terme pour éviter les utilisations contradictoires des matières premières gazières.

Chapter 5

SMR hybridisation value

The results of the two previous chapters show that without SMR, electrolysis costs would be much higher. As a controllable production technology, SMR can bring flexibility into the system, helping to decrease the total costs of the system when combined with electrolysis. In this section, we seek to confirm this hypothesis by defining an indicator, the "SMR hybridisation value", that would allow us to quantify the value of the service provided by SMR to the system.

In a second phase, we evaluate this hybridisation value in different contexts less favourable to the SMR: presence of large underground storage, unlimited potential to install renewables, high carbon tax and expensive gas feedstock. For all the tested scenarios, we also vary two parameters: the captured CO₂ post-treatment with a cheaper alternative, that should be in favour of a better hybridisation value, and the carbon tax, with a more expensive alternative that should decrease SMR hybridisation value.

5.1 Defining the hybridisation value indicator

We define the SMR hybridisation value as the average LCOH difference between a system allowing SMR and a system without SMR for the same scenario. It can be written as follows:

$$\text{SMR}_{\text{value}} = \text{LCOH}_{\text{scenario}} - \text{LCOH}_{\text{scenario w/o SMR}} \quad (5.1)$$

where LCOH is the average levelised cost of hydrogen for all production technologies as defined in Chapter 3. For the "w/o SMR" scenario, the first operation period (2020-2030) is the same, and from 2030, the SMR capacities are forced to 0.

5.2 SMR hybridisation value in the reference scenario

In a first analysis, we compare four different scenarios: the reference scenario and three scenarios where SMR are banned. The difference between the three is the moment from when SMR are banned: 2030, 2040 and 2050. This could represent the will of politics to move away from fossil fuels from a certain date.

Figure 5.1 shows the average LCOH as a function of hydrogen carbon content, and Figure 5.2 shows the cumulative CO₂ emissions for the planning horizon. The reference scenario with SMR (blue line) is less expensive for the 2030-2040 and 2050-2060 periods. It is also the one with the lowest total average LCOH over the four operation periods (2.3 €/kgH₂). However, it is also one of the most emitting scenarios. The hydrogen carbon content is divided by more than two between the first and the second operation periods (from 8.7 to 4 kgCO₂/kgH₂) thanks to investments in carbon capture, but emissions do not fall to zero in the last period like other scenarios. The final hydrogen carbon content is 1.38 kgCO₂/kgH₂ in 2050-2060 period.

If we look now at the scenarios that prevent the use of SMR, we see that the sooner SMR is banned, the more expensive the average LCOH for the whole planning horizon is (3.03 €/kgH₂ if banned in 2030, 2.68 €/kgH₂ if banned in 2040, 2.45 €/kgH₂ if banned in 2050). This is due to the decrease in electrolysis CAPEX over time. However, we see that the lowest cost in the 2050-2060 period is attained for the "Ban on SMR from 2030" scenario, meaning that anticipation in the deployment of electrolysis helps to decrease hydrogen production costs. More generally, we see a clear demarcation in costs and carbon content between production mix allowing SMR and one preventing the use of SMR, proving the hybridisation value. Comparing the reference scenario with the SMR banned from 2030 scenario, we can quantify SMR hybridisation value: about 0.74€/kgH₂ i.e. -32%.

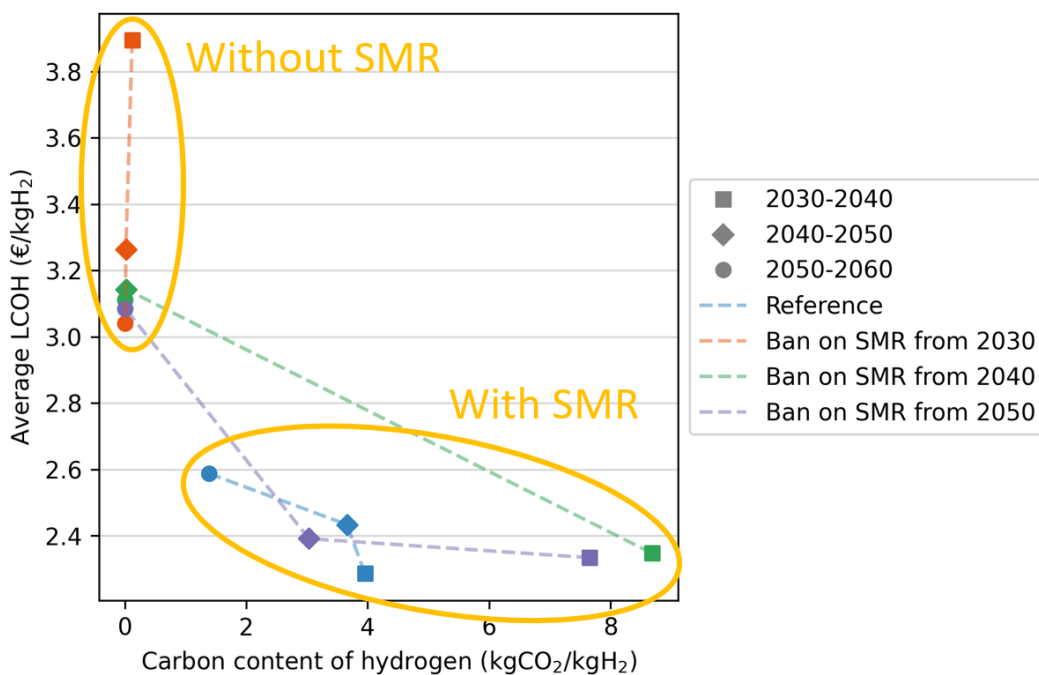


Figure 5.1: Average LCOH and carbon content evolution over the planning horizon for the reference scenario and the scenarios without SMR.

If we look at the cumulative CO₂ emissions (Figure 5.2), we see that as soon as the SMR are banned, the production becomes almost zero emissions. The only source of CO₂ emissions taken

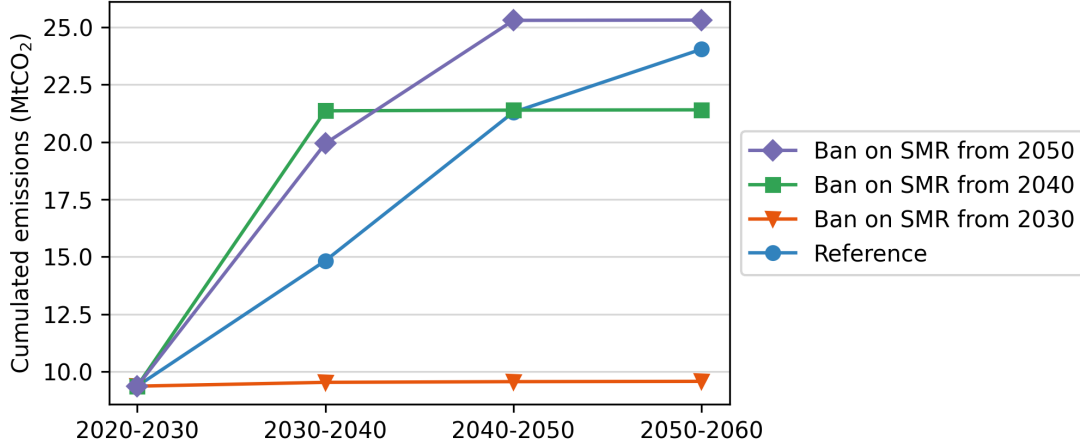


Figure 5.2: Cumulative CO₂ emissions over the planning horizon for the reference scenario and scenarios without SMR.

into account is the carbon content of the electricity coming from the grid. We see that the worst scenario in terms of CO₂ total emissions is the scenario without SMR from 2050. In fact, in that case, investments in carbon capture units are very small (114 MW), and for the first three operation periods (from 2020 to 2050), conventional SMR is used (27% of the production for 2040-2050).

