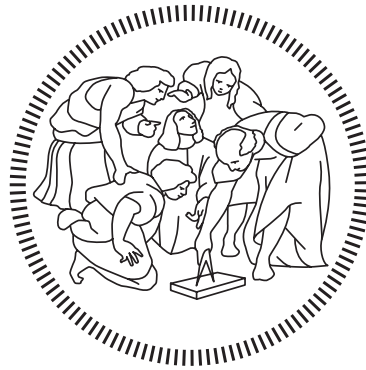


**Politecnico di Milano**

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SCHOOL OF INDUSTRIAL AND INFORMATION ENGINEERING  
Master of Science – Energy Engineering



**Development of an energy model to assess  
the potential role of hydrogen in the Italian  
energy system in a long-term scenario**

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# Sommario

Gli accordi internazionali per il 2030 hanno imposto una copertura dei consumi energetici finali di almeno il 32% da fonti rinnovabili. Per l'Italia il Piano Nazionale Integrato per l'Energia e il Clima (PNIEC) prevede circa il raddoppio della capacità installata di fotovoltaico e eolico rispetto all'attuale, determinando maggiori instabilità nell'equilibrio fra domanda e offerta. In uno scenario al 2050, con gli obiettivi proposti di decarbonizzazione completa, la penetrazione delle rinnovabili è attesa essere molto maggiore, con l'inevitabile sviluppo di eccessi di produzione stagionali. In questa ottica si inserisce la produzione di idrogeno e combustibili sintetici derivati dall'elettricità in eccesso. Tuttavia, la definizione di politiche nazionali efficaci per lo sviluppo e la diffusione di queste tecnologie risulta ostacolata dalla scarsità di previsioni che ne valutino le potenzialità.

In quest'ottica, questo lavoro si pone l'intento di sviluppare un modello pre-esistente e pubblicamente accessibile, implementando i processi emergenti legati alla produzione di idrogeno e suoi derivati. Tale modello è impostato sulla risoluzione di un problema di ottimizzazione lineare, perseguendo l'ottimizzazione delle risorse energetiche utilizzate attraverso la minimizzazione dei soli costi di approvvigionamento. Lo strumento sviluppato risulta quindi idoneo ad analizzare scenari al 2050, restituendo una simulazione di un anno solare con un dettaglio temporale orario. Il modello è applicato al sistema energetico italiano, il quale viene descritto con una risoluzione spaziale nazionale.

Viene così analizzato uno scenario nel quale si persegue la minimizzazione del consumo di risorse fossili (gas naturale) o non gratuite (biomassa), valutando il ruolo della filiera dell'idrogeno non solamente nel settore elettrico ma anche in altri settori come industria e trasporto.



# Abstract

The international agreements for 2030 have imposed a coverage of final energy consumption of at least 32 % from renewable sources. For Italy, the National Energy and Climate Plans (NECPs) made the projection of almost the doubling of the installed capacity of photovoltaic and wind power with respect to the current one, which will cause greater instability in the balance between supply and demand. In a 2050 scenario, with a complete decarbonisation target, the penetration of Renewables (RE) is expected to be much greater, with the inevitable development of seasonal over-generation situations. In this perspective, the production of hydrogen and synthetic fuels deriving from excess electricity is inserted. However, the definition of effective policies for the development and diffusion of these technologies is hindered by the lack of projections that evaluate their potential.

With this in mind, this work aims to develop a pre-existing and publicly accessible model, implementing the emerging processes related to the production of hydrogen and its by-products. The model is set on the solution of a linear optimization problem, pursuing the optimization of the energy resources used through the minimization of the supply costs only. The developed tool is therefore suitable for analyzing 2050 scenarios, returning a year-simulation with an hourly time-step. The model is applied to the Italian energy system, which is described with a national spatial resolution.

A scenario is therefore analyzed in which the minimization of the consumption of fossil resources (natural gas) or non-free (biomass) is pursued, assessing the role of the hydrogen supply chain not only in the power sector but also in other sectors such as industry and transport.





# Extended Abstract

## Introduction

In the most recent period, a growing interest has spread about the necessity to revolutionize the energy system, following a low-carbon emission target.

2030 international agreements set a deeper integration of intermittent Renewable Energy (RE) sources in the energy system to cover at least the 32% of final energy consumption. This determines a high level of instability in the energy grid, managed with higher electrification and battery storage.

From a longer-term perspective, the 2050 time-horizon, a full decarbonization would then be required, imposing a much higher REs presence in the energy system. The need to not waste excess energy produced in peak periods imposes the necessity to decouple production from demand. Electrification and battery storage likely will not be enough. Alternatives like hydrogen would play a key role.

In this context the energy system model presented in the paper was developed. The core of the thesis was to implement *Power to Hydrogen (P2H)* and *Hydrogen to X (H2X)* processes in the existing 2030 NEMeSI model [1], providing an enhanced open-source tool that could investigate role of hydrogen in a long-term scenario.

A consistent literature review on the main existing processes related to hydrogen and the most promising ones was conducted. Through the help of summarized global reports provided by IEA [2], Navigant [3], DEA [4] or SNAM [5], it was possible to frame the situation of hydrogen in energy sector.

From this perspective, a state of the art of the current hydrogen-related technologies is presented, starting from P2H. Water electrolysis is described in its multiple option: from the mature alkaline electrolyzers (AEC), passing through PEM electrolyser and solid oxide (SOEC) to the most recent anion exchange membrane ones (AEMEC) a detailed description is reported [2,6–9].

Thereafter the different  $H_2$  utilization pathways are investigated, from *Hydrogen to Gas (H2G)* with methane synthesis via catalytic thermochemical and biological methanation [6,10,11] to the wider *Hydrogen to Liquid (H2L)* world. Here several synthetic fuels are reported, namely jet-fuel, methanol, Dimethyl Ether (DME) and ammonia.

The former can be obtained from different processes, such as Fischer-Tropsch synthesis [4,12,13] or synthesis from methanol [12,14,15]. Methanol synthesis [14,16–18] and DME production [12,15,19] complete with ammonia synthesis [20–23] the overview of main electric fuel that can be obtained from green hydrogen.

Direct hydrogen utilization in power generation is then described in *Hydrogen to Power (H2P)*, focusing on Fuel Cell technologies currently available. Several technologies are mentioned, such as Alkaline FC, PEMFC, solid oxide ones and phosphoric acid

(PAFC) or molten carbonate based (MCFC) [2, 8].

Then, a literature review for different hydrogen storage option such as compression, liquefaction or transformation into metal hydrides is reported [2, 8, 24–28].

Lastly, to clarify the context in which the implemented model fits, a model classification is provided, highlighting the main features of the different classes.

## Model development

The implemented model is based on the *Oemof* framework [29], a Python-based open source flexible model generator. It allows several settings, enabling different time-step resolution or customized technological levels. It is structured to solve a Linear Programming (LP) optimization problem, with a cost minimization of the overall energy system, by minimizing the total annual cost for primary fuels (e.g. Natural Gas, biomass).

The original version of the model NEMeSI (National Energy Model for a Sustainable Italy), developed by the ReLAB Group of Politecnico di Milano was then enhanced with the implementation of P2H and H2X processes to analyze 2050 scenario.

The model describes the national energy system as a single node, with the zero-dimension (0-D) property, without considering inter-connections or different regional characteristics. It studies the Italian energy system in a 2050 time-horizon, with a year simulation with hourly time resolution.

In Figure 1 the main inputs-outputs of the model are presented, which pursues a cost minimization for the primary fuels.

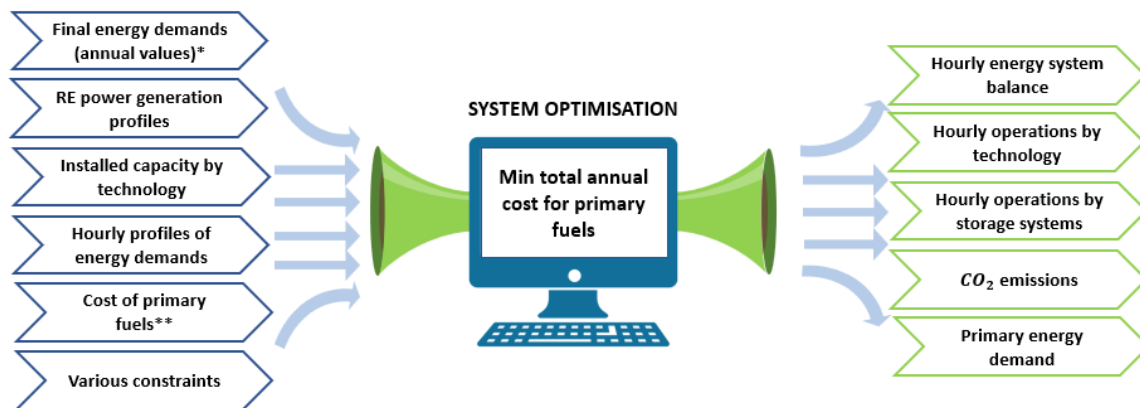


Figure 1. Main inputs and returned outputs of the model; (\*) by energy carrier,  $H_2$ , e-fuels, electricity etc; (\*\*) expressed in €/MWh

The logic structure behind the *oemof* framework can be described through three main concepts, in the model named *bus*, *flow* and *transformer* (Fig. 2). The first represents the commodities of the system, basically energy carriers, and their properties (e.g. emissions related, purchase cost etc). In order to represent the exchanges of the commodity used between different processes, the concept of *flow* is introduced. It expresses the quantity of a specific bus (commodity) that is consumed/produced by a technology. In the model represented flows are energy-based (MWh).

Last concept, the *transformer*, depicts the technology that change the energy carrier's properties. It receives one or more commodities in input and returns in output a

different one (or more) with other common features.

To completely describe an energy system, some other components are still necessary. Basically they are sub-classes of the *transformer* one, namely *source*, *sink* and *storage*. The former provides the information of where the first "raw material" bus comes from, while the second indicates where the last "final product" bus has to be supplied, the final demand. They are characterized by one single flow in output and in input respectively.

However, in a real-life system, generation and consumption are not always perfectly balanced. The *storage* class allows to decouple the supply from the demand, enabling the possibility to store a specific bus for a period of time-steps.

Lastly, two backup flows are implemented, *excess* and *shortage* flows. They come into play when the model cannot completely allocate a bus, like in over-generation situation (excess case), or when it has not enough quantity available of a bus and it has to create it in a fictitious way to fill the gap with the demand (shortage case).

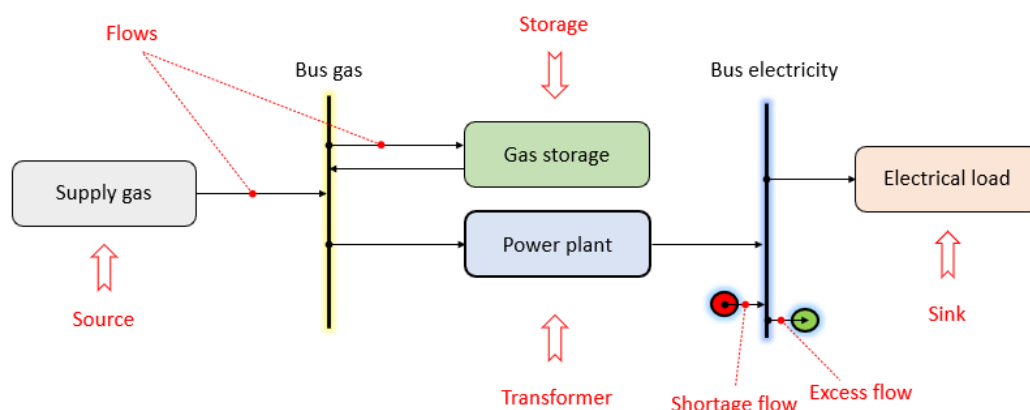


Figure 2. Example of logic structure of buses, flows and transformers

Several background hypothesis were assumed to define the structure of the energy system. The imposition of single technology option for each process described in the model was taken in order to keep the system representation as simple as possible and due to computational time increase issue that would derive from multiple technology options.

An exception was made for hydrogen storage. Due to its low-performing properties at ambient conditions,  $H_2$  requires some transformation. Three possibilities are then compared: physical storage (via compression and liquefaction) and material-based one (switching to metal hydride).

Another assumption is to consider the continued existence of the gas grid infrastructure, being the imported NG likely the only fossil fuel not banned. The grid is then supposed to continue its transmission and distribution role. The origin of the injected gas will be different. *Hydrogen to Gas (H2G)* and blending option are then considered as potential alternatives, such as some bio-based solutions (e.g. biogas upgrading). blending option consists in the injection into the gas grid of a  $H_2-CH_4$  mix with hydrogen content up to 20%vol. To maintain linear the optimization problem, the model has to be free to choose the hydrogen content to inject into the grid. Three different  $H_2$  contents were implemented (0, 10, 20%vol) with three different transformers. A problem of  $CO_2$  emission allocation imposed the implementation of a new customized

*transformer* class.

## Model application

The analysed scenario wants to represent the Italian energy system in 2050. Final consumption, supply sectors and annual profiles data for 2050 were estimated by taking advantage of the knowledge that the RELAB research team has developed during the last 5 years [30–33], comparing with long-term projections and adjusting with some projections made by the Author.

The aim of the scenario is to evaluate the potential role of hydrogen and its by-products in the energy system, pursuing a cost minimization for primary fuels (e.g. biomass and NG). The maximum reduction of fossil NG use is evaluated, with the constraint to avoid shortage situations during the year.

Some assumptions are introduced in order to determine the allocation of  $H_2$  and its by-products in the energy system. Starting from pure hydrogen demand, it is assumed the steel industry and the heavy transport sector as fueled by green  $H_2$ . The former was assumed as constant being steel plant typically always working. The latter, representing trucks and buses, needed some further investigation. First it was necessary to calculate the overall transport consumption, being available international long-term projections represented in aggregated form. The estimated overall transport consumption was divided into road, naval and aviation transport. An uncertainty level regarded the consumption in naval and aviation sector (due to the national v. international travel distinction issue). Considering only national transport, a minor role was attributed to them with respect to road transport.

For the latter, divided into heavy and light transport, where the second was assumed to be electrified and fueled by Dimethyl Ether (DME), two profile curves were estimated. The profile for hydrogen demand was obtained. Remaining synthetic fuel demands were assumed with a constant profile due to lack of information in aviation and naval consumption's partition during the year.

For power demand, that includes the net electrical load, cooling electrical requirement for buildings and demand for Battery Electric Vehicles (BEV) recharge, estimations were conducted by comparing original data with 2050 projections, with an adjusted profile for BEVs demand, as well as for heat demand, taking advantage from previous works of RELAB group [30–33].

For resource availability, the only available fossil fuel was assumed to be fossil NG. Its first round availability was calculated from actual data [34], to be further diminished during the simulations. It is likely overestimated, being the 2050 gas demand much lower due to energy efficiency and higher REs penetration in the energy system.

Regarding the latter, hydroelectric power and geothermal heat&power are unlikely expected to increase in installed capacity. The 2030 values of PNIEC [35] are confirmed. For biogas availability the same consideration are made, assuming to maintain the 2030 level available from literature review. The introduction of new H2G processes (e.g. biological methanation) modified biogas allocation, previously used mainly for upgrading and small Combined Heat-Power plants.

Strong variations were assumed in wind and Photovoltaics (PV) power generation.

Italian 2030 PNIEC [35] estimates almost a doubling for PV and wind power capacity with respect to today installed one to cover the 32% of total final consumption. In a 2050 scenario, estimations are more critical, due to the net decarbonisation target. Uncertainty is derived by the necessity to overcome the fossil NG availability reduction with synthetic alternatives. Higher green  $H_2$  requirement imposes high power availability in over-generation situations.

Regarding the installed capacity for the processes and storages already existing in the original NEMeSI version, basically the proportions were maintained the same as for 2030, by adjusting them to cover the 2050 final consumption. For the new P2H and H2X implementations, uncertainty was related to their very low or absent diffusion in the Italian energy system to date.

The installed capacity were calculated in order to be able to process and store the quantities required by the system without constituting critical bottlenecks. After a first attempt simulation set, load duration curve were evaluated to obtain orders of magnitude for capacities of these processes.

The aim of the presented scenario was to assess the role of hydrogen in an energy system with minimized fossil NG availability, pursuing a cost minimization. A first round of simulation was conducted to estimate the installed capacities of P2H and H2X technologies and to evaluate the overall gas grid requirements. The latter was composed by a part with a fixed profile and a free profile one, representing the situations in which model is obliged to use gas grid to produce power/heat (the former) and periods in which gas use is more convenient than alternatives (the latter).

Seasonal behaviours for hydrogen and gas were observed in the simulation. Initial storage level is set by the model to coincide with the value at the end of the simulated year. After the estimation of initial levels of  $H_2$  and gas storage, the model returned a minimum use of fossil NG of 166 TWh on the overall 370 TWh required to the gas grid. Below this level, the model was not able to cover entirely the power demand, presenting electrical shortages.

Obtained annual power generation is presented in Figure 3, with a total value of 806 TWh. Of this, more or less the 85% is provided by REs. The contribution provided by the gas grid ( $\sim 11\%$ ) has to be further investigated.

The total energy provided by the gas grid is equal to 371 TWh, with only the 45% supplied with fossil NG. Another 20% is composed by synthetic methane obtained from catalytic methanation, 19% from biomethane via upgrading and 10% from biologic methanation. The remaining part of energy is provided by  $H_2$  injected via blending option (6%). The final amount of power generation attributable to fossil NG is then only 39.4 TWh ( $\sim 4.8\%$  of the total).

Regarding power consumption (Fig. 3), it was divided into three terms: 347 TWh destined to the final demands (e.g. net electrical load, cooling demand, BEVs recharge), 342 TWh to *Power to X (P2X)* and 57 TWh to Power to Heat. The second term describes all power uses to synthesise  $H_2$  and its by-products.

For P2X, almost the totality of power was destined to directly synthesise green  $H_2$  (97.2%), while remaining consumption was accounted to hydrogen storage, H2G, and Direct Air Capture (DAC).