The total avoided CO₂ emissions between the reference scenario and the scenario without SMR from 2030 is 14 461 ktCO₂. It means a cost of CO₂ avoided of 32 €/tCO₂ which is much lower than the carbon tax implemented (from 90 to 165 €/tCO₂). We could question whether the society would agree to pay more for a faster decrease in emissions. However, we have to keep in mind that the electrolysis deploying rate is limited [22]. SMR can be a good alternative to tackle this challenge.

5.3 Limiting factor to hybridisation value

In a second analysis phase, we want to compare the hybridisation value provided by the SMR to the system to other flexibility means. We compare five different scenarios: with unlimited renewable potential, with the presence of large underground geological storage, a combination of both, with expensive natural gas and with expensive biomethane. These three scenarios are calculated with two variants to see the impact of these parameters on the value of the SMR service to the system: with cheap CO₂ post treatment (10 €/tCO₂) and expensive carbon tax (200 €/tCO₂). Table 5.1 recaps the characteristics of the scenarios analysed in this section.

Figure 5.3 presents the average hybridisation value as a function of cumulative CO₂ emissions for all of these cases. It is not easy to bring out tendencies, but we can see at first glance that the SMR hybridisation value is significantly impacted by the natural gas price. When natural gas is expensive, the SMRs are less used, so banning them has a smaller impact. For that scenario, we find a hybridisation value below 0.3 €/kgH₂. In contrast, the hybridisation value of SMR is particularly high for the expensive biomethane scenario. In fact, in that case, almost all remaining

Table 5.1: Synthesis for SMR hybridisation value analysis.

Scenario name	Renewable potential (MW)	Geological storage	Biomethane price (€/MWh)	CH ₄ average price after 2020 (€/MWh)
Unlimited renewables	∞	No	105/90/75	27
Geological storage	300	Yes	105/90/75	27
Unlimited + storage	∞	Yes	105/90/75	27
Expensive natural gas	300	No	105/90/75	67
Expensive biomethane	300	No	110/100/90	27

SMR capacity is improved with CCUS to reduce CO₂ emissions. Then, the hybridisation value is similarly a bit lower (around 0.55 €/kgH₂) for unlimited renewables potential and geological storage scenarios, with higher emissions for the unlimited potential one, meaning that these two configurations bring the same kind of flexibility to the system. When combining both scenarios (unlimited renewable potential and geological storage), the hybridisation value of SMR decreases to around 0.45 €/kgH₂. For reference, the SMR flexibility value for the reference case was evaluated around 0.74 €/kgH₂.

For variants, we can see trends: with a more expensive carbon tax, the hybridisation value of the SMR is reduced by 0.06 €/kgH₂ in average (-10%) for all scenarios, and the CO₂ emissions also decrease. For the cheap carbon treatment variant, we can point out two things: it increases the SMR hybridisation value by 0.12 €/kgH₂ in average (+21%), which was expected as it increased the competitiveness of SMR + CCUS, and it reduces total CO₂ emissions. Indeed, with that variant, it becomes interesting to install SMR + CCUS 90%

In Figure 5.3, the values presented are the average values for all periods. In Figure 5.4, the SMR hybridisation values are presented for the period. We see that the hybridisation value decreases over time. For the second period (2030-2040), if we exclude the expensive natural gas scenario, it varies between 1 and 2 €/kgH₂, while in the last period (2050-2060), the value is between 0.25 and 0.5 €/kgH₂ for all scenarios. This is to be expected, as electrolysis has a large share of the production in all scenarios in the last period.

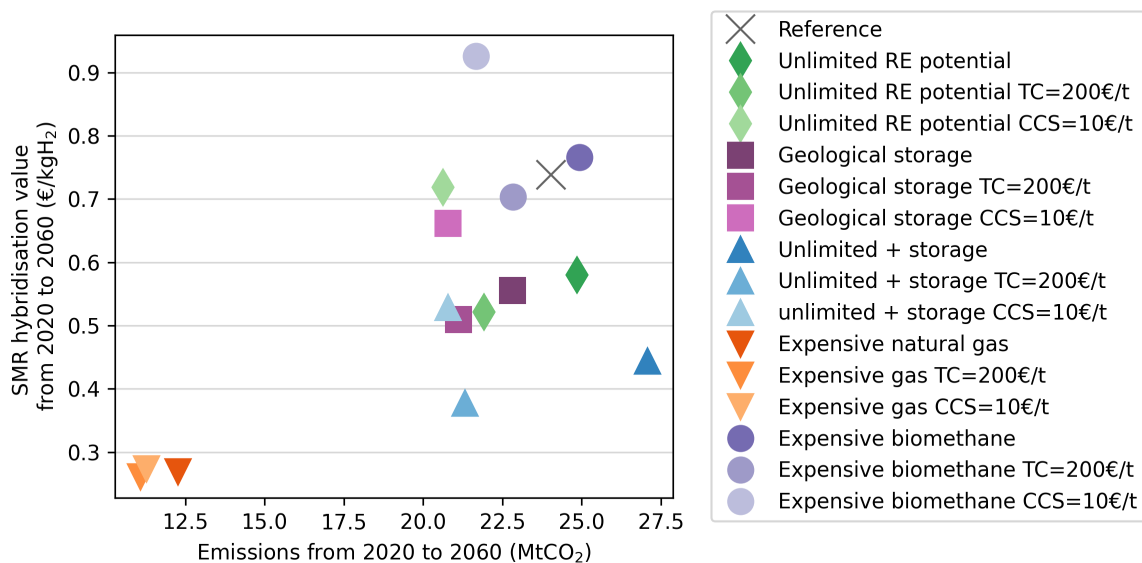


Figure 5.3: SMR average hybridisation value for the planning horizon for the unlimited renewables potential scenario, the geological storage scenario and the unlimited potential + geological storage scenario, with variant with carbon tax more expensive and carbon treatment less expensive.

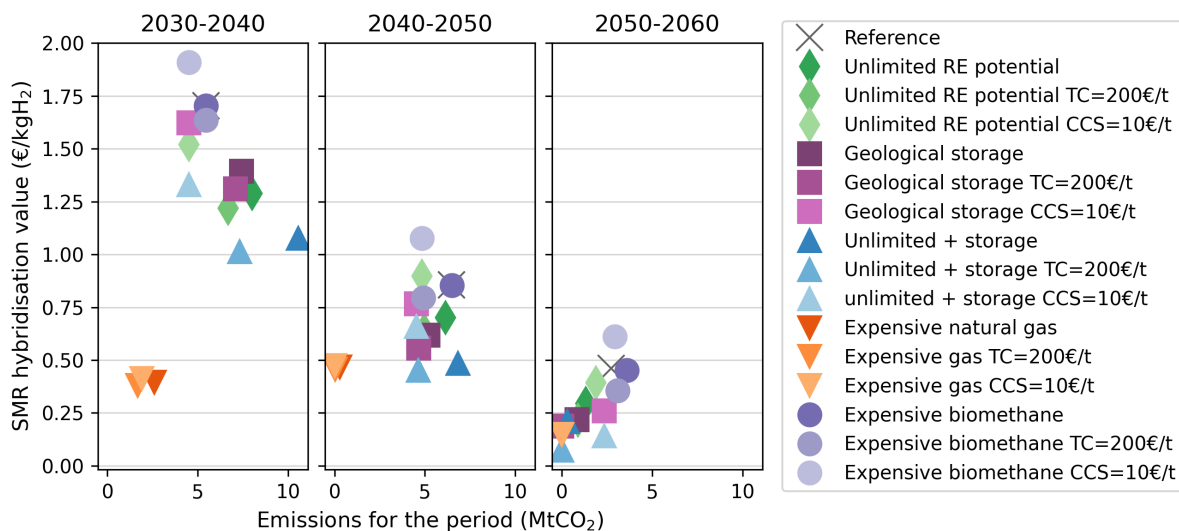


Figure 5.4: SMR hybridisation value per period for the unlimited renewables potential scenario, the geological storage scenario and the unlimited potential + geological storage scenario, with variant with carbon tax more expensive and carbon treatment less expensive.

5.4 Conclusion

In this chapter, we emphasise the key role that the existing steam methane reformer can play in the transition to keep hydrogen competitive. Because of the flexibility they bring to the system, maintaining the SMR helps decrease hydrogen LCOH. We defined the SMR hybridisation value as

the average LCOH difference between a system with SMR and a system where SMR are prevented, and all other parameters equal. For the reference scenario presented in Chapter 3, the hybridisation value of the SMR can be estimated at 0.74 €/kgH₂, i.e. 32% savings. This value can decrease below 0.3 €/kgH₂ if the natural gas is five times more expensive than the observed prices in 2019.

We point out that this hybridisation value is especially high in the 2030-2040 period and then decreases over time. Moreover, in the short or medium term, there will be fierce competition in Europe to access low-carbon hydrogen, and the electrolysis deployment rate may not be sufficient to supply the demand.

In the long term however, we must be careful not to develop incoherent uses of gas feedstock (be it natural gas or biomethane). Indeed, it would not make sense in most cases to produce hydrogen from CH₄ while doing methanation to produce CH₄ from H₂ at the same time. This could justify, say, by 2040, making the choice of closing SMR.

Schéma de raccordement optimal des EnR et des électrolyseurs - Résumé

Ce chapitre étudie les schémas de connexion optimaux entre les électrolyseurs et une zone de production d'électricité renouvelable dans le contexte d'un cluster industriel. Il s'agit de comprendre comment les choix en matière de transport de l'énergie influent sur les coûts de production de l'hydrogène, en examinant en particulier s'il convient de produire l'hydrogène à proximité des zones de consommation ou à proximité des zones de production d'électricité renouvelable.

Quatre schémas de connexion différents sont comparés :

- Électrolyseurs et énergies renouvelables dédiées (potentiel limité) dans la zone industrielle (ZI).
- Énergies renouvelables dédiées (potentiel illimité) à distance dans la zone d'énergies renouvelables (ZR), connectées à la ZI via le réseau électrique.
- Électrolyseurs et énergies renouvelables dédiées dans la ZR avec transport de l'hydrogène vers la ZI par un pipeline.
- Électrolyseurs et énergies renouvelables dédiées dans la ZR avec un grand stockage souterrain d'hydrogène également dans la ZR.

Les scénarios tiennent compte d'un potentiel renouvelable limité dans ZI, d'un potentiel illimité dans ZR et de la distance entre les zones. L'étude vise à identifier la configuration la plus rentable et la plus efficace pour la production d'hydrogène en tenant compte des différents potentiels renouvelables et des infrastructures de transport. En analysant les coûts du réseau et les configurations du système, elle donne un aperçu des compromis entre le déploiement de l'électrolyse et des énergies renouvelables à différents endroits.

Le coût de la production d'hydrogène varie entre 3,7 €/kgH₂ et 3,9 €/kgH₂ en fonction de la localisation des électrolyseurs et de la source d'électricité nécessaire à leur alimentation. Si un stockage massif d'hydrogène, tel que des cavités salines, existe à proximité de la production d'hydrogène, l'option la moins chère consiste à produire de l'hydrogène à proximité de la production d'électricité, à utiliser le stockage pour compenser la variabilité de la production, puis à transporter l'hydrogène jusqu'au lieu de consommation. Toutefois, dans une configuration où le stockage de l'hydrogène n'est pas disponible, la solution optimale dépend du contexte.

Avec l'hypothèse considérées, en dessous de 150 km, il est moins coûteux de construire des électrolyseurs à proximité de la zone de production d'électricité renouvelable et de transporter l'hydrogène. Au-delà de 150 km, le transport de l'électricité est plus intéressant. D'autres paramètres tels que les coûts de renforcement du réseau ou la possibilité de valoriser l'électricité excédentaire sur le marché peuvent également entrer en ligne de compte.

Chapter 6

Electrolysis and renewables optimal connection scheme

In the previous chapters, we pointed out that the optimal electrolyser deployment would include a dedicated renewable electricity supply. However, in the context of an industrial cluster, the available space to build renewable electricity production units is the limiting factor. Renewable electricity production units can be built further away, but in that case a choice has to be made between transporting the electricity and transporting the hydrogen.

In this chapter, we give some insightful elements about the development of electrolysis at the scale of an industrial cluster with respect to the availability of renewable/low-carbon electricity. The objective is to understand the impact of energy transportation on hydrogen production costs and the trade-off between producing hydrogen close to the hydrogen consumption zone or close to the renewable electricity production zone. To do so, we compared four different connection schemes for electrolyzers.

6.1 Description of the scenarios

For this particular study, the investment trajectory was not investigated. We take only one investment period (from 2020 to 2030) and one operation period : 2030-2040. We define two different zones: the industrial zone (ZI), where hydrogen consumption occurs corresponding to the Fos-sur-mer industrial harbour presented in Chapter 3, and the renewable electricity production zone (ZR), where the space to install renewables is considered unlimited. In the industrial zone, the renewable potential is limited to 250 MW in 2030 (100 MW for solar and 150 MW for wind onshore). The renewable zone is 150 km away from the industrial zone and there is the possibility to develop underground salt caverns (which corresponds to the real geological site of Manosque in the south of France). We consider a base-load hydrogen consumption of 525 MWh/h for the target period 2030-2040 (see Chapter 3 for details). The four different configurations investigated are presented in Fig. 6.1.

The first configuration is the reference scenario presented in chapter 3. In this scenario, the electrolysis capacity is located in ZI, as are the renewable capacities, directly connected to the