In Power to Heat instead, three terms are included. Electrical consumption in heat

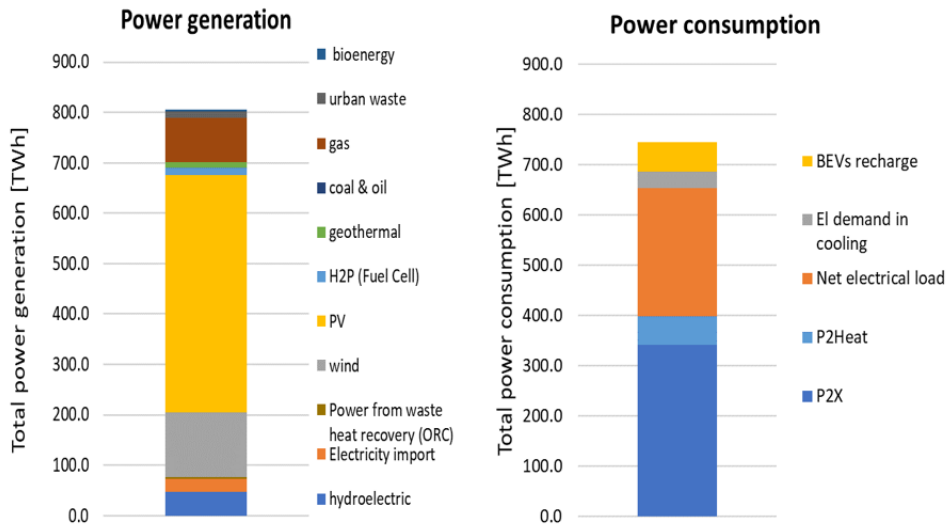


Figure 3. Annual power generation divided by source (left) and annual power consumption (right)

pumps to produce Domestic Hot Water (34%) is the former, then there is electrical consumption for heat pumps to cover space heating in buildings (62%), while the remaining 4% describes the power over-generation that is destined to Thermal Energy Storage systems in District Heating (DH).

Table 1. Hydrogen consumption in different utilization pathways

$H_2$ destination	Total energy provided [TWh]	Share on total $H_2$ produced
Final $H_2$ demand	68.3	27.9%
Gas grid injection	22.3	9.1%
H2Gas	115.7	47.2%
H2Liquid	16.6	6.8%
H2Power	22	9.0%
<b>Total</b>	<b>244.8</b>	

In Table 1 the green  $H_2$  allocation is presented. The pure demand covers less than the 30% of the total hydrogen production, being the dominant destination the H2G pathway (47%). An additional 9% is directly injected into the gas grid. These confirm the necessity of the system to compensate the limitation in fossil NG availability. The  $H_2-CH_4$  blending option in the gas grid is used at its maximum for almost the entire year.

Finally, less than 10% is directly used with Fuel Cell technology to produce power, being used only in period where RE power (e.g PV and wind) is not enough, during early morning and evening periods.

A seasonal storage for hydrogen is confirmed, starting from summer during frequent over-generation periods and being used in winter. Being assumed large storage ca-

capacities for both three  $H_2$  storage options, the model seems to promote hydrogen compression at 350 bar instead of its conversion to metal hydride or liquefaction. The latter is excluded due to its loss rate (e.g. boil-off issue), that weakens this solution for long seasonal storage.  $MgH_2$  metal hydride seems promising especially for stationary applications, however it still presents high energy consumption during its transformation process. By reducing their capacity storage, the model starts using all of them, by resorting to  $H_2$  liquefaction only when necessary.

It has to be stressed that the model does not consider investment or O&M cost for these technologies. Integrating an economic analysis could provide different results.

## Conclusion

The work of the thesis was to implement *Power to Hydrogen* and *Hydrogen to X* pathways in an existing energy system model. This enhanced version considers a more heterogeneous energy system, enabling the possibility to simulate multi-sector scenarios for the 2050 time-horizon. Several technologies in H2G and H2L are implemented and compared with bio-based alternatives. The potential role of hydrogen and electric fuels such as DME, methanol, jet-fuel or ammonia can be assessed. Moreover, the model is open-source and available for further implementations.

The single-node model returned a 2050 scenario with a year simulation and an hourly time-step. High levels of customization can be obtained in both spatial and temporal resolution, with multiple technology options that can be added.

Uncertainties are related to lack of detailed technical parameters for those technologies at early stage of market diffusion (e.g. e-jetfuel in H2L). The assumed values for these emerging processes might be underestimated, being at low TRL and then with likely margins of improvement. In future, their spread might allow more affordable and reliable information.

The zero-dimensional property translates that all the data provided and returned by the model are aggregated. As every single node model, there is a low level of detail when results have to be applied to a physical representation of the system. The solution would be to implement the multi-node characterization in the model. Also named regionalization, this addition would allow to describe n-nodes and their interconnections.

Following the example of the six bidding-zones for the power system, Italian energy system could be better described, with more precise characterization of heat/power demands and resources availability.

The single technology option for each process, might be strengthened with the inclusion of different alternatives, facing however with the increase in computational time and system complexity.

In the model application, assumed values for final demands were derived from international long-term projections, with a degree of uncertainty on allocation of consumption (e.g. naval or aviation transport). Better results could be achieved by integrating a specific study of long-term projection for the Italian energy system.

Lastly, economic consideration could include both  $C_{investment}$  and  $C_{O\&M}$ . *oemof* framework allows to do an optimization on investment. However, to date, the model generator does not allow to optimize all the period of transition from today to the

time-horizon (2050). Furthermore, economic parameter of new technologies will depend on many unpredictable factors (e.g. political and geographical). For this reason in the thesis only commodity costs were considered.



# Contents

<b>Ringraziamenti</b>	<b>iii</b>
<b>Sommario</b>	<b>v</b>
<b>Abstract</b>	<b>vii</b>
<b>Extended Abstract</b>	<b>ix</b>
<b>Contents</b>	<b>xix</b>
<b>List of Figures</b>	<b>xxi</b>
<b>List of Tables</b>	<b>xxiv</b>
<b>1 Introduction</b>	<b>1</b>
1.1 General framework . . . . .	1
1.2 Brief work description . . . . .	2
1.3 Thesis structure . . . . .	3
<b>2 Hydrogen processes network</b>	<b>5</b>
2.1 Power to hydrogen . . . . .	5
2.1.1 Alkaline Electrolyzer Cell (AEC) . . . . .	6
2.1.2 Proton Exchange Membrane Electrolyzer Cell (PEMEC) . . . . .	7
2.1.3 Solid Oxyde Electrolyzer Cell (SOEC) . . . . .	8
2.1.4 Anion Exchange Membrane Electrolyzer Cell (AEMEC) . . . . .	9
2.2 Hydrogen utilization pathways . . . . .	9
2.2.1 Hydrogen direct use . . . . .	9
2.2.2 Hydrogen to gas (H2G) . . . . .	10
2.2.3 Hydrogen to Liquid (H2L) . . . . .	13
2.2.4 $CO_2$ supply for H2G and H2L processes . . . . .	18
2.2.5 Hydrogen to Power (H2P) . . . . .	19
2.3 Hydrogen storage . . . . .	23
2.3.1 Physical hydrogen storage . . . . .	24
2.3.2 Material-based hydrogen storage . . . . .	26
2.4 Hydrogen transportation . . . . .	27
2.4.1 Compressed gas containers . . . . .	28
2.4.2 Liquid transport . . . . .	28
2.4.3 Pipeline . . . . .	28
2.4.4 Hydrogen blending in existing gas grid . . . . .	29

2.5	Use of excess heat from hydrogen processes . . . . .	30
2.5.1	Possible utilization pathways . . . . .	30
<b>3</b>	<b>Hydrogen in energy system models</b>	<b>33</b>
3.1	Review of energy system models . . . . .	33
3.1.1	Model classification . . . . .	33
3.1.2	Hydrogen in energy models . . . . .	36
<b>4</b>	<b>Model development</b>	<b>39</b>
4.1	Oemof framework . . . . .	39
4.1.1	Analytic background . . . . .	40
4.1.2	Oemof logic structure . . . . .	43
4.2	Scheme of Reference Energy System (SRES) description . . . . .	45
4.2.1	Processes involved in hydrogen supply chain . . . . .	48
4.2.2	Processes involved in methanol supply chain . . . . .	50
4.2.3	Processes involved in renewable methane supply chain . . . . .	50
4.2.4	Processes involved in dimethyl ether supply chain . . . . .	51
4.2.5	Processes involved in jet-fuel supply chain . . . . .	51
4.3	Model description . . . . .	52
4.3.1	Model structure . . . . .	53
4.3.2	Assumption of single technology option for each process . . . . .	56
4.3.3	Assumption on costs . . . . .	56
4.3.4	Assumptions on the gas infrastructure . . . . .	57
4.3.5	Multiple hydrogen storage option assumption . . . . .	59
4.3.6	Hydrogen-to-Power (H2P) assumption . . . . .	60
4.3.7	Assumption on waste heat recovery . . . . .	61
4.3.8	Assumption on hydrogen pipelines . . . . .	61
4.3.9	Assumption on biogas utilization . . . . .	62
4.3.10	Technological data assumptions . . . . .	63
<b>5</b>	<b>Model application</b>	<b>73</b>
5.1	Scenario definition . . . . .	73
5.1.1	Hydrogen demand in industry . . . . .	74
5.1.2	Energy demand in the transport sector . . . . .	75
5.1.3	Natural Gas constraints . . . . .	79
5.1.4	Assumption on total storage capacities for $H_2$ , $H_2$ -based products and $CO_2$ . . . . .	80
5.2	Input data description . . . . .	81
5.2.1	Final energy demand . . . . .	81
5.2.2	Available resources . . . . .	83
5.2.3	Technical parameters of $H_2$ and $H_2$ -based fuels synthesis technologies . . . . .	86
5.3	Results . . . . .	89
5.3.1	Energy required by the system from the gas grid . . . . .	89
5.3.2	Power generation and consumption . . . . .	94
5.3.3	Hydrogen production and utilization . . . . .	98

<b>6</b>	<b>Conclusions</b>	<b>105</b>
6.1	Areas of improvement . . . . .	107
<b>A</b>	<b>Input data tables</b>	<b>109</b>
	<b>Acronyms</b>	<b>113</b>
	<b>Bibliography</b>	<b>123</b>



# List of Figures

Figure 1	Main inputs and returned outputs of the model . . . . .	x
Figure 2	Example of logic structure of buses, flows and transformers . .	xi
Figure 3	Annual power generation and consumption . . . . .	xiv
Figure 2.1	Scheme of the chemical reactions occurring in a Alkaline Elec- trolyser Cell . . . . .	7
Figure 2.2	Scheme of the input and output flows in a catalytic methanation plant . . . . .	11
Figure 2.3	Scheme of the input and output flows in a biological methanation plant . . . . .	12
Figure 2.4	Scheme of the flows in the Fischer-Tropsch reactor to provide an output mix in the jet-fuel range . . . . .	14
Figure 2.5	Scheme of the flows required for methanol synthesis . . . . .	16
Figure 2.6	Scheme of the flows required for jet-fuel range output via methanol	17
Figure 2.7	Scheme of the flows required for DME synthesis via methanol dehydration . . . . .	17
Figure 2.8	Scheme of the chemical reactions occurring in a general fuel cell	20
Figure 3.1	Scheme of the market equilibrium between demand curve and supply one . . . . .	37
Figure 4.1	Scheme of the global Reference Energy System in the model .	47
Figure 4.2	Scheme of the Hydrogen Reference Energy System . . . . .	49
Figure 4.3	Main inputs and returned outputs of the model . . . . .	53
Figure 4.4	Model schematic approach . . . . .	54
Figure 5.1	Hourly profile of recharge for BEVs . . . . .	78
Figure 5.2	Load duration curve example . . . . .	87
Figure 5.3	Annual electrical shortage profile . . . . .	92
Figure 5.4	Storage of hydrogen and methane during the year simulation .	93
Figure 5.5	Annual power generation and consumption . . . . .	96
Figure 5.6	Hydrogen allocation in different uses . . . . .	100
Figure 5.7	Daily power generation and consumption curve . . . . .	100
Figure 5.8	Water electrolysis load duration curve . . . . .	101



# List of Tables

Table 1	Hydrogen consumption in different utilization pathways . . . . .	xiv
Table 2.1	State of the art of the different electrolysis technologies . . . . .	8
Table 2.2	State of the art of the different fuel cell technologies . . . . .	22
Table 2.3	Main properties and enegy consumption in the hydrogen storage options . . . . .	26
Table 4.1	Main technical parameters assumptions for Power to Hydrogen (P2H) pathway . . . . .	63
Table 4.2	Main technical parameters assumptions for methane synthesis processes in hydrogen to Gas (H2G) pathway . . . . .	64
Table 4.3	Main technical parameters assumptions for Hydrogen to Liquid (H2L) pathways . . . . .	66
Table 4.4	Main technical parameters assumptions for Hydrogen to Power (H2P) pathways . . . . .	67
Table 4.5	Main technical parameters assumptions for hydrogen storage transformation process . . . . .	68
Table 4.6	Main technical parameters assumptions for hydrogen storage . . . . .	69
Table 4.7	Main technical parameters assumptions for storage of remaining synthetic fuels . . . . .	69
Table 4.8	Main technical parameters assumptions for DAC and blending option . . . . .	70
Table 5.1	Assumed annual values for the main demands in the model . . . . .	82
Table 5.2	Assumed values for import, renewable and bio-based sources . . . . .	84
Table 5.3	Description of the aim of the main rounds of simulation and the obtained major results . . . . .	89
Table 5.4	Annual power generation from the different sources . . . . .	95
Table 5.5	Energy provided by the gas grid . . . . .	95
Table 5.6	Direct and indirect power consumption . . . . .	97
Table 5.7	Indirect power consumption: focus on Power to Heat . . . . .	97
Table 5.8	Indirect power consumption: focus on Power to X . . . . .	98
Table 5.9	Hydrogen consumption in different utilization pathways and total amount of final products obtained . . . . .	99
Table 5.10	Annual production and equivalent operating hours of the main implemented process in the model . . . . .	104
Table A.1	Main technical values assumed for System Heating and Domestic Hot Water technologies . . . . .	109

Table A.2	Main technological parameters assumed for the processes . . . .	110
Table A.3	Main technological parameters assumed for the storage technologies	111
Table A.4	Main technological parameters assumed for the processes with power and thermal outputs . . . . .	112



# Chapter 1

## Introduction

### 1.1 General framework

In the most recent period, a growing interest has spread about the necessity to revolutionize the energy system, following a low-carbon emission target. Starting from the 2015 Paris Agreement, towards the European target 2020, to the UN Sustainable Development Goal (SDG) to 2030, a wider awareness to the need to change explodes. The more and more extreme signals of climate change stressed the necessity to shift to a more sustainable way of living, driving the public debate to integrate specific policies of mitigation. In order to help policy-makers and industrial sector management to follow this goal, research activities started to focus on how to depict possible future scenarios.

A deeper integration of intermittent Renewable Energy (RE) sources determines a high level of instability in the energy grid, requiring large storage solutions. The need to not waste excess energy produced in peak periods imposes the necessity to decouple production from demand.

Increasing attention was accomplished by energy system models that study its interactions, trying to provide an optimized configuration and the possible pathways to reach the goal of decarbonisation.

The work of this thesis deepens the energy modelling environment, providing a study on the Italian national energy system for a long-term strategy to 2050. To meet this target, an energy model based on the open-source Python-based framework *Oemof* [29] was developed.

In the specific, the work was focused on the feasibility study of the supply chain of hydrogen and hydrogen-based fuels as a possible alternative solution to improve intermittent REs integration in the system.

The core of the thesis was to study the role that hydrogen could have in the next future in Italy, providing an extended open source energy system model able to deeply analyse the Italian energy system.

## 1.2 Brief work description

The work started with a consistent literature review of the main existing processes (and research focus) related to the hydrogen production pathway from renewable energy.

Subsequently, through the help of summarized global reports such as International Energy Agency (IEA) “The future of hydrogen” [2], SNAM “Generation H” [5] and “Gas for Climate: the optimal role for gas in a net-zero emissions energy system” by Navigant [3], it was possible to determine which technologies best suit the purpose.

Hydrogen as energy carrier can revolutionize the way of thinking not only the power sector, but also several other sectors such as transportation, industry and residential. From this perspective an helpful guideline was also provided by the 2018 EU technical report for the long-term strategy [36] and the Danish Energy Agency (DEA) "technology data for renewable fuels" [4].

The former firstly lists the already existing EU policies and the sectorial low carbon-guided transformation pathways, while the latter provides a review of the available alternative renewable fuels technologies.

Once the technological and international policy background was completed, it was possible to start developing a study on the hydrogen pathways at national level.

The main work relies on the implementation of hydrogen and  $H_2$ -derived fuels sector in an existing energy system model [1]. Subsequently, the developed tool was set to deeply investigate the interactions of *Power to Hydrogen (P2H)* in a highly renewable integrated energy system of the Italian country, studying its role as energy storage solution.

The implemented model analyses with a high level of detail the production mix in the Italian power sector, evaluating its interactions with the sectors demand during a year time horizon, with a hourly partition.

The implemented model returns the the generation mix by minimizing the resources consumption (e.g. fossil NG or biomass). Once defined the optimal system configuration, qualitative and quantitative information can be obtained in order to efficiently direct policy-makers and industry firms decarbonisation efforts.

Final observations are made to assess the capability to reach the zero-emission target for Italy, estimating the necessary requirements the country would need to make it possible.

Possible future developments could be the addition of sustainable technologies currently considered still at a laboratory Technology Readiness Level (TRL  $\sim$  1-4), or the implementation of the presented model for a regional characterization. In this way each one of the six Italian bidding-zones of the power market could be studied, with a focus on the interactions between each other.

Today, the model is limited to analyse the system at a national level, whose results however could be used to verify the consistency of the regional implementation.

## 1.3 Thesis structure

In this section the structure of the thesis will be presented. The Thesis is organised in the following manner.

the *Chapter 2* focuses on the description of the technologies related to the *Power to X (P2X)* pathway. The most common and the most promising conversion processes of the excess power are investigated, with an emphasis on the hydrogen as energy carrier.

*Power to Hydrogen (P2H)* and subsequent  $H_2$  utilization pathways are described, stressing on their strength and weakness points, limitations and main entry barriers, to help regulators to facilitate their introduction in the energy system.

Later, technologies to enable the decoupling between supply and demand, reducing wasted power during overload production are presented.

Fourth section provides a panoramic view of the main hydrogen transportation vectors, with some considerations on their ease of introduction in the grid.

A final focus was given on the waste energy reduction of the presented processes. Often waste heat is a by-product of the technologies previously described. Here possible utilization pathways (e.g. direct use in district heating or small power generation via Organic Rankine Cycle) are studied.

*Chapter 3* has the aim to provide a literature review of the main energy system models classification. Due to the high level of heterogeneity of existing energy models, some families are presented, where distinguishing features are underlined.

The chapter continues with a description of the current models that have already implemented the hydrogen handling in the studied system, with some technical report examples where first  $H_2$  feasibility considerations are made.

With *Chapter 4* the core of the thesis work is introduced, starting with a more detailed introduction of the model framework *oemof*. This allows to introduce the analytic background of the model structure.

With the information on the main logic components that describe the energy system, it is provided a description of the Scheme of the Reference Energy System (SRES). Here the main implemented process in the model are described in a general view.

Last part of the Chapter is destined to the analytical description of the implemented model, its structure and the main background hypothesis that differentiate it from the original version plus the main technical data assumptions for the technologies described in Chapter 2.

The *Chapter 5* has the goal to test the implemented model by defining a 2050 scenario setup for the Italian energy system. Baseline assumptions are presented, with a focus on the main hypothesis and the decision driver that lead the evolution of simulation's rounds.

Once that the scenario is defined, a detailed overview of the input data is provided. Last part is characterized by the comment of obtained results, their meaning and possible further implementation that would provide a more complete description of the simulated energy system.