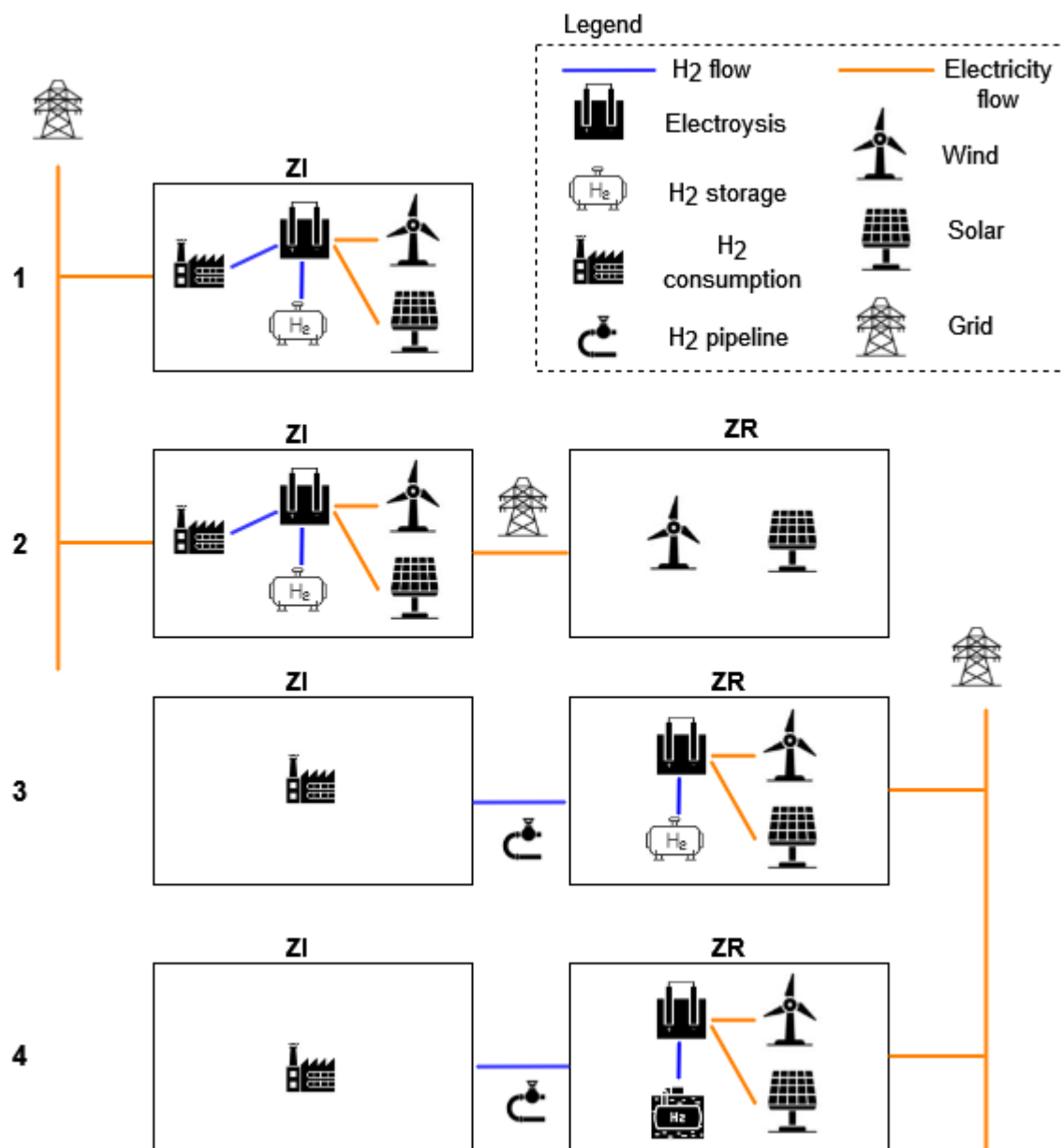


Figure 6.1: Graphic representation of the four investigated connection schemes.

electrolysers. In the second configuration, it is possible to install distant renewable electricity production means in ZR where the potential is much bigger. In that case, renewables are connected via the existing electricity network, and the network access rights have to be paid. In the third scenario, the electrolysers are located in the renewable zone, and the hydrogen has to be transported from ZI to ZR. To do so, a hydrogen pipeline has to be installed. Finally, in the last configuration, the electrolysers are also located in ZR but we also consider the presence of a large underground hydrogen storage in ZR. In all scenarios, electrolysers are also connected to the electricity network and the quantity of electricity imported from the grid at market price is optimised. Table 6.1 recaps the location of technologies for each scenarios.

Table 6.1: Location of the technologies for all scenarios.

Scenario	electrolysers	Renewables	H ₂ storage	H ₂ pipe
Scenario 1	ZI	ZI	Tank in ZI	-
Scenario 2	ZI	ZI & ZR	Tank in ZI	-
Scenario 3	ZR	ZR	Tank in ZR	150 km
Scenario 4	ZR	ZR	Underground in ZR	150 km

6.2 Network costs

The electricity network access cost is divided in two parts : a fixed part proportional to the power of the connection to the transmission network and a variable part proportional to the quantity of electricity flowing through the connection. The fixed part represent the distribution among the users of the cost of maintaining and improving the grid. We use the current network cost for the french transmission network, which is calculated every year by the french TSO [105]. The electricity network cost can be written as follow:

$$\sum_{t,h} \left[\theta_{h,t} I_{y,t,r} + (PS_{y,h} - PS_{y,h-1}) \psi_h \right] \quad (6.1)$$

where $\theta_{h,t}$ is the variable network cost for time slot h , $PS_{y,h}$ the maximum power of the connection to the grid for time slot h and ψ_h the fixed network cost for time slot h . In France, the grid access cost is different depending on the time slot considered. Usually, for industrial consumers there are five time slots: peak hours, winter/summer stress hours and winter/summer off-peak hours from the most expensive to the less expensive. The cost depend on the stress on the grid. Note that the fixed cost for time slot h is applying to the capacity difference between time slot $h - 1$ and time slot h where the time slot $h - 1$ is the one just a notch less expensive than the time slot h .

The hydrogen network costs are found in [23]. We take the cost for a new pipe capacity of 900mm of diameter with 75% compression capacity (3.6 GW H₂ (LHV)). With these hypotheses, the pipe cost depend on the distance as follow: 2.3 M€/km.

6.3 Results and discussion

Fig. 6.2 shows the optimised installed capacities of the production technologies for the four different configurations. The orange and purple bars represent renewable electricity production capacities. The green bars show electrolysis capacities with the respective load factors. In scenario 1, the electrolysis capacity is oversized to make the most of the limited local renewable electricity production. That's why the load factor is the smallest among all the scenarios. In this case, only 10% of the electricity used to power the electrolyzers comes from dedicated renewable electricity production, the rest is sourced on the market. This number goes up to 77% at in scenario 3, which is the one with the highest dedicated renewable electricity production capacity. Figure 6.3 shows the hydrogen production distribution between dedicated renewable electricity based electrolysis, grid based electrolysis and hydrogen importations, with the percentage representing the share for each. We can see that as scenario 1 is the one with the less potential for dedicated renewables, the share of hydrogen importations reach 23%, while it is only around 10% in scenario 2 and 3 and less than 1% in scenario 4.

In scenario 2, compared to scenario 3, the total capacity of dedicated renewable electricity production is a little bit smaller because of network costs that need to be paid for electricity transmission between ZR and ZI. It makes the market electricity and hydrogen imports a bit more interesting. Scenario 2 and 3 have a similar production mix with respectively 68% and 71% of renewable electricity based electrolysis, 22% and 21% of grid based electrolysis and respectively 9% and 8% of importations. We can conclude that with the chosen hypotheses there is not a big difference between transporting electricity or transporting hydrogen for a distance of 150 km. For both scenarios, the curtailment of the renewable production (lost electricity because it can't be used for electrolysis), is around 46 GWh, i.e. around 1% of the maximum renewable production.

Now, if we compare scenario 3 and scenario 4, we see that underground long term storage allows to reduce the investments in dedicated renewable electricity capacities by 28% as well as electrolysis capacity by 16%. The flexibility brought by the long term storage allows to decrease renewables curtailment to only 0.3% (13 GWh/yr) even without any valorisation of the surplus on the market. It is the scenario with the highest charge factor for electrolysis (55%), and the one that makes the most of the low electricity grid prices with 34% of grid electricity based electrolysis.

Fig. 6.4 shows the cost breakdown for all the investigated scenarios. As expected, for all scenarios, electricity supply account for a big part of the hydrogen cost, ranging from 36% to 65%. In this study, we compare three different electricity sources: the electricity market (scenario 1), the delocalised renewable electricity production with electricity transportation (scenario 2) and the delocalised renewable electricity production with hydrogen transportation (scenario 3). In scenario 1, the electricity mainly comes from the grid while in the other scenarios, it comes from dedicated renewable electricity production. As only low carbon production technologies are considered, we note the small share of the cost coming from the carbon tax.

With the electricity mix we considered (31% of renewables in 2030), hydrogen is the most expensive in scenario 1 and 3, at respectively 3.89 and 3.91 €/kgH₂. Hydrogen costs in scenario 2 and scenario 4 are a little bit lower, around 3.7 €/kgH₂. However these costs could significantly change if the excess renewable electricity production were to be sold on the market or if the distance

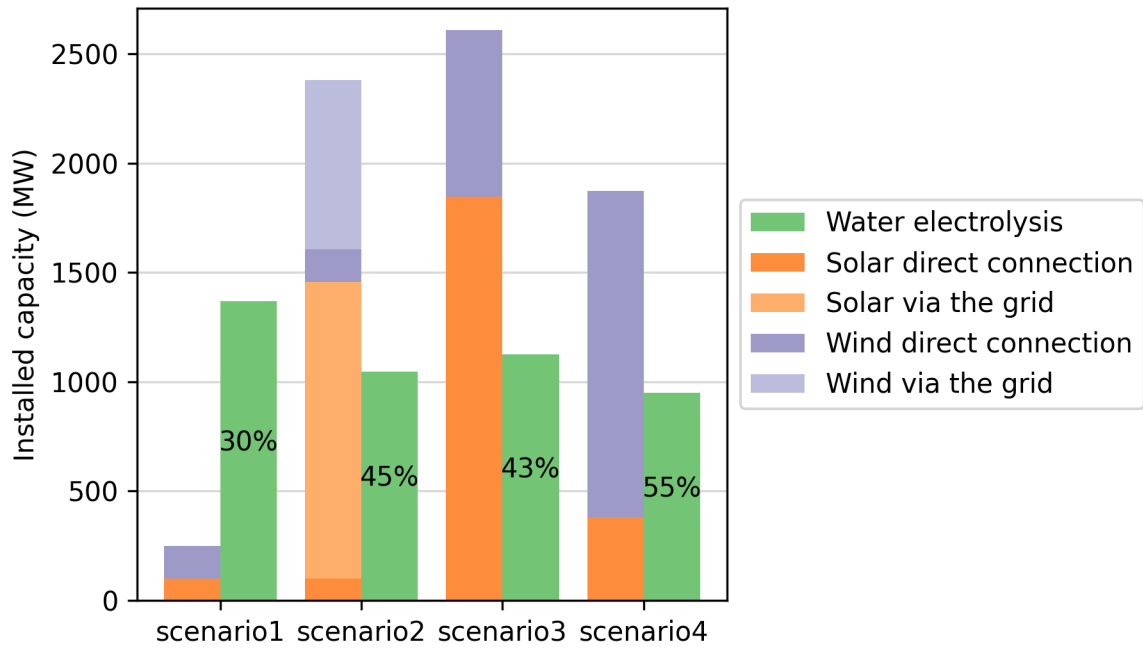


Figure 6.2: Optimised production capacities with load factors for electrolysis.

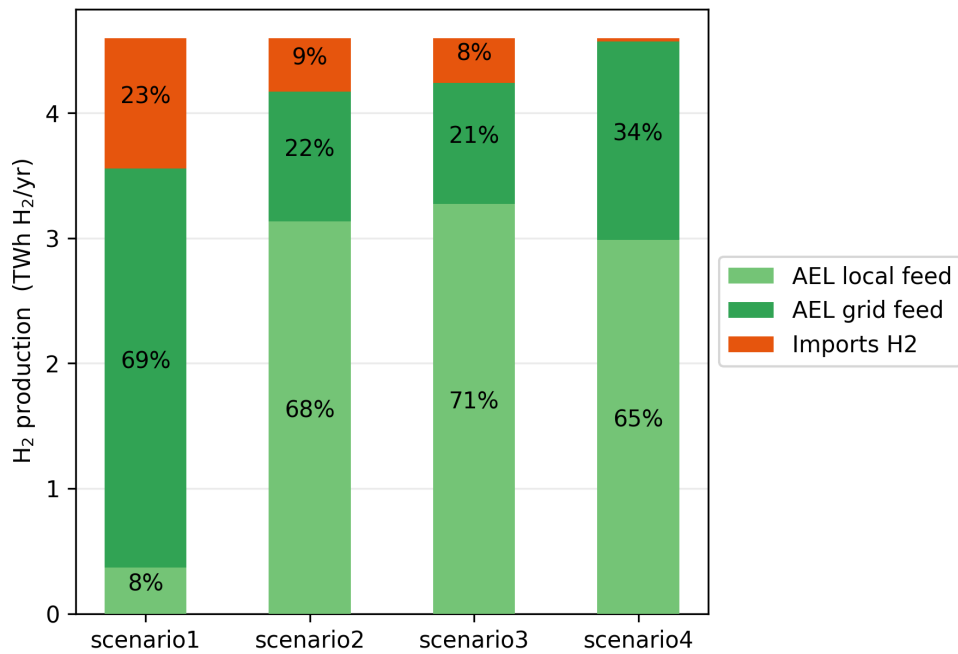


Figure 6.3: Optimised distribution of the hydrogen production.

between the two zones were to change. We note that even if the cost structure is different for all the scenarios, the final levelised cost of hydrogen is really close.

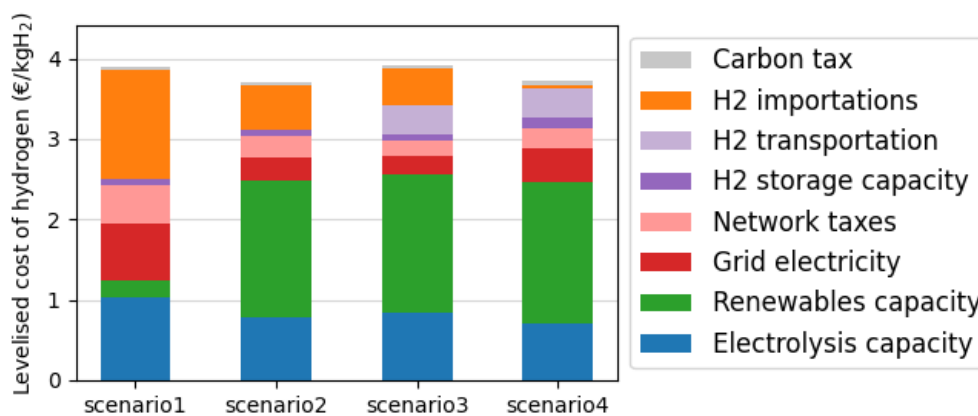


Figure 6.4: Comparison of the levelised cost of hydrogen breakdown between the different scenarios.

6.4 Effect of electricity and hydrogen transmission costs

Network costs are divided in three categories : a fixed part of the electricity network cost proportional to the grid connection power, a variable part of the electricity network cost proportional to the quantity of electricity flowing through that connection and the hydrogen pipeline CAPEX and OPEX (including the compression needs), considered proportional to the length of the pipeline.

We found that the total network costs range between 0.26 €/kgH₂ in scenario 2 and 0.60 €/kgH₂ in scenario 4, which account from 7% (scenario 2) to 16% (scenario 4) of the final hydrogen cost. Those costs are differently distributed between the three categories depending on the scenario, as shown in table 6.2.

Table 6.2: Distribution of networks costs for each scenario.

Scenario	Electricity network tax		H ₂ pipeline
	Variable	Fixed	
Scenario 1	81%	19%	0%
Scenario 2	19%	81%	0%
Scenario 3	22%	12%	65%
Scenario 4	31%	9%	59%

We found that for the scenarios where hydrogen is transported (scenario 3 and scenario 4), the cost distribution ranges from 59% to 65% for the hydrogen pipeline, 9% to 12% the grid connection (fixed part of network taxes) and 22% to 31% for the use of the connection (variable part of the network taxes).