Last Chapter summarises all the presented considerations, reminding what the implemented model allows to do. Its limits and its main characteristics, such as its availability or its setting, are recalled.

The thesis concludes pointing the possible future developments, explaining how the pillar assumptions could be improved and how to enhance the analysis.

# Chapter 2

## Hydrogen processes network

In this chapter a review of the state of the art for the main technologies related to the hydrogen world will be discussed. This is necessary in order to better understand what solution mix might be the most suitable for the further analysis in the model presented in Chapter 4.

The main topics of the thesis are about the possibility to facilitate the introduction of the technologies related to the hydrogen world in the context of the Italian electricity grid.

The final goal is the deeply integration of unpredictable renewable technologies within the grid: here hydrogen can bring lots of benefits in stabilization between demand and supply.

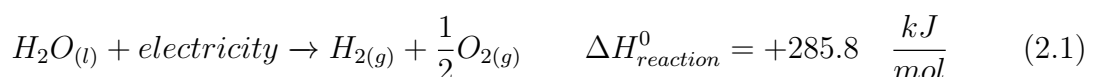
Here below the main possible process in which hydrogen is involved will be presented.

### 2.1 Power to hydrogen

In the text the process of hydrogen generation from renewable electricity, through the water electrolysis will be called *Power to hydrogen*.

Water electrolysis is the sum of different chemical reactions which bring to two output streams of pure hydrogen and pure oxygen giving as inputs electricity and a stream of pure water.

Water electrolysis reaction (Eq. 2.1) is the electrochemical splitting of the reactants by passing electric current between two electrodes, which are separated by an electrolyte to yield  $H_2$  and  $O_2$  [4]. It can be divided into 2 steps: the reduction reaction at the negatively charged cathode and the oxidation one at the positive charged anode. The two reactions depend on the electrolyte type, varying for each electrolyser. In the following, the overall reaction (Eq. 2.1), the reactions occurring for an Alkaline Electrolyser Cell (AEC) and for Proton Exchange Membrane one (PEMEC) on the two electrodes are reported, to point out the difference:



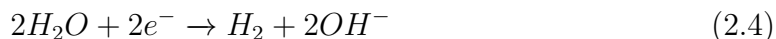
For the PEMEC, at the cathode:



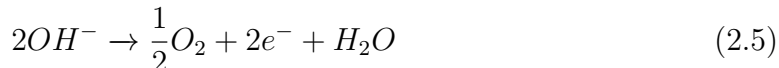
and at the anode:



While for the Alkaline electrolyser's cathode:



and at AEC's anode:



Depending on the type of electrolysis technology, the charge carrier can be  $OH^-$ ,  $H_3O^+$  or  $H^+$  or  $O^{2-}$ .

There are currently 4 main different types of electrolyzers:

- Alkaline Electrolyzer Cell (AEC)
- Proton Exchange Membrane Electrolyzer Cell (PEMEC)
- Solid Oxide Electrolyzer Cell (SOEC)
- Anion Exchange Membrane Electrolyzer Cell (AEMEC)

A schematic view of the general reactions occurring in Alkaline electrolyser is shown in Figure 2.1.

In the following sections the main characteristics of each one will be presented. For a comparison of the most common water electrolysis technologies see the next table 2.1.

### 2.1.1 Alkaline Electrolyzer Cell (AEC)

Alkaline electrolysis is the most mature technology, commercially available and used since 1920s. An aqueous alkaline solution (NaOH or KOH) is typically used as the electrolyte [2, 6, 7].

The lifetime of this technology is more or less the double than the PEMEC (80'000 operating hours v 40'000 h) and is expected to remain longer in the medium term [7]. However, Alkaline EC suffers of a lower flexibility and has a limit in the operating range: it goes from a minimum load of 10% to full design capacity [2, 7].

Being a consolidated technology with an established production volume and due to the avoidance of precious materials, AEC has lower capital expenditure (CAPEX) with respect to the other electrolysis technologies [2, 7].

This type of electrolysis produces an  $H_2$  stream at atmospheric pressure. Some AECs are under development to obtain pressurized hydrogen up to 15 bar, nevertheless with a negative consequence on the overall efficiency and output hydrogen purity [6].

The two main disadvantages of AEC are that it takes up to 10 min to restart the system following a shutdown [7] and that it uses highly corrosive electrolytes, needing high maintenance costs [6]. The main values are reported in Table 2.1.

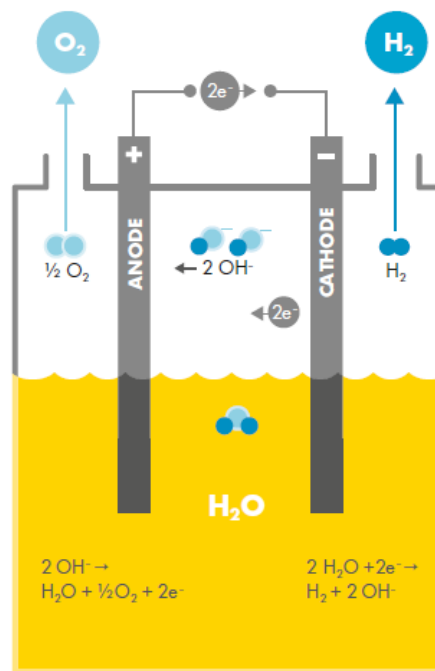


Figure 2.1. Scheme of the chemical reactions occurring in a Alkaline Electrolyser Cell (source [8])

### 2.1.2 Proton Exchange Membrane Electrolyzer Cell (PEMEC)

PEM electrolyzer systems are relative new technology, with first commercial applications in 1960s with General Electric [2]. Here the electrolyte is a solid polymer membrane (e.g. Nafion) with the advantage of producing a high purity  $H_2$ . Compared to AEC, other important advantages include a higher flexibility and better coupling with dynamic power systems. The fast response and the smaller size make them more attractive in dense urban areas [2]. The cold start can require up to 5 minutes, while the normal response is 1-2 seconds [6].

They produce highly compressed hydrogen (30-60 bar) and their operating range can go from zero load to 160% of the design capacity: this gives the possibility to overload the electrolyzer for a definite period of time, degradating however the system [2]. Please note that in the thesis the design capacity of a technology is considered the one that operates at the optimal condition. The overload means that the electrolyzer could produce more hydrogen than the expected at the optimal condition.

Main drawbacks are the need of expensive electrode catalyst, such as platinum or iridium and membrane materials, and a shorter lifetime (today "halved" with respect to the AECs) [2, 6]. Although they are modulable, PEMECs are available in the market only in smaller size compared to AECs.

Table 2.1. State of the art of the different electrolysis technologies [2, 9]

	<b>AEC</b>		<b>PEMEC</b>		<b>SOEC</b>		<b>AEMEC</b>
	Today	Long term <sup>a</sup>	Today	Long term <sup>a</sup>	Today	Long term <sup>a</sup>	Today
Electrical efficiency (% LHV)	63-70	70-80	56-60	67-74	74-81	77-90	40
Operating pressure (bar)	1-30		30-80		1		30
Operating temperature (°C)	60-80		50-80		650-1000		50-70
Stack lifetime <sup>b</sup>	60-90	100-150	30-90	100-150	10-30	75-100	N/A
Load range	10-110		0-160		20-100		N/A

<sup>a</sup> values obtained with projections with different system sizes

<sup>b</sup> thousand of operating hours

### 2.1.3 Solid Oxide Electrolyzer Cell (SOEC)

SOECs are the most recent and the least developed technology for water electrolysis. It is still at laboratory stage and is not commercialized yet. They use ceramics as electrolyte and have low material costs [2, 6, 7].

They operate at high temperature and they need steam water as input. For this reason they need a heat source, so they well couple with systems that produce waste heat, recoverable for the water evaporation (e.g. Fischer-Tropsch synthesis, methanation) [2, 6].

However, operating at high temperature means degrading conditions for the cells, with a direct impact on the lifetime due to the materials deterioration. Their need for heat sources might limit their utilisation in the *Power to hydrogen* pathway, allowing only renewable sources such as Concentrated Solar Power (CSP) or high temperature geothermal [7].

The main advantage is the higher electrical efficiency, compared to the two previous technologies. Furthermore, it has been proven the possibility to operate a SOEC in reverse mode as a fuel cell, converting hydrogen back into electricity: this enables the capability of the technology to provide balancing services to the grid, despite a lower conversion factor [2, 6, 7]. Another advantage is the possibility to use solid oxide electrolyzers to convert carbon dioxide  $CO_2$  to carbon monoxide  $CO$ . Thus, if water is electrolysed in the SOEC at the same time, it is possible to obtain as output the syngas, a mixture mainly of  $H_2$  and  $CO$  [4]. This can be particularly interesting in those application in which hydrogen and carbon monoxide are involved as inputs for obtaining a more complex energy carrier (e.g. jet-fuel synthesis via Fischer-Tropsch



reaction, discussed in Section 2.2.3) .

### 2.1.4 Anion Exchange Membrane Electrolyzer Cell (AEMEC)

The previous technology SOEC currently is the only that operates at high temperature. For the class of low temperature ECs, there is another typology, the *anion exchange membrane electrolysis*. This is still at R&D stage, with commercial availability for limited applications [8,9].

The structure is similar to the one of PEMEC, but with the main difference that in the electrolyte ions  $OH^-$  are transferred instead of protons  $H^+$ . Currently, the main advantages with respect to the PEMECs are the use of non-noble metal at the electrodes and the non-corrosive electrolyte. These two characteristics enable lower costs and the absence of leakages from the cell, with the direct consequence of producing high pressure  $H_2$  [9].

However, the main drawbacks are connected to the membrane degradation issue, which affects the durability. Furthermore, efforts on increasing current density and reducing the excessive catalyst loading are investigated by R&D.

## 2.2 Hydrogen utilization pathways

Once produced, hydrogen can be destined to different uses. It can be stored as an energy carrier and then reconverted into water, releasing electricity when necessary. It can be used directly as an energy carrier (e.g. transport sector) or for industrial purposes (e.g. steel production).

Otherwise, it can be used as an input for more complex compounds, like synthetic methane or liquid synthetic fuels (e.g. methanol, dimethyl ether DME or jet-fuel).

### 2.2.1 Hydrogen direct use

Before introducing all the possible *Hydrogen to X* pathways, it might be useful to introduce those sectors in which a direct use of green  $H_2$  could bring benefits.

The colour "green" is used to indicate the hydrogen production from renewable energies, for example PV and wind power, that supply electricity to electrolyzers.

To date, the global hydrogen demand is related to industrial applications. The highest  $H_2$  demand is in oil refining, immediately followed by ammonia production. Together, they cover  $\sim 60\%$  of the total demand. Other application uses are in the methanol production and steel production with the Direct Reduction of Iron ore (DRI) [2].

Currently more than 60% of hydrogen used in refineries is produced from Natural Gas (NG), through steam reforming reaction (Eq. 2.6), presented below:



The remaining  $H_2$  part is obtained as a by-product of coal use (gasification). Steel sector offers a wide potential for green hydrogen demand growth, from a perspective of emissions reduction [37].

Another possible direct use of hydrogen could occur in the transport sector. Currently the main barriers for Fuel Cell Electric Vehicles (FCEV) diffusion are the FC stack cost and the cost for on-board hydrogen storage. This problem can be downsized for heavy transport, where the long range requirements rules out battery electric vehicle solution.

While  $H_2$  FC electric forklifts are already commercially viable, there is an increasing interest in the public transport sector.

There already exists some pilot project of hydrogen fueled buses for public transport. During the period 2010-2016 a European Union project, named Clean Hydrogen In European Cities (CHIC) [38], was conducted in some EU cities, included Milan.

The transport system of the Italian city introduced a small number of buses fueled with hydrogen, locally produced in the deposit of San Donato Milanese with a rate of 200 kg/day through a system of water electrolysis coupled with a PV system.

A rapid growth is expected in the short term thanks to the large deployment driven by China, which has the goal to expand its fleet of thousands elements. Some other countries or delivery companies are following the same trend, introducing new heavy-duty trucks fueled by hydrogen [2].

From a net-zero GHG emission target perspective, the *Hydrogen to X* pathways can be very promising if  $CO_2$  (biogenic or coming from Direct Air Capture (DAC) systems) is coupled to this renewable  $H_2$ .

Depending on the final energy carrier obtained, it is possible to define different ways to use the formed hydrogen.

### 2.2.2 Hydrogen to gas (H2G)

This pathway deals with the synthesis of a gaseous energy carrier, mainly synthetic methane, which can bring a lot of push in the reconversion of the energy system.

The production of synthetic methane can get advantages thanks to the cost savings coming from the already existing infrastructures (e.g. transmission line, storage tanks etc).

Furthermore, converting hydrogen into  $CH_4$  allows to keep using the existing heat/power systems present in the grid (e.g. boilers, gas turbines etc), while the R&D of these technologies develop machineries able to manage higher  $H_2$  content input flows.

The synthetic methane can be produced from a chemical reaction which involves  $CO_2$  (or  $CO$ ) and  $H_2$ . Depending on whether carbon dioxide or monoxide is used, the reaction is called  $CO_2$  hydrogenation (Eq. 2.7) or  $CO$  hydrogenation (Eq. 2.8), which are following reported:





These reactions go under the name of methanation process, which will be analysed in the following Section.

### Catalytic thermochemical methanation

To date, the main application of the methanation process rely mostly on catalytic thermochemical methanation [2]. The main inputs-outputs are presented in Figure 2.2 below.

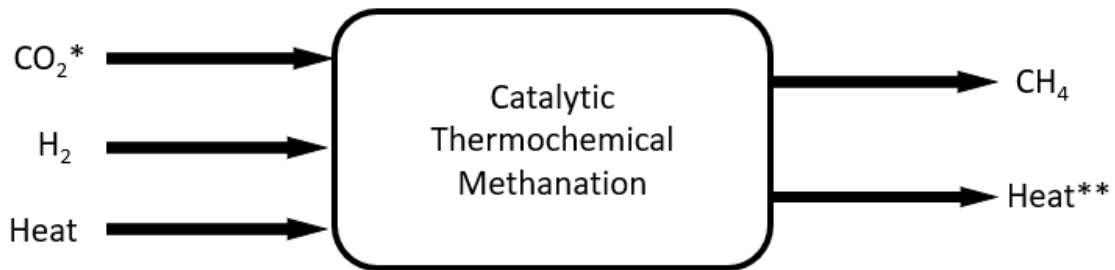


Figure 2.2. Scheme of the input and output flows in a catalytic methanation plant; (\*) the provided input can be also a biogas stream ( $CH_4$  and  $CO_2$ ), where carbon dioxide will be the only reactant while methane will behave as an inert [11]; (\*\*) the exothermic reaction of methanation can provide heat suitable for small power generation through an ORC, or it can be recovered to sustain the reaction operating conditions or to supply an external heat demand (i.e. district heating)

It is not the only possible process, in fact also biological methanation can be a solution. However, this second solution is still at an earlier stage of development. Further information will be treated in the next Section.

The thermochemical reactors typically operate at temperatures between 200°C and 550 °C, with operating pressures between 1 and 100 bar. Several metals are suitable as catalyst in the process, such as Ni, Ru, Rh and Co. However, the best trade-off choice between activity, good  $CH_4$  selectivity and low material price is nickel. The main drawbacks of this catalyst is the high purity requirement for the feed gas, with respect to sulphurous compounds [6, 10]. This would require some purification process before the injection in the reactor.

The process is highly exothermic, so there is the possibility to recover some of the heat (i.e. using for steam production in SOECs, for power generation through Organic Rankine Cycle or for district heating) [2].

### Biological methanation

Biological methanation (Fig. 2.3) is another solution for the *Hydrogen to Gas*, although less developed. There is no metal utilisation as catalyst, because this function is provided by methanogenic microorganisms [6, 10]. They operate in an anaerobic environment in which they convert the input hydrogen and carbon dioxide into methane [2, 6].

Compared to catalytic methanation, the process operates at much lower temperatures (between 20 and 70 °C) and at ambient pressure.

Before the synthesis of methane, the input feedstock, which is typically solid biomass, must be treated and gassified. This requires a biogas digester, an intermediate reactor in which there is the hydrolysis and separation of the organic substrate into simple monomers and then their conversion into biogas, mainly composed by  $CH_4$  and  $CO_2$  [6, 10, 39].

This technology has a lower overall efficiency compared to the catalytic one. Thus, due to lower rates of  $CH_4$  formation, the larger reactors' requirement makes this pathway more suitable for small-sized plants [10].

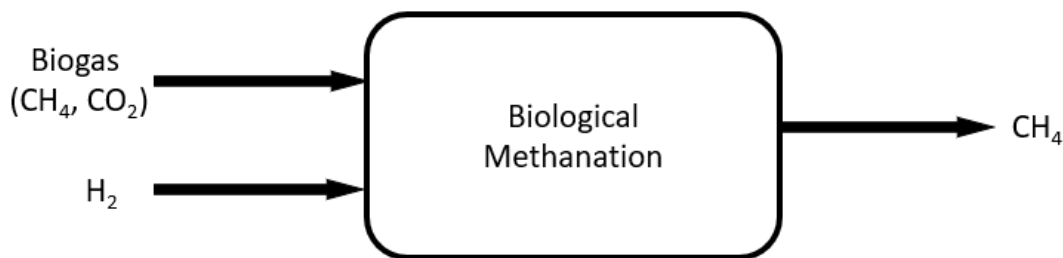


Figure 2.3. Scheme of the input and output flows in a biological methanation plant

Biological methanation can occur in two different configurations:

- *Biological methanation in situ*; in this P2G process, hydrogen is fed directly to the biogas digester. Here, a part of the carbon dioxide produced by the biomass gassification is converted to  $CH_4$ . However, the optimal configuration to enhance the  $CO_2$  conversion (elevated T and p) cannot be adapted to the operating condition of the digester.

Therefore, reaching a total conversion of the  $CO_2$  is difficult. Due to the low solubility of the  $H_2$  in the digestate, low hydrogen conversion factor occurs in the system, translating into a residual  $H_2$  content in the product gas ( $\sim 20\%$  vol) [6].

At the output there will be a stream mainly composed by methane, but with a small residue of hydrogen and carbon dioxide.

- *Biological methanation ex situ or in a separate reactor*; the main difference from the previous case is the presence of a separate methanation reactor, after the

biogas digester.

Here biogas and a hydrogen stream are fed to the reactor, where gases are converted by methanogenic microorganisms into methane.

This configuration enables to set those conditions which are optimized for the hydrogenotrophic methanogens, increasing the  $CH_4$  content in the output stream with respect to the *In situ* configuration [6].

The main drawback is the cost due to the need of an additional reactor, avoided in the previous configuration.

As seen before, the *biological* and the *catalytic thermochemical* methanation can play a role in substituting to those biogas upgrading plant, with the direct re-utilisation of the by-product  $CO_2$ . They could be considered as valid solutions when a new plant for biogas processing has to be built.