6.5. SENSITIVITY TO THE DISTANCE BETWEEN THE INDUSTRIAL CLUSTER AND THE RENEWABLE ELECTRICITY PRODUCTION

If we compare the scenarios where electricity is transported (scenario 1 and scenario 2), we see that the distribution between the fixed part and the variable part of the electricity network cost is opposed. In scenario 1, the power capacity of the connection for the peak time slot is more than triples compare to scenario 2 (2.05 GW against 552 MW). In scenario 2, the connection is used more unsteadily because most of the electricity flowing through is coming from renewable sources, while for scenario 1, the connection is used with a base-load profile. Because in scenario 1 the use of the connection has a flatter profile, the biggest part of the cost is carried by the fixed part, when it is the opposite for the scenario 2.

6.5 Sensitivity to the distance between the industrial cluster and the renewable electricity production

As previously mentioned, the cost of the hydrogen pipeline is highly sensitive to distance. We investigated this sensitivity by varying the distance between ZI and ZR from 10 km to 500 km. Fig. 6.5 shows the results of this analysis. We see that transporting hydrogen (scenario 3) is more interesting than transporting electricity (scenario 2) for distances shorter than 150 km. If underground hydrogen storage is present (scenario 4), the transport of hydrogen is more interesting up to 250 km.

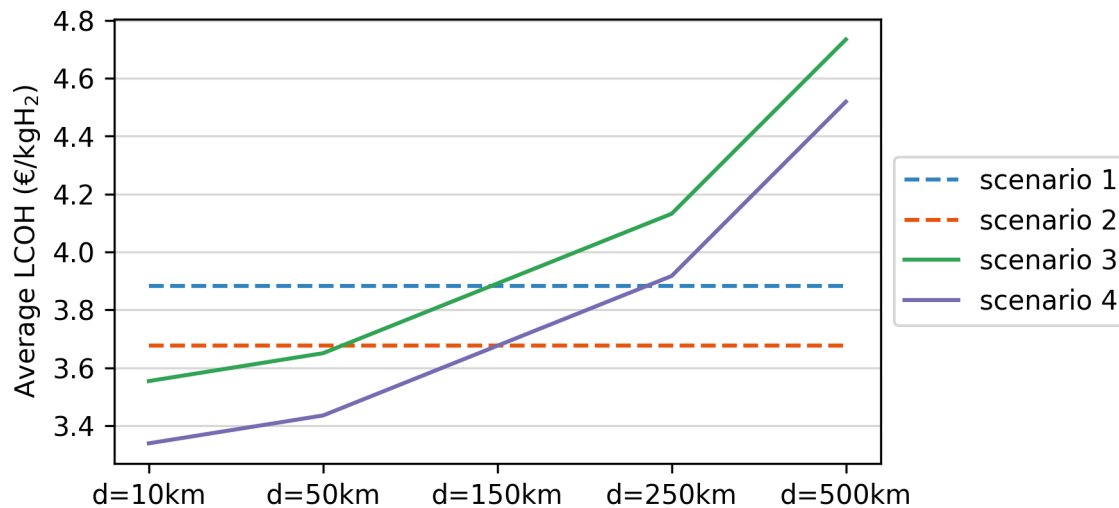


Figure 6.5: Sensitivity analysis of the levelised cost of hydrogen to the distance between the industrial zone and the renewable zone

Note that in Scenario 2 we considered that renewable electricity flows from ZR to ZI through the existing grid. Grid reinforcement costs are taken into account through the fixed part of the network cost, but are proportional to the connection capacity, not to the distance. That is why the distance between the two zones does not impact the hydrogen cost.

6.6 Sensitivity to the electricity network tax

Another parameter that can have a significant impact on the results is the price of the electricity network cost. To evaluate the sensitivity of our results to the electricity network cost, the fixed part of the cost was divided by two and multiplied by two for all scenarios. It could represent the optimist and pessimist grid reinforcement cost hypothesis.

We can see in Fig. 6.6 that this parameter impacts more significantly scenarios 1 and 2 for which more electricity is flowing through the grid. No major changes in the order of hydrogen costs are observed. However, with the optimist hypothesis, scenario 2 would be more interesting than scenario 4, and with the pessimist hypothesis, hydrogen becomes especially expensive in scenario 1.

For a distance of 150 km, we can conclude that it is always more expensive to transport hydrogen (scenario 3) than to transport electricity (scenario 2). However, if a large storage is present close to the hydrogen production site, it can become interesting to transport hydrogen instead of electricity. We should keep in mind that the electricity network tax changes every year and it is difficult to predict its value in 2030.

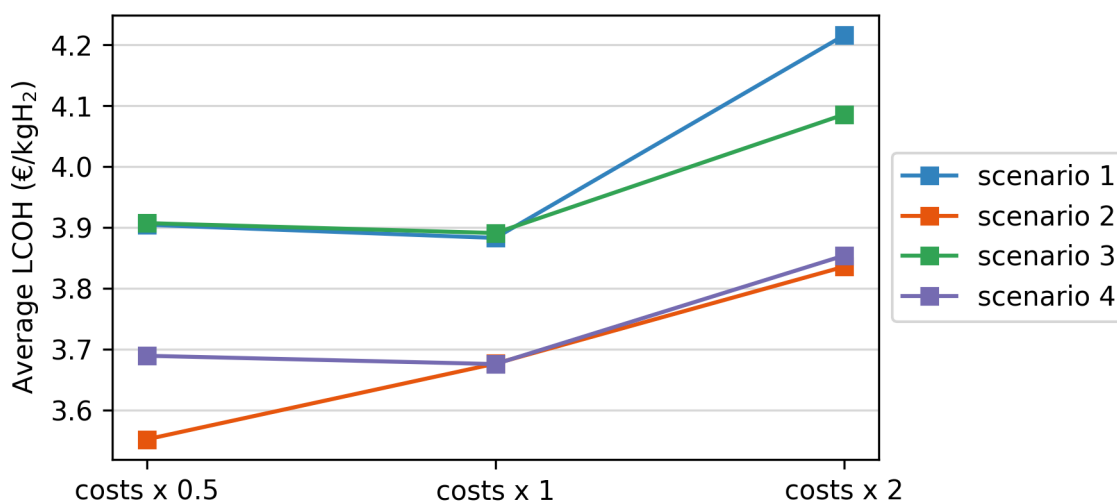


Figure 6.6: Sensitivity of the levelised cost of hydrogen to network taxes.

6.7 Conclusion

The cost of hydrogen production varies between 3.7 €/kgH₂ and 3.9 €/kgH₂ depending on the location of the electrolyzers and the source of the electricity needed to power them. If massive hydrogen storage such as salt caverns exists close to hydrogen production, then the cheapest option consists of producing hydrogen close to electricity production, using the storage to compensate for the variability, and then transporting the hydrogen. However, in a configuration where hydrogen storage is not available, the optimal solution depends on the context. With the considered hypothe-

ses, below 150 km, it is cheaper to build electrolyzers close to the renewable electricity production zone and transport hydrogen. Over 150 km, transporting the electricity is more interesting. Other parameters such as network reinforcement costs or the possibility to valorise excess electricity on the market can also come into play.

Conclusions et perspectives - Résumé

L'hydrogène est reconnu par les communautés publique et scientifique comme un élément crucial du futur paysage énergétique pour réduire les émissions de carbone. Toutefois, son statut actuel de produit chimique principalement utilisé dans l'industrie signifie qu'il est nécessaire de disposer d'outils de planification complets pour optimiser son déploiement en tant que vecteur énergétique. La littérature existante manque d'études détaillées sur la transition du système énergétique actuel vers un système optimisé. La plupart des modèles de planification à long terme sont limités par l'agrégation temporelle et spatiale et négligent le couplage énergétique.

Ce travail propose une méthodologie pour modéliser l'évolution des écosystèmes hydrogène à l'échelle locale en tenant compte de l'évolution de la demande, des facteurs technico-économiques et des contextes politiques. L'effort principal de modélisation consiste à développer un modèle d'expansion des capacités, multi-énergies dans un processus en trois étapes. Cette approche intègre la demande locale, les contraintes et les actifs existants.

L'estimation des prix horaires de l'électricité sur le réseau, cruciale pour le déploiement de technologies de production basées sur l'électricité comme l'électrolyse, est un défi essentiel à relever. Les incertitudes liées à l'évolution du marché de l'électricité nécessitent des méthodes pour obtenir les prix du réseau, ce que ce travail permet de faire en optimisant le fonctionnement du réseau national sur la base des capacités projetées.

L'étude se concentre sur le port industriel de Fos-sur-mer en France en raison de son économie historique basée sur le pétrole, ce qui le rend pertinent pour l'examen des stratégies de déploiement de l'écosystème de l'hydrogène. La proximité de sites géologiques appropriés pour le stockage du gaz et de capacités de production d'électricité renouvelable renforce encore sa pertinence en tant que zone d'étude. En estimant la demande d'hydrogène entre 2020 et 2060 et en tenant compte de diverses contraintes, l'étude déduit les trajectoires d'investissement optimales, les stratégies d'exploitation, les coûts du système et les incidences sur l'environnement.

Un scénario de référence basé sur des paramètres économiques réalistes est établi, et les résultats montrent qu'une combinaison optimale de production d'hydrogène entre l'électrolyse et le reformage du méthane (SMR) avec 50% de capture du CO₂ est viable. Les capacités de SMR adopteront des unités de capture du carbone d'ici 2030, tandis que l'intégration de l'électrolyse se fera plus tard en raison des coûts élevés associés à l'électricité renouvelable.

Des analyses de sensibilité sur des facteurs clés tels que les prix du gaz, le prix des technologies, le potentiel des énergies renouvelables et les politiques en matière de carbone, révèlent une combinaison résiliente d'électrolyse et de SMR dans divers scénarios. Le développement parallèle de

l'électrolyse et des capacités renouvelables renforce la robustesse du système. Pour mieux analyser le service que peut rendre le SMR au système, un indicateur représentant la différence de coût avec et sans intégration du SMR est défini (0,74 €/kgH₂ dans le scénario de référence). Toutefois, cette valeur varie en fonction de facteurs tels que les coûts du gaz naturel et la proximité des sites de stockage, ce qui a un impact sur la combinaison technologique optimale.

La méthodologie développée fournit des informations précieuses sur le territoire étudié mais présente des limites qui doivent être prises en compte pour l'améliorer. Il est nécessaire de quantifier les avantages de la résolution horaire dans l'optimisation du système et d'étendre le modèle à une version multi-nœuds pour une meilleure modélisation des prix de l'électricité, en incorporant les interconnexions électriques mondiales et les variations météorologiques.

L'inclusion de facteurs tels que les accords d'achat d'électricité pour les électrolyseurs et la modélisation de l'infrastructure de transport de l'hydrogène peuvent conduire à une réduction des prix de l'électricité, favorisant ainsi le déploiement de l'électrolyse. La concurrence entre l'utilisation du stockage stratégique local et mondial doit également être étudiée.

La caractéristique incertaine des nombreuses hypothèses appelle à l'optimisation stochastique ou robuste. Des améliorations dans la modélisation de la demande, l'inclusion de diverses technologies (par exemple, le craquage de l'hydrogène, le reformage auto-thermique, l'électrolyse PEM), la prise en compte détaillée des impacts environnementaux et l'optimisation multicritères sont suggérées pour une analyse plus complète.

Le modèle d'optimisation multi-énergies existant peut intégrer des vecteurs énergétiques supplémentaires tels que la chaleur, l'ammoniac et le CO₂ pour une meilleure modélisation du traitement du CO₂ en aval. La prise en compte de facteurs non économiques tels que le bien-être social, les risques de sécurité et les impacts environnementaux est cruciale et pourrait être intégrée par les biais de techniques d'optimisation multicritères.

Les outils et la méthodologie développés sont génériques et évolutifs, encourageant des méthodes systématiques et automatiques utilisant des systèmes d'information géographique pour analyser les scénarios énergétiques sur différents territoires à l'échelle mondiale, relevant ainsi le défi de la régionalisation des stratégies énergétiques de manière efficace.

Chapter 7

Conclusion and perspectives

7.1 Conclusion

7.1.1 Contributions

It is commonly agreed among public and scientific communities that hydrogen will be a part of the future energy mix to help decarbonise society. However, today hydrogen is not an energy carrier but a chemical product that is used mainly in industry. With the diversity of hydrogen production pathways, storage technologies, and transportation technologies, as well as dependencies on other energy resources, there is a need for planning tools to optimise hydrogen deployment. According to the literature review, few works have studied the transition path between the existing energy system and an optimised system in the future. Moreover, most of the existing long-term planning models are temporally and spatially aggregated, and do not consider energy coupling.

In this work, we proposed a methodology to simulate the evolution of hydrogen ecosystems at a local scale given the evolution of hydrogen demand and the techno-economic and political contexts. The main part of the modelling effort is the development of a multienergy capacity expansion model. Our three-step methodology allows us to take into account local demand and constraints and to consider the existing assets of the studied territory. To easily modulate the model by adding constraints and varying the parameters, we chose to develop an in-house integrated single node planning and operation model.

A major challenge in this work was the estimation of hourly grid electricity prices, which is an essential part of the modelling. Indeed, it was important to take into account the evolution of the electricity grid which is expected to happen in the next 30 years to discuss the deployment of electricity-based production technologies such as electrolysis. However, the evolution of the electricity market is uncertain. In our methodology, we presented a method to obtain grid prices by optimising the operation of the national grid based on projected installed capacities.

In this work, we were able to discuss the role of hydrogen in the energy transition in the industrial sector. The territory that was chosen to develop and test the methodology throughout this work was the industrial port of Fos-sur-mer in the south of France. With its historically oil-based economy, this territory is a good case study for examining the key characteristics that can have an impact on the hydrogen ecosystem deployment strategy. Moreover, the area is favourable

to the deployment of renewable electricity production capacities and is close to a geological site suitable for gas storage (both for hydrogen and natural gas).

For this territory, we estimated the evolution of hydrogen demand from 2020 to 2060 and looked for the optimal supply chain needed to satisfy it considering economical, environmental, social, political, geopolitical, and technological constraints. We were able to obtain the optimal investment trajectory, the optimal hourly operation of the system for each period, the costs of the system and the environmental impact of the system.

7.1.2 Synthesis of the analyses

First, we define a reference scenario built using the economic parameters that we found to be the most realistic in the literature. The results show that in the considered techno-economic context, the optimal final hydrogen production mix is evenly distributed between electrolysis and SMR with 50% CCUS. From 2030 onwards, the existing conventional SMR capacities are equipped with carbon capture units; electrolysis arrives later (from 2040). The average levelised cost of hydrogen including production and storage is found to be 2.3 €/kgH₂, with an electrolysis load factor of around 30%. The limiting factor for the deployment of electrolysis seems to be the need for lower electricity prices resulting from a highly renewable mix, in which case the optimal deployment strategy for electrolyzers would be to connect them directly to dedicated renewables or to use them when renewables are marginal on the market.