A normal biogas upgrading plant filtrates the raw biogas coming from a digester in order to inject into the gas grid a stream of pure methane.  $CO_2$  and other impurities (e.g. water moisture, particles, ammonia  $NH_3$  or hydrogen sulphide  $H_2S$ ) must be removed, in order to reach the technical requirements of the grid [4].

Thanks to further development and decreasing cost, it will become feasible to reconvert these upgrading plants into direct methanation ones, as reported in the study of the Swiss Federal Office of Energy [11].

### 2.2.3 Hydrogen to Liquid (H2L)

This second pathway can be relevant in those sectors in which a decarbonisation through electrification might be hard to achieve. Typical examples are the aviation transport, the heavy road transport and the maritime one.

As for the *Hydrogen to Gas*, if the  $H_2$  coming from renewable electricity is coupled with captured (or neutral) carbon dioxide, this solution can contribute to a GHG emission reduction. Furthermore, there is the additional advantage to produce fuels that are compatible with the current engines, using the existing transmission and storage grid, without particular adjustments.

The fuels of this class are typically called *electrofuels*, which potentially constitute a zero-emission alternative. However, as of today their use is likely to remain limited in the short term, due to their high production cost ( $\sim 3$  to 6 times more expensive than kerosene) [2, 40].

These are not the only potential solution for the GHG emissions reduction in those sectors where fuels are necessary. Furthermore, to date, to cover the demand of these fuels with zero-emission alternatives, electrofuels won't be enough.

A possible help to cover the fuel demand could come from bio-based fuels. These are obtained from solid biomass, vegetable oils, hydrogenated fats and recycled waste. Here a secondary stream of hydrogen is used in last transformation steps to achieve the final product, but the main input remains the bio-based feedstock.

This hydrogen supply could be provided by water electrolysis, while at present is mostly obtained by steam methane reforming reaction.

This bio-based pathway is typically called *Biomass to Liquid (B2L)*.

It might be useful to divide these input streams into different categories, depending on their origin:

- *First generation feedstocks*, all the vegetable oil plantations that are in competition with the food supply chain.
- *Second generation feedstocks*, mainly animal fats, used cooking oils, waste oils and agricultural scraps.
- *Third generation feedstocks*, oils derived from algae and waste.

While the first one is an already well consolidated supply chain, there are strong efforts to make cost-competitive the second and the third generation pathways from a sustainability perspective (i.e. in the refinery sector).

Interesting italian examples are the ENI bio-refineries of Venice [41] and Gela [42].

Among the HtL fuel chain, two are the main production pathways: the Fischer-Tropsch (FT) pathway and the methanol one.

### Fischer-Tropsch to synthetic liquid fuels

The Fischer-Tropsch pathway to synthetic liquid fuels is a consolidated process in the coal and gas sectors, known under the class of gas-to-liquid (G2L) and coal-to-liquid (C2L). Also starting from the biomass is possible (B2L), because all the three pathways give syngas as intermediate product, a mix of hydrogen with, carbon monoxide and some  $CO_2$ .

FT synthesis requires carbon monoxide and hydrogen as inputs, as shown in Figure 2.4.

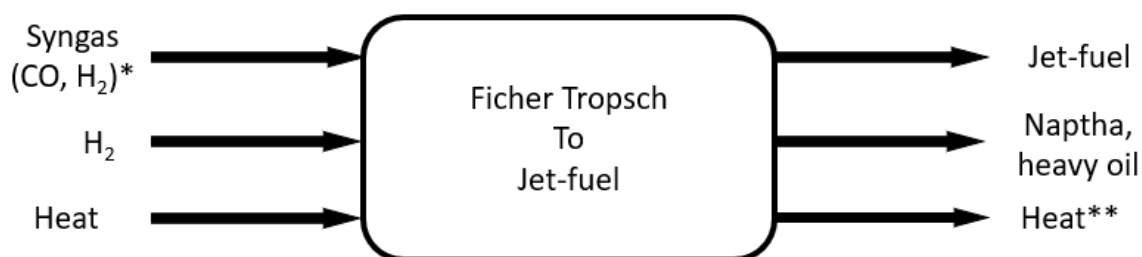


Figure 2.4. Scheme of the flows in the Fischer-Tropsch reactor to provide an output mix in the jet-fuel range; (\*) input flow is a syngas mix of  $CO$  and  $H_2$ , but also  $CO_2$  is feasible, converted via reverse Water-Gas Shift (WGS) reaction (Eq. 2.9); (\*\*) the FT synthesis is highly exothermic [43], thus generates recoverable heat for self-sustain the process, produce electricity through an ORC or to supply an external heat demand (e.g. district heating)

Thus, the residual  $CO_2$  can be converted to  $CO$  via the *reverse water-gas shift* process, as follow:



Once obtained the output FT-derived crude product, some other refinery processes are required to get the final fuel mix. They are hydrocracking, isomerization and then distillation [12].

The first two steps are required in order to increase the cold flow properties of the fuel, hydro-isomerizing and hydrocracking the normal paraffins produced after the FT synthesis [4, 12]. The final distillation is made to separate jet fuel from other products of the final mix. The share of output streams suitable for jet fuel use is about 50 to 60 % of the output energy [12]. In the thesis work the process will be analysed only to produce jet-fuel (see Section 4.3.10)

The FT process can be divided in two categories: high temperature Fischer-Tropsch synthesis and low temperature one. The first class operating condition is around 310-340 °C, and the main products are gasoline and olefins, while the low temperature pathway operates at 210-260 °C producing main kerosene and diesel oil [13].

### Hydrogen to methanol

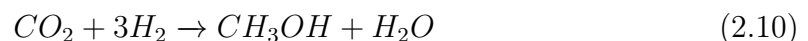
Another possibility of  $H_2$  conversion is to produce methanol. Methanol ( $CH_3OH$  or MeOH for short) has important potential as fuel but not only. This can be an interesting solution for energy carrier purposes or as an intermediate product for more complex fuels (e.g. DME or jet-fuel discussed later).

This can be relevant particularly in the maritime sector. It can be blended with gasoline [18] (or used pure in recent methanol engines) or could be used in fuel cell [17], with the advantage of better transportation and storage properties with respect to pure hydrogen [16]. It can be stored in standard fuel tanks for liquid fuels, because is liquid at ambient temperature and easily transported by trucks or bunker vessels.

There exist two pathways to synthesise methanol from carbon dioxide:

- direct hydrogenation of  $CO_2$  (Eq. 2.10)
- $CO_2$  conversion into  $CO$  and further hydrogenation of  $CO$  (Eq. 2.10 )

The main difference is the sequence of chemical reactions that occur in the reactor. The first route can be explained with the following chemical reaction:



The second pathway requires first a reverse water-gas shift (Eq. 2.9), then the following one:



Common commercial catalysts are  $Cu$ ,  $ZnO$  or  $Al_2O_3$  [14]. As other metal catalysts, they are sensible to temperature variation and their maintenance can be difficult. In fact the reaction of methanol synthesis (Fig. 2.5) is highly exothermic and an important issue is the removal of the excess heat, in order to avoid catalyst degradation and to shift the chemical equilibrium towards the products [14].

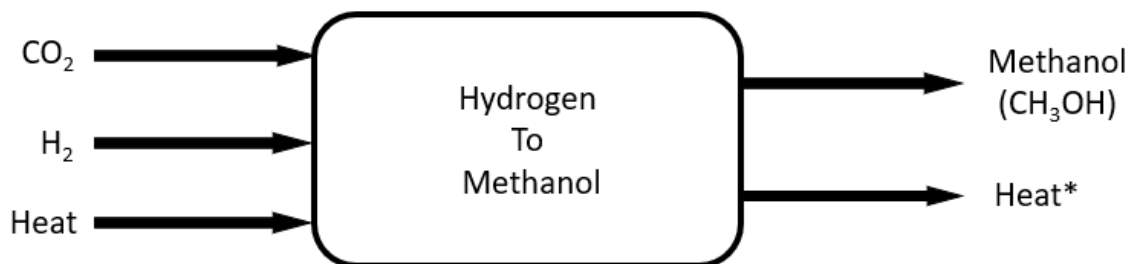


Figure 2.5. Scheme of the flows required for methanol synthesis; (\*) Heat generated by the exothermic reaction can be used for self sustain the reactor, to produce electricity through an ORC or to supply an external heat demand

There already exists an industrial *hydrogen to methanol* plant, the George Olah Renewable Methanol Plant in Iceland [44], with an annual *MeOH* production rate of  $\sim 4$  Gton.

### Methanol to jet fuel

A different pathway from the previous FT synthesis is the *methanol to jet fuel* illustrated in Figure 2.6. As shown in the previous section, there is an industrially proven knowledge regarding the methanol synthesis, in large-scale applications [12, 14].

Its upgrading to jet fuel generally undergoes a four-step process: olefin synthesis, oligomerization, hydrotreating and a final distillation.

First, the methanol is dehydrated to generate olefins. Subsequently, there is the oligomerization of the olefins, through the presence of a catalyst, to obtain a middle distillate.

This last intermediate product is hydrogenated with a hydrogen stream to get the jet-fuel-ranged hydrocarbons, which will require a final distillation [12, 13].

To date, no jet fuel has yet been commercially produced via methanol pathway (Fig. 2.6), although the necessary process steps are already available, being used at large-scale in refineries [12].

Further information about the process steps can be found in Bradin [15].



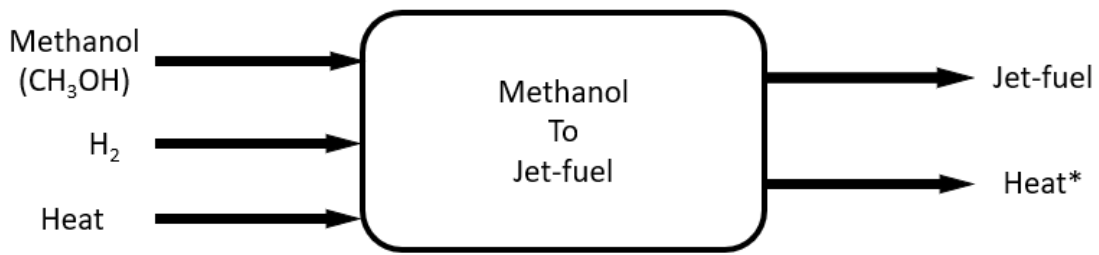


Figure 2.6. Scheme of the flows required for jet-fuel range output via methanol; (\*) Heat generated by the exothermic reaction can be used for self sustain the reactor, to produce electricity through an ORC or to supply an external heat demand

### Methanol to DME

In the previous sections the pathways to synthesize jet fuel from syngas or from methanol were analysed. However, from this last one intermediate product, it is possible to produce Dimethyl Ether (DME), a possible cleaner alternative to petroleum diesel in transport sector.

Typically, the DME is produced in a two step process, starting from syngas and generating the intermediate product of methanol (i.e. methanol synthesis). This last one is then converted to dimethyl ether (as depicted in Figure 2.7) by methanol dehydration, according to the following equation:

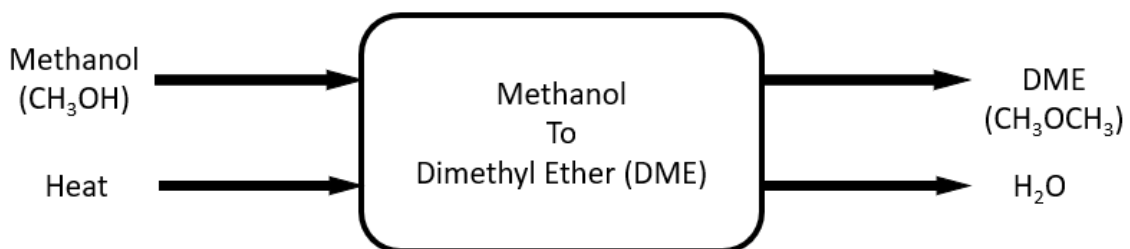


Figure 2.7. Scheme of the flows required for DME synthesis via methanol dehydration

However, there is the possibility to have a direct DME synthesis from the syngas, using a dual catalyst system, in which can occur both the methanol synthesis and its subsequent dehydration [15]. The main advantage is to avoid the need of MeOH isolation and purification. An existing facility in California produces DME directly from biogas [19].

Both the pathways are commercially available, but with a preference on the two-step process due to its lower start-up costs and structural complexity [12, 15].

### 2.2.4 $CO_2$ supply for H2G and H2L processes

In order to have significant GHG emission reduction in those specific sectors which use as input a stream of carbon dioxide, it has to be neutral the latter. This means that the  $CO_2$  required, which is produced almost entirely from the combustion of fossil fuels, could be captured from this source or come from the biogas upgrading, (in this case is called *biogenic  $CO_2$*  which will be analysed later).

Coming back to the option of  $CO_2$  acquisition from the combustion of fossil fuels, there are several industry plants which offer concentrated carbon dioxide streams (e.g. cement and steel production) [2].

For this reason there exist a theoretical upper limit of 50% emissions reduction: the carbon molecule contained in the original fossil fuel can be used twice to produce energy. First, it is used in the industrial process, releasing energy and giving as output  $CO_2$ . The captured carbon dioxide is then converted to synthetic methane/synthetic hydrocarbon fuel, which, if combusted, will provide energy for the second time and release again the  $CO_2$  in the atmosphere [2].

There are other possible ways to supply the carbon dioxide needed. When  $CO_2$  is obtained from non-fossil sources, (i.e. from biomass), is called *biogenic  $CO_2$* . It is the definition for the stream that comes from the combustion of a feedstock or its downstream product which has captured  $CO_2$  in the "previous life". Vegetable plant species do the photosynthesis process, using the solar irradiation to convert the carbon dioxide into carbon and oxygen as by-product. However, during the night hours, the process is inverted, releasing again a part of  $CO_2$ . Although this negative contribution, the net  $CO_2$  absorption balance of each plant species is positive (otherwise their carbon-based trunk would not grow each year).

Finally, was estimated that the total amount of carbon dioxide released after the combustion of biomass or of its products (e.g. biogas) coincides with the total net  $CO_2$  captured by the tree during its life: for this reason can be considered "neutral".

For the biomass sector, systems of CCU are particularly developed in the biogas upgrading sector.

To date, there are five main upgrading technologies, listed in order of decreasing commercial maturity [4]:

- *Water scrubbing*; a stream of water is sprayed to the biogas flow. This washes out the carbon dioxide and the  $H_2S$ , more soluble gases than methane.
- *Amine scrubbing*; here the upgrading process is chemical absorption of  $CO_2$  in amines, which have to be separately regenerated.
- *Pressure swing adsorption (PSA)*; it is the last common upgrading technology, which uses a high pressure environment plus an adsorbent material to capture the carbon dioxide and other impurities of the biogas. The material is then regenerated with a switch to a low pressure environment.
- *Membrane separation*; basically a hollow fibres membrane, in which methane and nitrogen cannot pass through except of a very low extent, while the main impurities pass it and then are captured.

- *Organic physical scrubbing*; the concept is the same of the water scrubbing, with the difference that is used an organic solvent for the absorption of  $CO_2$ .

It is remarkable to notice that it might not be necessary to separate the carbon dioxide if the hydrogen can be directly introduced in the gasification product [2, 11]. In addition to the previous ways to carbon dioxide supply, there exists the possibility to capture the  $CO_2$  directly from the atmosphere. The technology is called Direct Air Capture (DAC), whose main drawback is the higher energy requirements with respect to the other technologies [2]. That is because there is a much lower carbon dioxide concentration in the air with respect to industrial or gassification processes.

Another important parameter regarding the competitiveness and the sustainability of the process is the water demand between bio-based synthetic fuels and *hydrogen to liquid*.

The net water demand of biofuels is significantly sensitive towards the bioenergy feedstock. For example, if the resource comes from agriculture (i.e. first generation biomass), synthetic fuel requires more water than the *hydrogen to liquid*, with a factor of 400 to 15000 [12].

### 2.2.5 Hydrogen to Power (H2P)

The last possible utilization pathway for hydrogen is its reconversion to power, through a Fuel Cell (FC), or a turbine.

Regarding the first solution, it is the opposite reaction of the one that occurs in the electrolyte, where water molecule is split into hydrogen and oxygen consuming electricity. Equation 2.13 reports the overall reaction for FC technology. Here the chemical energy of  $H_2$  is reconverted into electricity, combining with an oxidizing agent (typically oxygen) through a pair of reduction and oxidation reactions (Fig.2.8).



Fuel cells produce electricity, heat and water, without direct emissions. They can reach electric efficiencies of over 60% (LHV-based), with higher efficiency in partial load than full load [2]. This is a particular attractive characteristic especially in flexible power systems.

Here below the main FC technologies for stationary applications will be presented. Please refer to Table 2.2 for the main technical parameters of each technology.

#### Alkaline Fuel Cell (AFC)

Alkaline fuel cell is the oldest fuel cell technology, being developed for space applications. It is a low temperature FC (60-90°C) with the main advantage of low cost material used for the catalysts (base metals) [8].

It suffers carbon dioxide contamination of the input streams and for this reason only

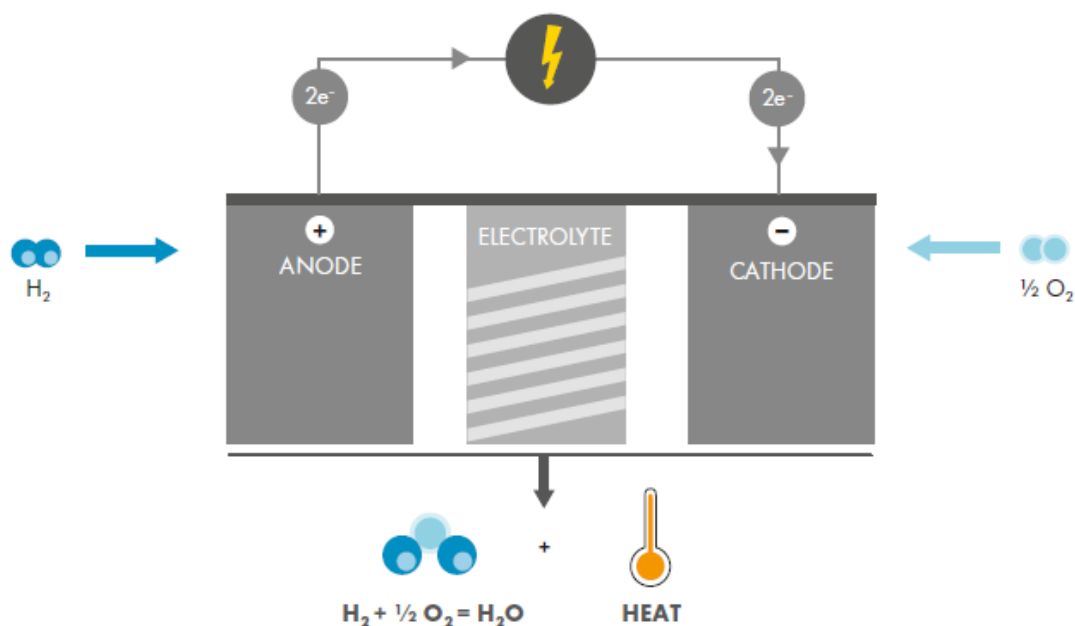


Figure 2.8. Scheme of the chemical reactions occurring in a general fuel cell (source [8])

pure oxygen can be fed. It has a lower durability and output power capacity compared with the following presented technologies.