In a second phase, we used sensitivity analysis to examine our assumptions for fundamental factors such as gas prices, CAPEX parameters for different production units, renewable resource potential of the area, and carbon regulation policy, among others. We also tested the robustness of different scenarios by stressing them with unanticipated events. We highlighted two points:

- in spite of the uncertainties, the hydrogen production mix tends to be a combination of electrolysis and SMR
- scenarios where electrolysis capacities are developed in parallel with dedicated renewable capacities tend to be more robust than others.

In light of these results, we defined an indicator for the value of SMR hybridisation, representing the hydrogen production cost difference between a system with and without SMR (all other parameters being equal). The SMR hybridisation value was found to be 0.74 €/kgH₂ for the reference scenario, but this value can be lower depending on the context. For instance, if natural gas is expensive or if there is suitable geological storage close to the hydrogen production site.

The conclusions of both the sensitivity analyses and the SMR hybridisation value analysis pointed out that electrolysis capacities should be fed with renewable electricity. In many cases, the renewable electricity potential might not be located near the hydrogen consumption site. This led us to study in greater detail the connection between electrolyzers and dedicated renewable electricity production capacities when they are not directly connected, and the trade-off between building electrolyzers close to electricity generation or close to hydrogen consumption sites. The results show that for the period 2030-2040, for separation distances of less than 150 km, it is more cost effective to locate electrolysis at the renewable generation site and transport hydrogen. With

the added possibility of installing a large volume of hydrogen storage at the demand site, this configuration remains attractive for separation distances of up to 250 km.

To conclude, we highlight three key attributes of a territory favourable to the deployment of a hydrogen ecosystem: a high industrial hydrogen demand (especially if there are existing production assets in the territory), large potential renewable energy resources, and significant geological storage located close to the consumption site. It is clear that geography plays a key role in an optimised investment strategy.

7.2 Ongoing work and perspectives

7.2.1 Ongoing work

Thanks to the methodology developed, we were able to obtain a number of insights about the territory of interest. However, this work presents some limitations.

First, it would be useful to quantify the advantage of having an hourly resolution for the optimisation of the operation of the system by doing a convergence study. If the number of time steps could be reduced without significant loss of precision, this would allow for the same analyses to be carried out with a reduced computational burden. The possibility of changing the time step has been implemented in the model, but this analysis is incomplete at the time of writing.

We also began to work on a multi-node version of the model. A global geographic scale can improve the modelling of electricity prices by taking into account the effect of electricity interconnections with neighbouring countries and other flexibility means, the importance of which should not be overlooked [35]. Moreover, a multi-node model would allow for the use of different weather time series depending on the location, and thus enhance analyses with respect to electricity sourcing. Power purchase agreements for powering electrolyzers could also be included. Including these factors could lead to reduced electricity prices, which would in turn point towards more favourable results for the deployment of electrolysis.

Multi-node modelling would also be useful at a local scale, allowing us to take into account hydrogen transportation infrastructure. An improved modelling of hydrogen interconnections could add significant value to the results. Moreover, large underground storage capacities (such as the site in Manosque) could also be used as strategic storage at a European scale. It would be interesting to investigate the competition between use for the local area and use for the global system. Placing the studied area in a broader context could also allow us to consider the possibility of long distance transportation of hydrogen.

7.2.2 Perspectives

Note that all of the results presented are highly dependent on the chosen hypotheses. For this reason, we have proposed several sensitivity analyses, but it would be beneficial to consider uncertainties in a stochastic or robust optimisation [106]. Further work on the modelling of the weather data could improve the reliability of the results and bring some new elements to the debate.

In the presented work, the modelling of demand was not systematically addressed. We considered an exogenous hydrogen demand assuming that it is a requirement to reduce global CO₂ emissions. It would be interesting to compare hydrogen solutions with other solutions that could also meet the same demand (for example, electrifying or using CH₄ in the DRI steel production process). By endogenising the demand, we could compare hydrogen technologies to alternatives through the optimisation of the energy system as a whole. This would allow us to define priorities in the deployment of infrastructure and different technologies considering their relative costs and environmental impacts.

The modelling could be improved with the consideration of more technologies, for example hydrogen cracking or auto-thermal reforming or high temperature electrolysis. We talked a lot about the importance of maintaining SMR in the system, but another technology might also have a significant value we need to consider in the planning of hydrogen ecosystems. Moreover, the modelling of each technology could be more detailed. For instance, we considered the lifetime of electrolyzers without considering its use. A mixed-integer formulation could be added to the model to take into account technical constraints such as a lower operating bound (SMR and electrolysis depending on the technology).

Furthermore, modelling could also be improved by a life-cycle approach to environmental impacts. In our work, we only take into account fugitive emissions and direct emissions, but it is also essential to consider embodied emissions. Including other types of environmental impact beyond CO₂ emissions would also contribute to the completeness of the study. This approach would bring a new perspectives to the work, especially if combined with improved demand modelling.

The developed optimisation model is multienergy, so everything is ready to add more energy vectors such as heat, ammonia, and CO₂. This would allow us to take into account more coupling between the different vectors. Thus, we could better model the downstream chain of CO₂ treatment.

We can also question the choice of performing the optimisation on purely economic cost factors. Decision makers often consider a variety of other factors such as social welfare, safety risk, visual pollution, and many more. Multi-criteria optimisation could be used to take into account these diverse considerations [58, 107]. It could be really interesting to also consider the territory use with criteria such as land use, water use, or employment because they can be as critical as the cost of the system.

The tools and methodology are generic, and we purposely developed them in order to be able to use them for other territory and even other countries. It would be interesting to develop systematic and automatic methods, for instance, with the help of geographic information systems, for a large number of territories across the world, as the regionalisation of energy scenarios is an important challenge to be addressed.

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RÉSUMÉ

L'objectif de cette thèse est de développer des méthodes et des outils d'aide à la décision pour assister les acteurs de la transition énergétique à l'échelle territoriale. A travers l'optimisation du système énergétique, notre approche permet d'évaluer le rôle et l'évolution de l'hydrogène, un produit chimique et un vecteur énergétique clef de la transition. Le modèle est adapté à l'étude de l'évolution des *cluster* industriels, où des synergies ont lieu entre les différentes industries. Nous avons testé notre méthodologie sur le cas du port industriel du Fos-sur-mer. Les résultats montrent l'intérêt de faire coexister les technologies fossiles avec l'électrolyse, sensible à l'évolution des prix de l'électricité. A travers différentes analyses, nous avons pu mettre en lumière les facteurs clefs à prendre en compte dans le développement des écosystèmes hydrogène : le prix du gaz, le coût de capture du CO₂ ou encore l'espace disponible pour construire des parcs renouvelables dédiés.

MOTS CLÉS

Coûts actualisés de l'hydrogène (LCOH), Optimisation, Modélisation intégrée, Systèmes énergétiques locaux, Décarbonation industrielle, Couplages énergétiques, Transition énergétique

ABSTRACT

The objective of this thesis is to develop a methodology and tools to help investors and decision makers in the energy transition at the scale of a territory. Through energy system optimisation, our approach allows to understand the role of hydrogen, a key chemical and energy carrier. Our model is especially suitable for studying the evolution of industrial clusters, where synergies can be formed between industries. We tested our methodology on the use case of the evolution of Fos-sur-mer industrial harbour. The results show that there is an interest in keeping fossil fuel based technologies together with electrolysis because it is very sensitive to electricity prices variability. Thanks to different analyses, we learned that the key factors to take into account when developing hydrogen ecosystems are the gas prices, the CO₂ treatment and storage price and the space available to build renewables dedicated to hydrogen production.

KEYWORDS

Levelised cost of hydrogen (LCOH), Optimisation, Integrated modelling, Local energy system, Industrial decarbonisation, Energy coupling, Energy transition