More recently this technology got back in the public eye thanks to its suitability to generate power from ammonia. Coupled with a cracker to convert ammonia back to hydrogen, they show interesting characteristics as alternatives to current diesel-based off-grid generators.

Existing pilot projects are running in Kenya and South Africa, where off-grid ammonia AFCs are replacing existing diesel generators [2].

### Polymer Electrolyte Membrane Fuel Cell (PEMFC)

PEMFC is a low temperature fuel cell, operating in a T-range of 80-100°C, with a quick start-up time. As for the PEMEC (see Section 2.1.2), the used catalyst is mainly platinum, leading to high construction costs [2, 8].

It requires as input a pure hydrogen stream. Currently, this technology is the most diffused in world market, however there is a rising interest in the Solid Oxide FCs discussed later [8].

### Phosphoric Acid Fuel Cell (PAFC)

This technology falls into the category of the medium temperature range ( $\sim 160$ - $220^\circ\text{C}$ ), with power outputs in the 100-400 kW range [2, 8].

The main difference with the PEMFC is their heat production (at about  $180^\circ\text{C}$ ), which could be used in district heating. The electrical efficiency (LHV) would be relatively

low (40%), but with heat recovery they would reach higher overall efficiencies of about 80% [2, 8].

They have high material requirements, making them less suitable for small outputs range (e.g. mobility sector). They are instead mostly diffused as large stationary applications [8].

### **Molten Carbonate Fuel Cell (MCFC)**

MCFCs operate at higher temperatures (600-700°C), allowing a lower purity requirement for the feeded hydrogen, which can be obtained directly inside the fuel cell, without an external reformer to transform the hydrocarbon fuel (e.g. syngas, MeOH) into  $H_2$  [2].

This advantage marks all the FC technologies which operate at high temperature (like the solid oxide FCs presented below). They present high electrical efficiency (around 55-60%), with the possibility to increase the overall one if HT waste heat is recovered and used for additional electricity generation (up to 85%) [8]. The recovered heat can be used for district heating purposes in buildings too.

Molten carbonate FCs are used in the MW scale for electricity generation

### **Solid Oxide Fuel Cell (SOFC)**

Solid oxide fuel cells present some characteristics which arouse a day by day growing interest in the power generation market, becoming to date the second most important FC type after the PEMFC.

They operate in a high temperature range (800-1000°C) with the possibility of internal reforming of the hydrocarbon fuels like the MCFCs [2, 8].

The main drawback of operating at high temperature conditions is the requirement of appropriate resistant materials and a long start-up time.

However, like MCFCs, they have high electrical efficiency (around 60%) with the possibility to recover the heat for a downstream power generation process or for district heating [8].

They have applications in power generation areas, often at smaller scale in the kW range (e.g. micro co-generation, off-grid power supply) but with increasing output capacity size [2].

Table 2.2 above reports the main characteristics of the most diffused and the most promising FC technologies.

### **Hydrogen turbines**

Hydrogen turbines are an emerging technology well suitable for larger scale electricity production. It has been demonstrated that burning up to 100% hydrogen in a Gas Turbine (GT) is technically feasible.

However, due to its high flammability and flame velocity, high temperatures are reached in the combustion chamber, with material resistance criticisms and  $NO_x$  emissions [2, 45, 46].

A pioneer project in Japan successfully achieved the world's first delivery of electricity

Table 2.2. State of the art of the different fuel cell technologies (Source Shell, 2017 [8])

Technology	Temperature [°C]	Output capacity	Fuel	Oxidant	Efficiency (LHV $H_2$ )	Lifetime	Market development
AEC	60-90	up to 250 kW	$H_2$	pure $O_2$	50-60%	5,000 to 8,000	Mature (space applications)
PEMFC	50-90 (LT)	Up to 400 kW	$H_2$ , gas, bio-gas, syngas, MeOH	$O_2$	30-60%	60,000 (stationary)	Mature
PAFC	160-220	Up to several 10 MW	$H_2$ , gas, bio-gas, syngas, MeOH	$O_2$	30-40%	4,000 to 5,000	Mature
MFCF	600-700	Up to several MW	$H_2$ , gas, bio-gas, syngas, MeOH	$O_2$	55-60%	4,000 to 6,000	Early market
SOFC	700-1000	Up to several MW	$H_2$ , gas, bio-gas, syngas, MeOH	$O_2$	50-70%	3,000 to 4,000	Mature (volumes rising)

and heat using a 100% hydrogen-fueled gas turbine. A 1.1 MW hydrogen GT installed in a cogeneration system was able to provide 1.1 MW of electricity and 2.8 MW of heat to a district of the Kobe city [47].

An Italian project has successfully developed a prototype of a pure hydrogen fueled GT burner, facing with the problem of  $NO_x$  emissions [45].

As for the gas fuel-based GTs, exhaust gas recirculation is considered as possible solution to reduce combustion chamber temperature and nitrogen oxides formation. Another pilot project was conducted in the Italian power sector: in 2010 ENEL, an Italian power supplier, promoted the installation of an innovative hydrogen-fuelled combined cycle power plant at Fusina (Venice) [48]. It provided an output of 12 MW, supplying high-temperature steam to a nearby coal-fired plant.

The project was successfully carried out. However, in 2018 the power plant was closed, being changed the scenario [49]. The hydrogen supply was provided by coal-gasification coupled with a system of Carbon Capture in the power plant of the nearby Porto Marghera.

More recently, South Australian government started a pilot project in Port Lincoln. The hydrogen power plant is composed of a 15 MW Alkaline electrolyser, coupled with a 10 MW pure hydrogen GT and a 5 MW fuel cell [46].

## 2.3 Hydrogen storage

There is a growing awareness in the scientific community about the hydrogen role in the decarbonisation of the energy sector. One issue related to its diffusion is its storage.

Hydrogen can help to manage the grid instability given by non-programmable renewable sources, using the excess electricity in water electrolysis. Furthermore, it can provide a solution in the opposite situation, when there are shortages in peak load situations.

This decoupling between production and demand imposes the need of hydrogen storage.

Before starting to analyze the main storage technologies, it is useful to make a comparison between  $H_2$  energy density and other energy carrier (e.g methane, diesel, gasoline).

Assuming to consider the energy content of each source in a lower heating value basis (LHV), there are two ways to define the specific energy content of a fuel:

- gravimetric energy density [MJ/kg], where energy is specific to the mass
- volumetric energy density [MJ/l], the equivalent volume-based option

Hydrogen has the highest mass-based LHV (120 MJ/kg) with respect to the other fuels ( $\sim 43$  MJ/kg for diesel and gasoline or 50 MJ/kg for methane). However, its volumetric energy density is much lower (0.01 MJ/l), especially if compared with other competitors' range (30-40 MJ/l, with the lower exception of methane, very low too). This property is mainly due to the physical state of  $H_2$  at ambient condition: hydrogen

and  $CH_4$  are gaseous, while diesel and gasoline are at liquid state. It becomes then necessary to increase its density, to make feasible its storage or to find different solutions to limit the problem.

There are two main classes of hydrogen storage:

- physical storage
- materials-based storage

In the following sections the main technologies for the first class, the most mature, and a brief description of the other material-based methods will be presented.

### 2.3.1 Physical hydrogen storage

Physical storage covers those pathways which modify the physical state of hydrogen due to a specific combination of temperature and pressure. It does not require another material (liquid or solid) as storage carrier, simplifying the process.

Hydrogen has a very low freezing temperature ( $-253^\circ C$ ), so the liquefaction pathway is possible, but will require high energy cost in order to reach the final product.

There is also the possibility to store  $H_2$  through compression, reaching high pressure in order to increase its volumetric energy density. Finally, combining these two technologies, cryo-compressed final product is achievable.

Compressed hydrogen ( $CH_2$ ) can be then transported through lorry or via pipeline, whereas Liquid Hydrogen ( $LH_2$ ) via lorry (see Section 2.4).

Below the different possible transformation pathways will be described.

#### Compressed Gaseous Hydrogen ( $CGH_2$ )

Hydrogen pressure between the different steps (i.e. production to end user) assumes different values. Usually, when stored at gaseous physical state,  $H_2$  pressure reaches the highest value in the pathway.

This is due to the necessity, as mentioned above, to increase the energy content minimizing the volume occupied. Modern solid steel or steel composite vessels can reach pressures up to 1000 bar [8]. However, stationary storage applications most common are in the range of 350-700 bar (e.g. stationary hydrogen refuelling stations). For these range of pressure, the volumetric energy density is between 2.9 and 4.8 MJ/l [8].

It has to be noted that when large amounts of gaseous  $H_2$  have to be stored, the pressure does not exceed 100 bar in vessels and 200 bar in underground storages [24]. This is basically due to material properties and operating costs.

Hydrogen can be an interesting solution in the transport sector, with the application on Fuel Cell Electric Vehicle (FCEVs). These vehicles require on-board  $H_2$  storage tanks, which operate at 350-700 bar. Its compression requires the equivalent



of 6-15% of the hydrogen energy content [2, 8, 24].

In large scale industrial applications (steel, chemical) there could be a high  $H_2$  demand. To date the needed hydrogen is obtained through steam methane reforming, where methane is supplied by pipelines.

If renewable  $H_2$  should be introduced, it would become particularly difficult to match its production (or supply) with its demand, especially if a specific dedicated grid is economically unfeasible.

This requires high storage capacity, making the steel vessels to be not competitive. The best solution is underground storage: namely salt caverns or, in absence, exhausted oil and gas fields, aquifers or artificial dedicated structures.

Salt caverns are the best choice because of their tightness and low risk of contamination [2]. Unfortunately, only a small number of these available large reservoirs are salt caverns, being the depleted gas field the most common form of underground storage [8]. The latter would present the additional problem of possible hydrogen contamination, which would require additional costs for filtering.

### **liquified Hydrogen ( $LH_2$ )**

As mentioned before, there is the possibility to store cryogenic hydrogen in the liquid state. The main advantage with respect to the  $CGH_2$  is the almost doubling of the volume-based LHV (8.5 MJ/l) [8].

To achieve the change of physical state of hydrogen, the energy carrier must be cooled down to  $-253\text{ }^\circ\text{C}$  and the main consequence is the high amount of energy required for the process.

To date, more or less 25-35% of the initial  $H_2$  energy content (LHV basis) must be spent. To make a comparison with liquified natural gas, this last process consumes around 10% of the initial amount of natural gas [2, 8, 25, 28].

The liquid hydrogen is then transported through cryogenic trucks and pumped into the tanks of the point of use. When it is needed, it is extracted and evaporated through an heat exchange with the ambient environment, without energy penalties (being liquid at  $-253^\circ\text{C}$ ). However, in addition to the higher energy consumption during liquefaction, this technology suffers from another drawback.

During the store, the problem of "boil-off" arises. It is the spontaneous evaporation inside the tank due to the non-perfect thermal insulation that causes the phase change of small fractions of hydrogen. In order to avoid a dangerous increase of pressure, that would result in a ripple effect of evaporation, the gas  $H_2$  fraction has to be removed. Andersson et al. [24] estimate this loss in  $\sim 0.1\%$  of the hydrogen content per day.

### **Cryo-compressed Hydrogen ( $CcH_2$ )**

There is a possible pathway which consists in the combination of the two previous storage methods. Thanks to the Gay-Lussac's law, reducing the temperature of an ideal gas and keeping the pressure constant, the volume decreases proportionally to the first.

In this way volume reduction is possible due both to the compression and the cooling

process, gaining in energy density at the expense however of additional energy inputs of about the 9-12% of the final  $H_2$  energy (LHV basis) [8, 50].

$CcH_2$  is then transported through insulated trucks to the final tanks of point of use where it is injected.

In Table 2.3 the main properties and energy penalties for hydrogen storage technologies are reported.

Table 2.3. Main properties and energy consumption in the hydrogen storage options

Technology	Volumetric energy density	Current energy penalty <sup>a</sup>	Ref.
$H_2$ compressed ( $CGH_2$ )	2.9-4.8 MJ/l (350-700 bar)	6-15% of $H_2$ energy content	[2, 8, 24, 50]
$H_2$ liquified ( $LH_2$ )	8.5 MJ/l	30% of $H_2$ energy content	[2, 8, 24, 50]
$H_2$ cryo-compressed ( $CcH_2$ )	> $CGH_2$ case	9-12% of $H_2$ energy content	[2, 8, 24, 50]
$H_2$ in metal hydride ( $MgH_2$ )	~ 10.2 MJ/l	~32% of $H_2$ energy content <sup>b</sup>	[2, 8, 24, 50]

<sup>a</sup> on a hydrogen LHV basis

<sup>b</sup> composed by a power consumption during the storage ( $0.7 \text{ kWh/kg}_{H_2}$ ) and a heat amount required for the release ( $10 \text{ kWh/kg}_{H_2}$ ) [24]

### 2.3.2 Material-based hydrogen storage

This class of storing methods involves the necessity to store hydrogen in solids, liquids and on surfaces. Being these technologies still in development, they will be only mentioned.

Material-based media can be divided into three main classes:

- Metal hydride storage
- Liquid organic hydrogen carriers (LOHCs)
- Surface storage systems (sorbents)

The first typology uses metal surface in which hydrogen is adsorbed and forms interstitial compounds with the metal, releasing heat. The further extraction can be obtained through an heat input. Typical metal used are palladium, lanthanum and magnesium [8]. The most promising elemental metal hydrides for large-scale stationary storage are magnesium hydride ( $MgH_2$ ) and aluminum hydride ( $AlH_3$ ) [24].

To date, they are the only reversible solid-state  $H_2$  storage commercially available. This solution could be especially attractive for stationary storage. This because it has a very low-performing gravimetric energy density due to the high metallic presence [27].

However, the main advantages of the metal hydride storage are the wide operating pressure range, which enables to have excellent compatibility with fuel cells and electrolyzers and the high volumetric energy density [27].

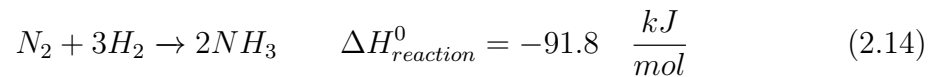
LOHCs are an interesting option, because they are chemical compounds with good hydrogen absorption properties. They have similar properties to crude oil and oil products. They absorb  $H_2$ , transport or store it and then release it in pure form. The key advantage is the possibility of transportation without particular difficulties. However, most of them cannot be reused once hydrogen is created back at the end of the process and must be sent back to their place of origin [2].

Last material-based storage class includes all those materials with high specific surface areas that enables the hydrogen adsorption. For further information on material-based hydrogen storage, please refer to [26].

### Hydrogen to ammonia ( $NH_3$ )

Hydrogen can be stored not only in its physical pure form or through the utilization of external materials. As seen before, it can be transformed into different energy carriers (e.g. methanol), which are much easier to be transported and stored. They can be then reconverted to produce  $H_2$  in fuel cells (see Section 2.2.5).

Another interesting possibility in hydrogen storage is its transformation into ammonia, using the industrial Haber-Bosch process. The chemical reaction is the following:



The obtained  $NH_3$  can be stored and transported in liquid conditions at non-prohibitive conditions ( $\sim 9$  bar and  $20^\circ C$ ), allowing the use of inexpensive pressure vessels [20].

Ammonia can be used as a liquid fuel in some internal combustion engine, in particular in the naval sector. It has an easier handling with respect pure hydrogen, because of its narrower flammability limit and lower burning velocity [16, 20].

As a  $H_2$  carrier for fuel cells, ammonia can be reconverted through thermal decomposition and electrochemical process, obtaining compressed hydrogen ( $\sim 20$  bar) [23].

The  $NH_3$  production from hydrogen reaches a total energy efficiency of about 67%, with the main advantage that the system can cover its own consumed electricity, without the need of an external supply [20].

Further information can be found in [21, 22, 28].

## 2.4 Hydrogen transportation

There are different ways to transport an energy carrier like hydrogen, depending on its physical condition.

As mentioned above, material-based  $H_2$  storage is suitable more for stationary applications, thus in this Section only physical hydrogen transportation will be discussed.

Compressed gaseous hydrogen ( $CGH_2$ ) has currently two main ways to be transported: through lorry or via pipeline. Liquid hydrogen ( $LH_2$ ) instead is transported by lorry.

It is important to remark the distance range that has to be considered: our analysis is confined in the national border of Italy. The overall distance is in the order of magnitude of 1400 kilometers.

When longer distance has to be covered, other solutions could become more suitable, with respect to transportation by trucks: pipelines or shipping could be interesting options.

It must be kept in mind that to date the majority of  $H_2$  demand is either produced and consumed on-site ( $\sim 85\%$ ) and only a small fraction is transported ( $\sim 15\%$ ) [2]. Here are presented the most common option for transport.

### 2.4.1 Compressed gas containers

Compressed gaseous hydrogen can be transported in small-medium quantities in specific pressurised containers by a lorry.

To date, the largest tank volume for  $CGH_2$  transport is 26 cubic meters at 500 bar, which means roughly to 1,100 kg of hydrogen [2, 8].

However, this weight is rarely achieved in practice, because of the limit on the maximum allowable pressure. This sets a maximum transported load of 280 kg of  $H_2$  [2]. They are currently a cost competitive solution for distances less than 300 km [2].

### 2.4.2 Liquid transport

Highly insulated cryogenic tank lorry can carry much higher amounts of hydrogen (up to 4000 kg), thanks to its higher density in liquid phase. Today, they are a common option for distances up to 4000 km [2].

Above this distance problems of  $H_2$  heating and spillovers arise, making this option not suitable anymore.

For longer distances a possible solution could be the shipping. However, there are currently no ships that can transport hydrogen in pure form [2]. Their structure would be similar to LNG ships.

If hydrogen has to be shipped overseas, there could be two more competitive ways than liquified  $H_2$  transportation: it could be shipped as ammonia or in a Liquid Organic Hydrogen Carrier (LOHC) [2].

### 2.4.3 Pipeline

Pipelines are likely to be the least-costly solution for distances below 1500 km in the long term, given a sufficiently large and localised demand [2, 8].

The main drawback is the need of a high initial investment, justified only if a large hydrogen volume is involved. On the other hand, they present low operational costs and a wide lifetime (between 40-80 years) [2].

Developing a new hydrogen transmission grid would require strong coordinated investments by many different market players, which could be really challenging to be implemented. For this reason a different solution which involves existing structures could be considered.

#### 2.4.4 Hydrogen blending in existing gas grid

This could be an interesting option to avoid the significant capital expenditures required to build a new dedicated  $H_2$  transmission grid.

Hydrogen could be blended with methane and transported through an already existing and well diffused grid.

The upper limit for hydrogen blending depends on many factors, but basically the component of the  $H_2$  chain (from the supply to the end-user included) with the lowest tolerance will determine the hydrogen limit [2].

For example, cooking appliances and gas heating systems are currently certified for a blending of  $H_2$  up to 23% (volume basis) in Europe, while in the industrial sector limits are lower. The existing control systems in power generation (e.g. with gas turbines) are not designed for hydrogen properties, thus they can tolerate only a 5% blending, rising to 10% with limited investments [2, 5].

The Italian NG transmission operator SNAM has successfully conducted a pilot project in the province of Salerno to supply 5% blending of hydrogen in the Italian gas transmission network to two industrial companies [51], recently increased to 10% [52]. The new compressors and turbines could work with  $H_2$  blending up to 30%, as long as this percentage is kept stable. Current pressure gas pipeline can handle blends up to 10%, with the possibility to increase up to the transmission of pure hydrogen with limited investments [5].

Hydrogen blending could be considered an option to supply  $H_2$  to end-users which need it in a pure form.

Some hydrogen separation membranes, based on a heated metal foil (typically a palladium alloy) are under investigation. They offer the possibility to separate the blended  $H_2$  from the mixture of methane. However, they require a minimum hydrogen concentration ( $\sim 15\%$ ) and specific operating conditions to be effective [53]. In Section 4.3.4 the background hypothesis behind the application of this technology will be discussed.

## 2.5 Use of excess heat from hydrogen processes

In the previous Sections the main processes related to the hydrogen and its related hydrogen-based fuels pathways were presented. The main supply steps from the production, transportation and possible storage were analysed.

However, many technologies are characterized to have an highly exothermic process. In the reactors the temperature management is often a criticism, in order to keep the kinetics under control and to avoid catalyst material degradation.

The generated heat in excess must be taken out the reaction environment. In the following section the different possibilities will be considered, stressing their application limits and their strength.

### 2.5.1 Possible utilization pathways

There are thus two good reasons to recover this excess heat previously proposed. The first is more physically related to the main reaction operating conditions management. The second is the possibility to increase the overall process efficiency, by diminishing waste energy, with the non secondary effect to supply an additional power/heat external demand.

Recovered heat can be used in two different ways. It can play the role of an hot source for a bottom power generation cycle or can be directly used as heat carrier.

In the following Section these two possibilities will be described, with their strength and main drawbacks.

#### Power generation via Organic Rankine Cycle (ORC)

When there is the availability of a sufficient thermal energy, one possibility to increase the overall process is to consider this source to produce additional power. For example, in large Combined Cycle Gas Turbine (CCGT) power plants the hot exhaust gases are recovered to supply heat in a bottom Steam Rankine Cycle (SRC).

For those cases where hot recoverable source has unfeasible characteristics for the use of water steam, other working fluids had been investigated.

There exists a wide family of organic working fluids, each of which with specific properties optimised for a specific operating condition.

Rahbar et al. [54] provide a list of the most common organic working fluids categorizing them based on heat source temperature and their critical temperature.

The fluids are grouped in three main classes:

- Low-temperature fluids, those ones resulting the optimal choice with hot sources providing heat at temperature  $< 150^{\circ}\text{C}$ ;
- Medium-temperature fluids, where the hot source stays in a range between  $150\text{-}250^{\circ}\text{C}$ ;
- High-temperature fluids, with temperature range between  $250\text{-}400^{\circ}\text{C}$ ;

The maximum evaporation temperature is imposed by the critical temperature of the organic working fluid. This is one of the decision parameter to identify the best configuration of an ORC, given the heat source properties.

Another point to be stressed is the difference with the classic Steam Rankine Cycle: due to its properties, water requires superheating to avoid condensation problems in the expander. Organic fluids typically do not have this problem, resulting in less technology complexity of the cycle [54].

ORC are suitable with a wide range of hot source temperature, covering many potential excess heat production technology.

Feasible coupling structures are the cooling system and the exhaust gases from Internal Combustion Engines (ICE), or small GTs with exhaust gas temperature too low for the combination with a normal steam Rankine cycle [55].

To date, there is a growing interest with renewable sources such as geothermal energy, solar irradiation or biomass.

This solution suites well for those application where small power production is needed. However, excess heat coming from the hydrogen related processes has different properties (e.g. temperature and capacity) for each case.

This implies the necessity to study which organic working fluid is more suitable for the specific heat recovery, with expensive computational energy.

### **District Heating (DH)**

The second possible type of use of the excess heat produced by the mentioned exothermic reactions is its application to supply a heat demand. It results necessary to exchange the heat from the hot source (e.g. exhaust gas of an industrial process) to an energy carrier that is subsequently stored.

In literature there are three developed DH generations. The first generation, established until 1930, used steam as heat carrier.

Successively system based to pressurized water as heat carrier emerged and diffused until the 1970s. They were characterised by supply temperatures higher than 100°C [56]. The latter generation was introduced during the 1970s, replacing the major share of the systems in the 1980s.

The main differences were the possibility to use system of prefabricated insulated pipes directly buried into the ground and a supply temperature typically below 100°C.

In the most recent period there had been a focus on lowering the distribution temperature, reaching a new temperature frontier, with supply temperature below 50-60°C. This new class represents the 4<sup>th</sup> generation DH [56].

To date, there is a consistent heat recovery potential from various renewable sources, such as solar thermal energy and geothermal one, in addition to the industrial waste heat and the exhaust gases from a GT installation.

The main advantage of this fourth low temperature generation class would be the easier integration with a wide range of excess heat systems. Their combination could be increased with a system of Thermal Energy Storage (TES), which would decouple

the heat supply with its demand.

There are two families of TES connected to district heating networks: a practical review of their main differences can be found in [57].

The first class is the daily storage, typically used to shift the daily peak of heat production to fill the daily thermal lows. A common solution are water tank storages, distributed along the network.

The second family is represented by long-term TES, which enable the possibility to store thermal energy in hot season (but also cold in winter) and release it when necessary. They can be pit, tank or aquifer storages [58].

There are different types of seasonal thermal energy storage:

- Sensible heat storage, a technology widespread and with a consistent background;
- Latent heat storage, that is still in development at a laboratory level. Compared to the first class, it offers a higher thermal density;
- Chemical storage, still at a research level, which offers high thermal density and very low thermal losses.

One important drawback concerns thermal losses, due to the long storage period. This determines the low temperature store of heat to lower thermal losses.

District heating systems are generally located near densely population areas, thus the need of large TES could represent a limit in terms of space requirements. However, the possibility to link DH network to the processes related to hydrogen generation can be a driver in the choice of their location and size. Several variables should be considered, such as where the demand is located, the availability of renewable electricity, the transmission costs, land usage and the possibility to recover heat.



# Chapter 3

## Hydrogen in energy system models

The aim of this chapter is to present and summarize the existing methods that describe the current energy system and return possible evolution scenario. There will be a classification of the most important characteristics of an energy system model, underlying their strengths and weaknesses.

The chapter continues with a description of the current models that have already implemented the hydrogen handling in the studied system.

### 3.1 Review of energy system models

Once the definition of the possible pathways and the main processes allowed in the energy system is accomplished, a wider awareness about the feasible scenarios becomes necessary.

Energy system must be studied from a global perspective to define which possible evolution could be achieved. For this purpose, energy modelling has been implemented since the 90's.

Forecast analysis of large-scale energy systems has gained increasing attention in the recent years, trying to study what are the possible future scenarios, given projected evolution trends.

The typical main focus of these models is the integration of the unpredictable renewable energy in the system and the transformation of the existing one that would occur as a consequence.

#### 3.1.1 Model classification

There exist many different classes of models, each one developed to try to answer to a specific need. It is necessary to clarify the goal: different purposes lead to different designs and hypothesis, with the result of different models.

Secondly, models are different in terms of scale. They can operate at national or regional scale, with a different level of detail and time horizon.

All these distinctions make impossible to compare all kind of models directly. It becomes clearly necessary to focus on a limited number of models with comparable characteristics.

### **Time horizon, time interval and time step**

In this Section will be depicted the differences related to different time horizons. As mentioned before, there exist lots of possible classifications for the energy models. This implies a concrete risk of misleading or overlapping in definitions.

The main distinctions driver between the classes can be the time horizon and the analysed level of detail.

First, it is necessary to better distinguish between time horizon, time interval and time step.

The former wants to represent the event period that the model has to simulate (e.g. the period today-2050) . The time interval notion describes the boundary within the model returns the results (e.g. at distance of 5 years), while the latter, time step, is the level of detail at which the model analyses the scenario (e.g. annual values).

There exist models that are designed to analyse transition scenarios. Typically these scenarios cover long-term periods, requiring a long time horizon (e.g. the period 2020-2050).

To limit computational problems and to reduce the data matrix to be computed, they use a lower time-step degree of detail (typically annual).

When the time horizon can be limited, the main gain is the possibility to strengthen the time step. Model can use an hourly time step (or even more detailed one).

The main consequence is the possibility to analyse all the daily fluctuations between demand and supply, what technologies are involved and the required storage.

However, it is possible to implement an analysis combining two models with different time characteristics: a model with a hourly time step can be used to analyse more in detail the annual results coming from a model with a long time horizon. It is the case of the model presented in this thesis work, in which the analysed time horizon is the single year 2050, providing annual results with an hourly time step. Further information can be found in Chapter 4

### **Optimisation v. simulation models**

In literature, there exist plenty of classification criteria. Lund et al [59] introduce two macro classes: optimisation models and simulation ones.

. The first type has an objective function that has to be optimised given a set of constraints. They often use the current energy system as a starting point to identify the optimal solution in the long term, i.e. the optimal evolution of a number of decision variables (typically, installed capacities and related investments). [59].

The objective's choice has a significant impact on the result of the final energy system design. It's important to define the inputs in the most accurate possible way, existing a high uncertainty related to some hard to predict variable (e.g. technological innovation,

future fuel price fluctuation).

For this reason optimisation models use the current system as a starting point, being very detailed for the current energy system [59].

While optimisation models are searching for the optimal way of reaching a specific goal (typically the least-cost solution), given certain assumptions and constraints, simulation models based on an accounting approach are used to evaluate the performance (e.g. primary energy demand, CO<sub>2</sub> emissions, costs) of alternative energy system configurations [60]. Broader simulation models can also be used to study the effects of the adoption of possible energy policy measure [61–63].

### Top-Down v. Bottom-Up models

Another useful classification is given by Herbst et al [64], where the *Top-Down* model and the *Bottom-Up* one are defined.

The former tries to use the economy of the system at global scale as the driver for the definition of the results, assessing the effects of energy-related policies in monetary units.

Energy sector and its economy are then analysed in an aggregated view, being the energy technologies not explicitly represented in the model [64].

They are part of a more general class, called *Computable General Equilibrium (CGE)* models, whose characteristic is the bundling of the sectorial classes in homogeneous macro-groups.

The absence of this detailed sector characterisation sets strong limits of application for this kind of models, especially in long-term analysis with strong deviation from the benchmark scenario [65].

Most energy system models are *Bottom-Up* models. This class has a relatively high degree of technological detail with respect to the former, in order to better evaluate future energy supply and demand.

They can give detailed evaluations of technology-specific policies (e.g. prerequisites and consequences for PV diffusion). However, this high level of detail implies a heavy dependency on the data availability.

In addition, another limit of this class of models is the neglect of macro-effects given by the radical introduction of a specific technological change on the overall economic activity [64].

This type of model belongs to the general class of *Partial Equilibrium (PE)* models, where the constraints to match demand and supply is limited only to the energy sector.

They need socio-economic data (e.g. GDP, population's growth) in input, in order to return as result the least cost energy system configuration that reaches the goal.

There is the possibility to benefit from the strengths of both model types by combining their analysis. Long-term macro-economics considerations can be obtained as an output from the results of the CGE model and become inputs for a *Bottom-Up*

one. The latter will analyse the required scenario and define the technology mix required by the energy system to reach the target.

The model presented in the thesis will benefit from the macro-level information obtained by a *Bottom-Up* long-term energy model to deeply analyse the Italian energy system in a confined time period in the future. This will be possible thanks to the characteristics of the *Bottom-Up* class explained before.

### 3.1.2 Hydrogen in energy models

In this Section there will be a focus on those models that started to implement the hydrogen handling following the distinction criteria mentioned above. An example of existing long-term horizon model and a short-term one will be presented.

A very diffused long-term class is the International Energy Agency (IEA) model generator TIMES: the acronym means The Integrated MARKAL-EFOM System. It was developed by the IEA-ETSAP, the Energy Technology Systems Analysis Program, an international community whose goal is the in-depth energy system analysis [66].

TIMES is a *Bottom-Up* model generator, which results the least-cost energy system given a list of constraints over a typically long-term time horizon. It represents with high technological detail all the energy supply chain from the primary resources to the final end-users.

This class is composed of three element types:

- Commodities, all the products that characterize a multi-steps process. They include energy carriers, related emissions and monetary flows.
- Processes, the representations of the involved technologies for converting a commodity into another one (e.g. a power plant which produces electricity from a fuel).
- Commodity flows, substantially the link between the commodity and the process which produces/consumes it. This category has the same nature of the commodity one, but is used to indicate the specific energy carrier related to a specific process. A clarifying example could be the following. Coal is the general commodity, the coal pulverized power plant the process and as commodity flow the specific quantity of energy carrier (coal) that is consumed in the time-step by the technology.

The model generator always starts from a reference scenario, obtained with a first run without any type of constraints.

It is important to note that often the obtained scenario differs from the national energy projections, which are based on simulating future energy demand and supply, this because TIMES provides the least cost optimization solution [66].

An interesting version is the JRC-EU-TIMES model developed by the European Union Joint Research Center [67].

It is a linear optimisation bottom-up technology model that represents the EU energy system from 2005 to 2050. Each country represents one region. The model considers both the supply and demand sides and the equilibrium is driven by the maximization of the total surplus, the sum of producer surplus and consumer one.

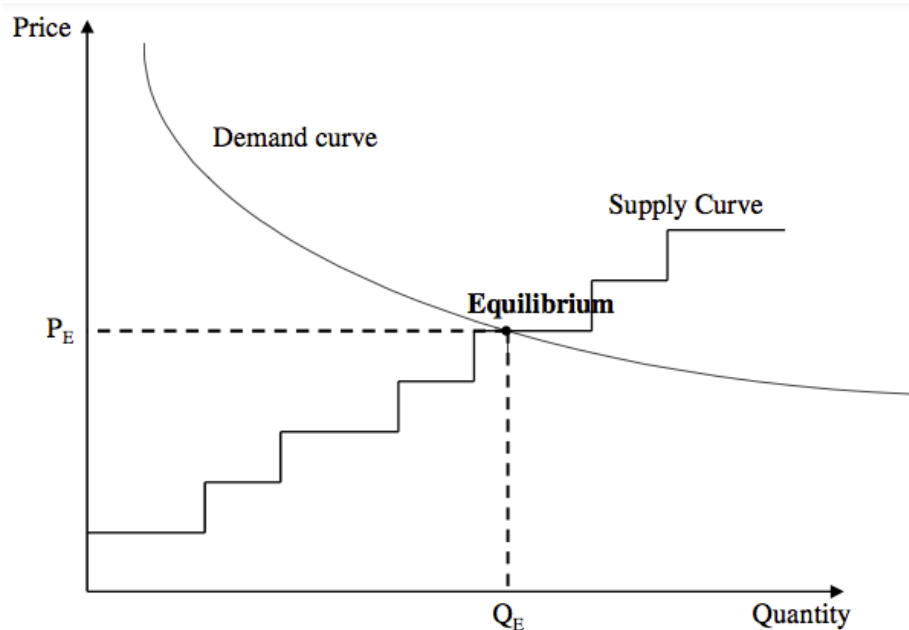


Figure 3.1. Scheme of the market equilibrium between demand curve and supply one (credits to [68])

As can be seen in the following graph (Fig. 3.1), the demand curve represents the sum of willingness to pay of each consumer for a given commodity, the maximum price a user will be able to buy the product. The supply curve consists instead on the reservation price, the minimum price at which a producer will sell its product. The price obtained by the optimal equilibrium is called equilibrium price ( $P_e$ ) and is the market one at which products will be sold and bought. Finally, the consumer surplus is the integer of the differences between each willingness to pay and  $P_e$ , while the producer one is the integer of the differences between  $P_e$  and each reservation price.

As *Partial Equilibrium* class, JRC-EU-TIMES does not model the economic interactions outside the energy system. It does not return a macro-economic analysis, but the detail of used technology, the involved commodity flows for each energy carrier for each region and every time step.

Economic outputs (e.g. operation and maintenance cost, investment costs, commodities prices) are obtained for every time step [67].

It is important to underline that this long-term model has an annual time step, and each year is further divided in 12 time-slices. The latter represent an average of day, night and peak demand for each one of the seasons: this means that there will be a

summer day demand, a summer night and a summer peak one [67].

Short-term time horizon models have a more specific time step frame. For example the model that will be presented in the thesis has an annual horizon with a hourly time-step.

This enables the possibility to deeply analyse the fluctuations between demand and supply, making considerations on what technologies are involved and the required storage capacities.

Another example of existing energy models that implemented the hydrogen discussion was proposed in the technical report of Navigant [3], where scenarios for optimised gas supply chain are presented.

The main focus is on the production and retail of methane from sustainable alternatives with respect to the fossil-based one.

However, to meet the decarbonisation goal, not only methane-based pathways were analysed. In addition to biomethane, also biofuels and hydrogen were studied.

Navigant energy system model is built using Analytica software, which allows the study of various decarbonisation scenarios options in a multi-sector system. Providing the minimal societal cost given the availability of  $H_2$ , biomethane and biofuels, the model falls into the optimization class.

The objective function has the goal to minimize the energy system costs, using as decision variables the sectorial technology shares and the deployment of gas-fired power plants in the power sector. The model has to respect specific constraints such as the equilibrium between allowable energy carrier demand and its feasible supply [3]. The characterization has an high level of detail, with the possibility to distinguish different sectors and several subsectors, with a detailed description of the technologies involved.

This means that the presented model takes part of the previously described *Bottom-Up* class.

One strong limitation of this study is the fact that only results and a brief description of the model performing steps are presented, while its core is not publicly available. No considerations on the hypothesis or modifications on the code can be made.

In long-term projections any collaboration between different entities can only have positive effects on the knowledge spillovers. Furthermore, the latter can increase society awareness of what has to be done in order to reach the decarbonisation targets. It is also for this reason that the model presented in the thesis is in the public domain, welcoming any possible external improvement.

# Chapter 4

## Model development

The aim of this Chapter is to introduce the conception of the problem and its schematic design before to get into detail of the model development.

The goal is to develop a model in which to implement all the process related to hydrogen production and consumption. In the first part a detailed introduction of the model framework *oemof* is presented, in order to clearly define the analytic background and then the logical structure of the Scheme of the Reference Energy System (SRES) scheme. This latter wants to illustrate all the relevant flows that characterize a specific process transformation.

Once the setting of the logic structure is complete, the initial structure of the model is introduced, followed by the implementations added to the origin.

Subsequently, there will be the definition of the background hypothesis and a detailed description of the technological data assumptions will be provided.

### 4.1 Oemof framework

In this Section the pillars of the model will be presented, starting from its working framework, *oemof*.

Oemof framework, whose acronyms means Open Energy MOdeling Framework, is an open source flexible model generator, with many interesting characteristics [29].

It allows cross-sectoral multiregional analysis of the energy system, with the possibility to set different time-step resolution.

It is implemented in Python, using several Python packages that allow to reach high temporal and spatial resolution. This results in a more realistic representation of the technology mix and its interconnections in the energy system that has to be studied. Energy system models often do not have publicly accessible source code and often are developed for a limited specific application, making difficult its adjustment to other requirements.

Thus, its flexibility and the possibility of external implementations were important drivers to develop the model presented in the thesis using this framework.

In the following sections first the analytic background and then the logical components of *oemof* framework will be illustrated.

### 4.1.1 Analytic background

The model generator is structured to solve a linear optimization problem, using Linear Programming (LP). This method allows to achieve the best outcome in a mathematical problem represented by linear relationships.

The goal is to optimize a linear objective function, whose examples typically are profit maximization or lowest cost configuration, given some linear constraints.

The problem to solve is an optimization problem wherein the objective function is a linear function, which has the form

$$f(x_1, x_2, \dots, x_n) = c_1x_1 + c_2x_2 + \dots + c_nx_n \quad (4.1)$$

for some  $c_i \in \mathbb{R}$   $i = 1, \dots, n$ .

The feasible region is the set of solutions to a finite number of equality and inequality constraints, of the form

$$a_{j1}x_1 + a_{j2}x_2 + \dots + a_{jn}x_n \geq b_j \quad j = 1, \dots, s. \quad (4.2)$$

and

$$a_{j1}x_1 + a_{j2}x_2 + \dots + a_{jn}x_n = b_j \quad j = s + 1, \dots, m. \quad (4.3)$$

Typically there is an additional constraint set, that is the non-negative condition for the decision variables:

$$x_i \geq 0 \quad \forall i = 1, \dots, n \quad (4.4)$$

The formulation can be expressed in the matrix form:

$$\min\{\mathbf{c}^T \mathbf{x} \mid \mathbf{A} \mathbf{x} \geq \mathbf{b} \wedge \mathbf{x} \geq 0\} \quad (4.5)$$

Before starting the declaration of the problem structure in the studied LP, it is useful to better define each mathematical expression.

It will be called *decision variables* those variables that represent levels that the decision maker would like to determine, such as production, consumption, transportation rates of specific energy carriers. They are the unknowns of the model and their optimum values are obtained as result of the optimization process.

To each decision variable ( $x_i$ ), a cost per unit change in the variable ( $c_i$ ) is associated. These values are named *Cost coefficients*.

The core of the optimization problem is the *objective function* (Eq. 4.1), an equation that represents the cost (or the profit) related to the decision variables. Being the goal of the model to return the least cost configuration mix of the energy system, the objective function would pursue a minimization cost objective.



Once decision variables and their coefficients are defined and have constituted the objective function, there might be the necessity to add *constraints*. They represent the restrictions or limitations on the decision variables. They are not required if resources are unlimited, but it is not the case of a general energy system, where availability of resources has a strong impact on the overall balance.  $a_{ji} \forall j = 1, \dots, m$  and  $\forall i = 1, \dots, n$  are the technological parameters while  $b_j \forall j = 1, \dots, m$  are the known coefficients.

Last typical definition regards the *non-negativity* constraint for the decision variables. In a LP problem, they typically should take non-negative values.

The problem analysed by the model is a minimization cost one, where the LP is used to determine the least cost configuration of the overall energy system. Oemof framework allows a high level of cost settings. In this work the core of the analysis is to define the power generation mix that respects the given constraints, returning the lowest cost requirements. Equation 4.1 represents the typically cost function that can be expressed as follows:

$$C_{Total} = C_{Investment} + C_{Operating\&Maintenance} \quad (4.6)$$

Where the first term represents those expenditures that do not rely on the production output (e.g. CAPEX), while the second ones are the costs which depend on the level of output, here energy carriers.

An important clarification on cost definition is here mentioned, but it will be better explained in the Section 4.3.3. The goal of the thesis was to develop a model with which it was possible to define the most convenient power generation mix of the system from the point of view of pure energy consumption, that would be necessary to meet the decarbonisation targets.

Following this driver, only operating cost related to raw material supply were considered in the model. Costs concerning the building and the maintenance of each technology were intentionally excluded from the analysis.

Oemof however, allows to make a cost optimization considering both  $C_{investment}$  and  $C_{O\&M}$ , returning the optimized installed capacity for the investigated technology. Here below the investment optimization option is presented.

### Investment optimization

In this Section the economics background of the *Investment optimization option* is presented.

Oemof allows different linear optimization settings, enabling the possibility to compare different analysis using the same open-source framework.

An interesting customization is the opportunity to consider the capital expenditures related to a technology in order to define the trade-off of its installed capacity. This can be particularly helpful to compare processes which produce the same output that might be in competition, especially if they are not commercially available yet (with a

low TRL).

The option needs few information to work.

First the economic parameters are presented. It is necessary to estimate the capital expenditure (CAPEX) referred all to the same quantity, typically the output capacity (e.g. € per MW of product).

The second and more difficult to be determined is the *WACC*, the Weighted Average Cost of Capital. This is the expected average rate to be paid by a company to its holders to finance a specific project.

It can be expressed with the following equation:

$$WACC = \frac{D}{D + E} C_{debt} + \frac{E}{D + E} C_{equity} \quad (4.7)$$

where  $D$  is the total debt,  $E$  is the total shareholder's equity,  $C_{debt}$  is the cost of debt, and  $C_{equity}$  is the cost of equity.

Once economic coefficients are estimated, the following step is to define the expected lifetime of the analysed technology. With this three information, it becomes possible to estimate the *EPC*, the Equivalent Periodical Cost of the investment.

The latter represents the amount of the investment that has to be repaid for each period of time considered. Thus, if the simulation covers a year, this cost coincides with the equivalent annual costs.

It is calculated as follows:

$$EPC = CAPEX * \frac{WACC * (1 + WACC)^{lifetime}}{(1 + WACC)^{lifetime} - 1} \quad (4.8)$$

Once the economic parameters are set, two other input data are required by the investment optimization option. The former regards the capacity of the investigated technology that already exists in the system, while the latter determines the maximum capacity that can be installed in the system.

As reported before, the main criticism of this option is the estimation of the economic parameter, especially the *WACC*. If a technology has a low TRL, meaning that there are no commercially available installations, it becomes difficult to estimate the possible cost of capital.

The estimated CAPEX expected for the time horizon (e.g. 2050) might be over or underestimated with respect to the real one, that would be consequence of the spread of that technology. An example might be the fall in capital expenditures required for BEVs during the last period or the PV technology during the last 15 years.

For these reasons and for assumptions presented in Section 4.3.3 in the scenario setup presented in the following Chapter 5, investment optimization will not be used.

### 4.1.2 Oemof logic structure

Once the analytic background of the framework has been defined, the next step is to introduce the logical components that constitutes the model generator. This becomes relevant to explain the logical behaviour that is behind the SRES structure.

In the following Section, the three main concepts of *bus*, *flow* and *transformer* and their subclasses will be presented.

#### Bus

Introducing the TIMES model generator structure (see Section 3.1.2), three pillars were mentioned: commodity, commodity flow and process. The first one, which typically represents the energy carrier and its properties, can be described through the *bus* concept.

Basically it represents exactly the same characteristics covered in the TIMES model generator. In the SRES scheme, buses represent all the energy carriers generated or used by those processes.

Bus is the tool that collects all the specific properties (energy content, emissions related, extraction costs etc.) of a commodity.

In reality, frequently more than one single transformation process is required to supply power at the desired conditions to the end-users.

There will be necessary a bus for representing the raw material (e.g. biogas) going in the first transformation plant (e.g. biologic methanation power plant). The exiting energy carrier (methane) requires a new bus to bring its information to the following transformation process (e.g. a Combined Cycle Gas Turbine (CCGT) power plant), where is finally converted into electricity, delivered to the final user with a third bus. However, the interconnections between different technologies and the mentioned commodities have to be described through a different concept, which will be presented below.

#### Flow

As anticipated in the previous Section, oemof framework is very similar to the TIMES model generator. Once a commodity has been defined, its link with the process must be defined.

*Flow* concept represents all the quantities of a specific commodity that are consumed or produced by a technology. It indicates all the exchanges between processes and a bus. In the previous example, it quantifies the consumption and production rates of each energy carrier within each technology in the supply chain.

#### Transformer

Once the commodities and the linked flows are defined, it's time to define the technologies that change the energy carrier's properties. They are called *transformers*.

Their nomenclature is quite effective in defining their function. A transformer is the tool required to generate one or more outputs with specific common features, fed different commodities in input.

A distinction had to be implemented in the model to distinguish processes with different properties. In the schematic representation the only useful distinction was the one between *transformer* and *transformer with n outputs*.

The former has one single output, while the second class has more than one.

There however exist other subclasses of *transformers*, with some peculiarities, which will be described below.

### Source and sink

It might seem that the information provided by the *buses* (representing the commodities), *flows*, that show the rates of a used/produced commodity, and the *transformers* (to define the involved processes) would be enough to completely represent the energy system for the hydrogen path.

However, two information are still missing: where the first "raw material" bus comes from and where has to be used the final energy carrier. They can be described with two subclasses of transformers.

Keeping the left to right logic of the scheme, the former is implemented in the *source* class.

This tool is characterised to have only an output flow, and can be seen as the representation of all those steps from the extraction of the energy carrier to its purchase to the energy system (i.e. import, extraction, production).

In a similar manner to *source* tool, the last step of the energy system, the final demand, can be represented through the *sink*.

This latter has the same particular configuration, allowing this time only a single stream in input. It represents the demand of the pure energy carrier at its pure form.

### Storage

Last class that completes the energy system describes the possibility to store the energy carrier for a specific period of time. *Storage* is the tool that allows the decoupling between the demand and the supply.

It comes into play in those situations like over-generation, when there is an excess of intermittent renewable energy production (e.g. PV during a clean-sky day in summer), or in the opposite case when there is a peak in the demand (i.e. a winter afternoon). It enables the accumulation of a resource to be used when necessary. For this reason, it allows only one input and one output. Furthermore, the exiting flow has to have the same

### Excess and shortage flows

Buses allow to transfer the properties of a commodity from a process to the next one. However, in the energy system processes are not the unique receivers or producers of

the mentioned commodity.

There can be a situation in which source, sink and storage classes are not enough to allow the model to reach the energy system equilibrium. This happens when the model cannot allocate each bus to all its destinations in the specific time-step.

For example, a fixed source (e.g. a wind power plant) might generate a too big output commodity flow (e.g. electricity) that in the specific time-step cannot be managed by the grid.

In this situation, there would be a quantity of the flow electricity that should be "wasted" in order to allow the model to continue the optimization.

For this reason *Excess flow*, a fictitious commodity flow was introduced. The latter has a complementary solution, the *Shortage flow*.

Shortage flow is required in those situation in which the produced commodity flow is not enough to supply a subsequent transformer/sink. For example, if a constant demand cannot be supplied by the technology mix in the specific time-step, the model would not return the results.

In a high temporal resolution model, if the equilibrium mismatch happens in a single time-step, this could make the optimization process conclusion impossible.

It results then necessary to enable the model to bypass the obstacle, without losing the information of when and where the mismatch occurred.

In an ideal perfect structured energy system representation, the excess and shortage solutions should be obviously unnecessary. However, to guarantee a minimum flexibility to the model, especially because of uncertainties related to hypothesis or limited data availability, for some commodities excess and shortage are considered.

## 4.2 Scheme of Reference Energy System (SRES) description

Once the specific commodities and the processes are presented in their different categories, the SRES representation can be introduced.

SRES, whose acronym means Scheme of the Reference Energy System, is a way to represent the interconnections and the links between different technologies and different sectors. Through its structure, becomes more intuitive the representation of the energy system implemented in the model.

For the definition of what technologies had to be implemented in the SRES, it was necessary to define and estimate what demand they had to supply. A process starting from the bottom, the end-user, was thus required to firstly answer to the question "what demands do exist?", followed by the consequent "how these demands can be supplied?".

The first logical step was to list the considered demands and clarify which consumers they should supply. Basically, there are three kinds of demand classes: power demand, thermal one and the pure energy carrier one.

While the first two describe the required electricity and heat, the latter represents all those final products that can be used to produce further power/heat (e.g. hydrogen and synthetic renewable fuels).

For computational time and scheme simplicity, aggregate demands were considered for different sectors. This means that for a macro-area (e.g. tertiary sector) different demands classified per type were defined.

In the model, several sectors are defined, depending on their demand: industry, residential, tertiary sector and transport one.

For the net electricity load, a global demand was considered, with the exclusion of the power needed for Space Heating (SH), DHW heating, cooling and for transport via electric vehicles.

For industry sector only heat load was considered, while for residential and for tertiary ones several demands are represented: power required for space cooling, heat for individual space and hot water heating and heat for DH. Finally, for transport, electricity load for electric vehicles was estimated.

Once the final uses are defined, it is possible to focus on the segment of energy supply chain, which means to represent the processes needed to supply these demands. The SRES shows different technologies, that can be grouped depending on the final products required. There are power plants, combined heat and power ones, installations for centralized heat generation and for individual heating systems.

Last segment of the SRES is the left part, which shows all the primary supply or import of the raw materials that constitute the feedstock of the technologies for heat and power generation mentioned above.

In the following Figure 4.1 the SRES originally implemented in the model is presented. Please note that the figure shows exclusively the processes originally studied before this thesis work. For sake of nomenclature, it will be called *Global SRES*. Technologies that involve the hydrogen utilization and its derived products had to be depicted in a subsequent scheme (Fig. 4.2) to ease the graphic representation. The model discussed in the thesis considers the Reference Energy System as composed by the two representations together.

The logic of both schemes is to represent all the relevant flows that characterize a specific process transformation.

Starting from left to right of the scheme, it is possible to notice the pathway an energy carrier covers to reach the end-user at its final form.

Figure 4.2, which will be named *Hydrogen SRES*, represents in a detailed level the processes implemented in the model, whose technological background was described in Chapter 2.

In Chapter 2 those pathways that allow to limit grid overload due to the electricity produced by intermittent REs are described. The latter has the potential to be converted into different energy carriers (e.g.  $H_2$  or synthetic fuels).

As for the general demands shown in the global SRES (Fig. 4.1), similar consid-

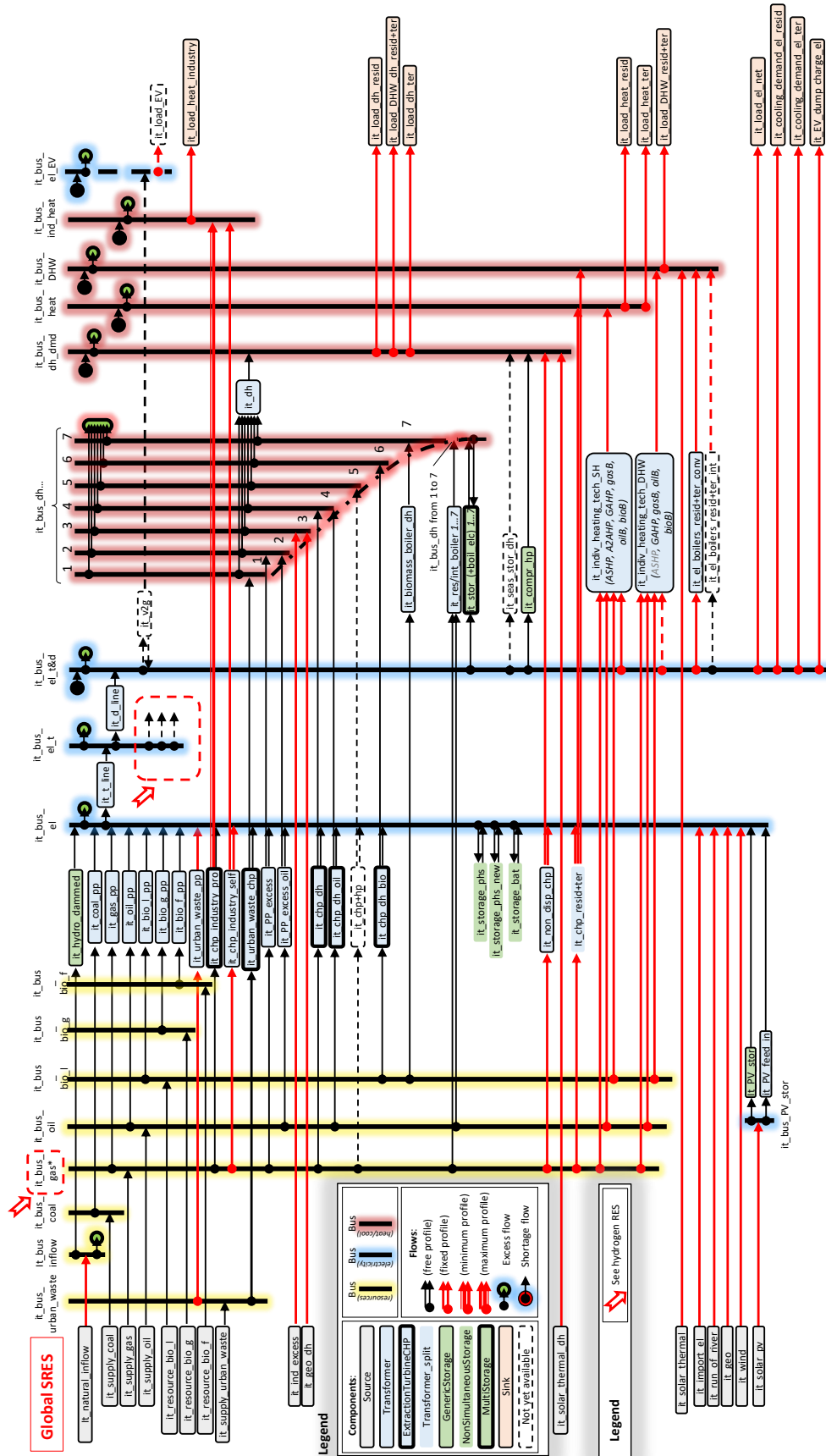


Figure 4.1. Scheme of the global Reference Energy System in the model: please note that for sake of representation, the implemented part discussed in the thesis is represented apart in Figure 4.2

erations have to be done for the ones reported in Figure 4.2. Here demands of pure energy carriers are reported.

The hydrogen demand consists on the pure demand in the transport sector (e.g. heavy transport) and for the industry (e.g. steel and cement facilities).

Jet-fuel and DME demands cover the part of the transport sector that are powered by these electric-fuels. The former for the aviation sector, while the latter is considered to cover the road transport that is not fuelled by hydrogen or electricity.

Methanol demand represents the quantity of e-fuel used in industry (e.g. chemical) to substitute oil-derived products in non energetic use as reactants, while ammonia consumption regards the small portion of naval transportation with  $NH_3$  fed into ICEs.

As for the first scheme, a common description method will be followed for the second one. For each final energy carrier, it is useful to focus on the production pathways possible.

### 4.2.1 Processes involved in hydrogen supply chain

Starting from hydrogen, it is current produced via water electrolysis. In the reality different electrolyser typologies exist for producing  $H_2$ .

In the model a single EC technology is considered: low temperature Proton Exchange Membrane electrolyzers are supposed to become more relevant in the EC market, thanks mainly to their flexibility (see Section 2.1.2).

The inverse process, hydrogen utilization to produce again electricity occurring in a fuel cell, is modulated with a single component too. Here again, several FC technologies are already on the market, but projections [2, 8] suggest a dominant role of PEMFCs shared with Solid Oxide Fuel Cells (see Section 2.2.5).

Water electrolysis and its reverse process release low temperature heat and they are characterized by a link with electricity bus. In one technology power is provided in input (water electrolysis), while for the opposite is the main process output.

Hydrogen bus can be destined to the pure energy carrier demand or can be used as input for the synthesis of more complex fuels. Furthermore, multiple storage options were considered in order to strengthen its production during the overload given by REs, with a consequent benefit for the grid stability.

Three storage technologies are considered: literature reviews suggest the use of metal hydrides and  $H_2$  liquefaction for stationary applications, while compressed hydrogen more suitable for transport sector. For further information see Section 2.3.

In Section 4.3.5 the hypothesis made on different hydrogen storage possibilities will be presented.

Finally, another utilization pathway is considered: the blending with methane and distribution in the already existing gas grid. We will come back on this solution in the section 4.3.4.



## 4.2. Scheme of Reference Energy System (SRES) description

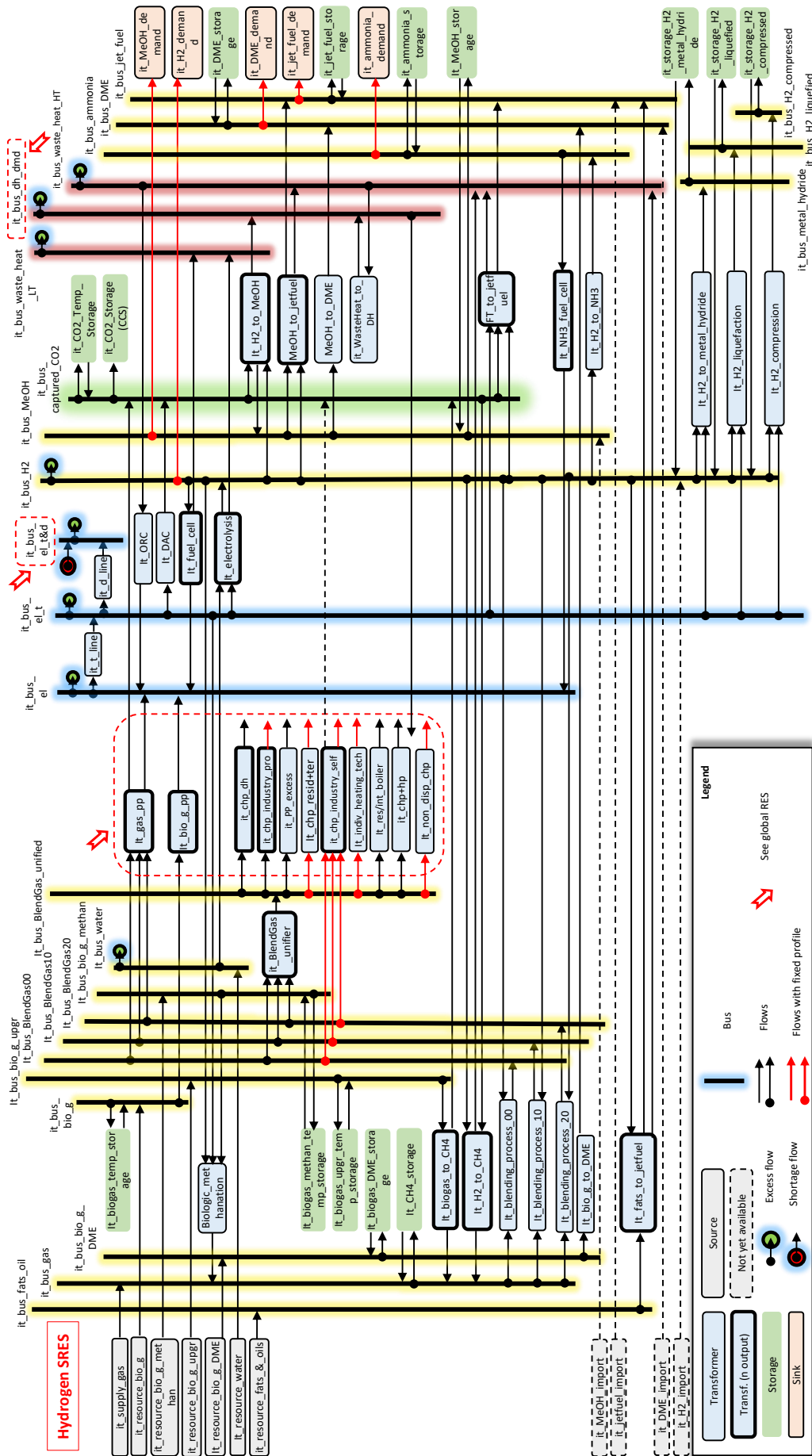


Figure 4.2. Scheme of the Hydrogen Reference Energy System that has a focus on the hydrogen and hydrogen-based fuels supply chains

### 4.2.2 Processes involved in methanol supply chain

A first hydrogen conversion can occur in methanol synthesis, where  $H_2$  molecule is reacted with carbon mono/dioxide.

As described in section 2.2.3, two different reactions are possible for MeOH production. The hydrogenation of  $CO_2$  or of carbon monoxide. However, these two different chemical reactions can be described by a single transformer in the SRES, that involves hydrogen and  $CO_2$ . This is possible thanks to Water-Gas Shift (Eq. 2.9) that eventually converts the carbon molecule into carbon monoxide.

As for hydrogen pathway, a pure methanol demand is present, as mentioned before mainly destined to industry, with a storage option to optimize the unbundling between production and consumption. The production of more complex fuels (e.g DME or synthetic jet-fuel) are possible with methanol too.

### 4.2.3 Processes involved in renewable methane supply chain

The dominant part of gas currently injected in the grid is fossil-derived. In Chapter 2 only renewable production ways were presented and the same logic structure is reported in the SRES.

In the scheme two processes of  $CH_4$  production from biogas are considered: biogas upgrading and biological methanation. For the technology description please refer to Section 2.2.2 and 2.2.4.

The first one is the filtering and separation of the existing methane part of biogas by the other impurities (carbon dioxide and  $CO$ ). Output  $CO_2$  and methane flows will be captured.

For the biological methanation,  $CO$  and  $CO_2$  present in biogas are reacted with hydrogen in a chemical reactor, adding their energy content to the existing methane part. The reaction takes place at low temperature, thus no waste heat can be recovered.

A different situation occurs in catalytic thermochemical methanation (see Section 2.2.2), where a stream of hydrogen is fed in a reactor with carbon dioxide, releasing heat thanks to the exothermicity of the reaction.

In the current model version, catalytic methanation receives a stream of  $CO_2$  in input. However, also biogas is a possible feedstock [11]. This implementation might be object of further developments.

It is assumed that all the methane has to be blended with hydrogen. At the exit of the blending process, the resulting blended gas bus reaches the same transformers previously fed by normal gas.

The methane (natural gas fossil, biomethane from upgrading, synthetic methane from the methanation) is then blended with a fraction of hydrogen, obtaining an output mix that is distributed to different transformers. Hydrogen blending is feasible at low percentage volume-basis (see Section 2.4.4). To keep the problem a linear one, it was necessary to let the model decide the blended fuel mix, imposing a minimum and a maximum share.

For this reason 3 blending processes with same technical parameters were implemented,

each one with a different volume mix (0%, 10% and 20%vol  $H_2$ ). This enables the model to decide the best %vol of hydrogen to be blended with methane for each time step of the optimization problem.

This may lead to a misunderstanding when comparing the two schemes. In Figure 4.2 is reported the blending process, the new three buses that supply all the technologies that previously were fueled by pure gas.

In Figure 4.1 the "it bus gas" has a outlined box to underline that in the model all the processes fed by gas are fed by the new mix of hydrogen and methane. Blending process was not illustrated in the global SRES always to ease the graphic representation. As mentioned above, for the hypothesis related to the blending option, please refer to the Section 4.3.4.

#### 4.2.4 Processes involved in dimethyl ether supply chain

The logic structure of this supply chain and the one for jet-fuel are the same. Starting from a pure fuel demand, a storage is illustrated to represent the decouple between DME production and consumption.

The typical DME synthesis reaction is the methanol dehydration (Eq. 2.12). The process is represented in Figure 4.2, however, it is not the only DME production pathway.

It is already on the market a supply chain that starts from biogas [19], obtaining methanol as intermediate product and giving the final DME. This transformer was included in the supply chain for dimethyl ether.

To date in Italy, the most part of diesel used in transport is imported and it is likely to expect that internally produced renewable synthetic fuels will not be able to cover the entire fuel demand. For this reason, a DME import has been included in the model.

However, to date these two alternatives are not considered by the optimization process yet, but will be suitable for future developments.

#### 4.2.5 Processes involved in jet-fuel supply chain

As mentioned above, for  $H_2$  and hydrogen-based fuels the same component classes are involved. Starting from the pure jet-fuel demand, that basically covers the aviation transport, a storage was considered to represent the current structures designated for aviation fuel store.

To synthesize jet-fuel, Fischer-Tropsch process is typically used. This transformation pathway starts from a syngas mixture of hydrogen,  $CO$  and  $CO_2$ .

Different feedstock can be thus considered, assuming different initial steps to obtain the required FT inputs. For this reason, several jet-fuel synthesis pathways are possible, starting from the classic FT one (see Section 2.2.3). Carbon dioxide and hydrogen are provided to the transformer, to obtain jet-fuel and some waste heat.

Another possible solution is the synthesis from methanol, with the only difference that an inverse  $CO_2$  hydrogenation (Eq. 2.10) is required, to split MeOH back to a syngas made by  $H_2$ ,  $CO_2$ ,  $CO$ . Again, similar outputs to the FT process are obtained. For the sake of completeness, also the *Biomass to Liquid* (see Section 2.2.3) has been implemented. Bio jet-fuel is obtained from used cooking oils and waste fats. Outputs are comparable to the classic ones obtained through Fischer-Tropsch process.

EU Aviation Agency projections [40] predict an increasing role of electric jet-fuel and bio-based one in the market, underlying however the risk to not completely supply the aviation fuel demand. This would require an external import, that has been included in the model but not implemented yet.

The main criticism of aviation transport consumption allocation is to separate national from international flights. The big issue is to understand to which country allocate fuel consumption and related emissions. In Section 5.1.2 the consideration on national aviation transport are reported.

A possible upgrade would be a more specific study on aviation demand and supply.

Finally, an alternative hydrogen storage possibility was included:  $H_2$  conversion to ammonia.

In Section 2.3.2, the Haber-Bosch process was considered as an interesting option to lower the criticism related to hydrogen storage, especially thanks to the recent development of the inverse process, i.e. liquid ammonia electrolysis to obtain compressed hydrogen.

To date, an ammonia demand was included, representing the naval ICEs fueled by  $NH_3$  of the national naval transport considered in the model (see Section 5.1), coupled with a storage option, which offers an attractive option to convert hydrogen into this final energy carrier, overcoming the issue related to pure  $H_2$  storage.

### 4.3 Model description

In the Section 4.2 the logic structure of the work was presented. The model was developed starting from the open access model NEMeSI, whose acronym means National Energy Model for a Sustainable Italy, developed by the ReLAB Group of Politecnico di Milano.

The model is based on the open-source oemof framework, introduced in the previous Section. Its original version simulated the Italian energy system, limited to the generation and use of electricity and thermal services with current technologies.

It describes the national energy system as a single node, with thus the characteristic of a zero-dimensional (0-D) system. It does not consider inter-connections and the different regional characteristics that may emerge in reality between North and South Italy (e.g. solar irradiation, heat demand for industries). All the represented components, flows and buses are aggregated.

The work of the thesis was to include the part related to hydrogen and hydrogen-based by-products generation and use, assessing their role for decarbonisation target purpose. New customized components and solutions had to be implemented in order

to enable the  $H_2$  counting in the energy system. The model code and the full dataset are available online at <https://doi.org/10.5281/zenodo.3743316>.

### 4.3.1 Model structure

In Figure 4.3 the main inputs and the returned outputs of the model are presented. By considering the commodity costs for primary energy carriers (e.g. fossil NG, biomass), the model pursues a cost minimization of the system, as it will be described in Section 4.3.3. In order to return the hourly energy system balance, defining the technology production mix with a hourly detail, several inputs are needed.

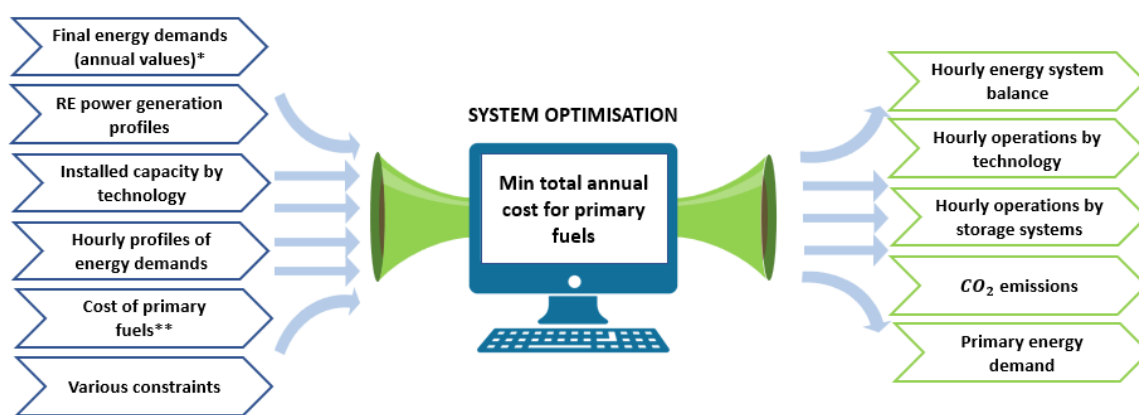


Figure 4.3. Main inputs and returned outputs of the model; (\*) by energy carrier,  $H_2$ , e-fuels, electricity etc; (\*\*) expressed in €/MWh

Returning the model a year simulation with an hourly time-step, final energy demands must be provided with annual demands and hourly profiles. The availability profiles of some power generation implemented as *Sources* (e.g. PV, wind power, geothermal) have to be provided, as for the assumed installed capacities for the implemented technologies. Cost of primary fuels and various constraints such as the presence of fixed production profiles or initial level of storage capacity complete the required inputs.

Before introducing the main hypothesis the model is based on, it is useful to introduce the model structure by defining the main steps. With the help of the diagram presented in Figure 4.4 it is possible to describe the main phases of the process.

Starting from the left, the first action required by the model represents the input data acquisition. In order to ease the management of a big amount of input data, they were organised in a spreadsheet file (e.g. Excel), divided by categories. The logic behind this classification follows the one of the subsequent step of the model.

Input data are divided depending on the type of information they provide. For example, annual values for final demands that define the final uses the model has to supply without shortages (as it will be described in Section 5.1) are grouped together,

but they are differentiated from resources availability.

The two groups define the energy that have to be supplied and that can provide during the year, some of which following a fixed profile. It is the example mentioned before of REs availability, that in the model are described through the oemof class *Source*. Hourly profiles are then grouped into another Excel spreadsheet, where all the profiles for demands, sources and processes are included.



Figure 4.4. model schematic approach

Input data for the technologies related to power and heat generation and for the *Hydrogen to X* pathways are grouped by similar input characteristics. For example, technologies that have as outputs a power flow coupled with an heat one (e.g. co-generation processes) constitute a single Excel spreadsheet, while *Transformers* that process a single input returning a single output are pooled into another spreadsheet. The structure of the overall input data follows the same logic. The model works with decision variables that are energy-based (MWh), returning the hourly energy system balance. For each time-step of the simulation, the optimal generation mix that pursue a cost minimization is provided, defining the hourly operation of each implemented technology.

The input data have then to define the energy penalty or conversion efficiency that occurs in each process, described in oemof through *Transformer* class. Input flows must be set, outlining the energy carriers that are processed and the resulting output ones with the buses of destination.

For each technology, the installed capacity have to be defined, unless they are object of investment optimization as described in Section 4.1.1. In this case, the latter would be additional decision variables (though not used in the present application - see Section 4.3.3).

Other information required by the model concern the load flexibility of each technology. Although the model has a national spatial resolution with aggregated input data, in order to define the hourly energy system balance, load operation ranges have to be defined.

With the exception of a specific case that will be discussed later in Section 4.3.4, for technologies that process multiple inputs, a ratio between them has to be provided. Lastly, in order to keep track of  $CO_2$  emissions related to each energy carrier, information on carbon content are described, expressed in kg of  $CO_2$  produced per MWh of energy.

The model code begins with the import of the required packages. For example, in order to open and to process data in Python the *pandas* package is used. To build the interconnections between different *transformers* and *buses* of the system and to

solve the linear optimization problem obtained, the oemof's package *solph* is imported. Lastly, oemof's *outputlib*, a package that allows to group and print the optimization results, is imported.

In order to collect input data and to organize them, a secondary function, named "nodes\_from\_excel", is defined. This function imports data from the Excel file and it builds the components required to describe the energy system. *Buses*, *transformers*, *sources*, *sinks* and *storages* classes are defined, collecting information of the input parameters. In this way the different interconnections between the elements that constitute the SRES described in Section 4.2 are defined.

Inside this function, some modifications with respect the original model version were required to enable the model to process *Power to Hydrogen* and *Hydrogen to X*. For example, for all processes in H2G and H2L where in addition to hydrogen a carbon molecule is needed, then carbon dioxide consumption was defined. Referring to Figure 4.2, a bus for the carbon resource was implemented, namely "it bus captured  $CO_2$ ". From this, the processes of H2G and H2L consume carbon dioxide, with a ratio defined in the input data Excel file, expressed in kg of  $CO_2$  per MWh of produced energy. Regarding carbon dioxide emission allocation, a further problem arises with the blending option of hydrogen and methane in the gas grid, requiring the development of a customized *transformer* class, but this will be resumed in Section 4.3.4.

Another modification dealt with the recovery of waste heat from hydrogen-related processes. A distinction on temperature range imposed the definition of a Low Temperature waste heat, such as for water electrolysis and Fuel Cells (see Section 4.3.2), and a High Temperature waste heat. The latter includes H2G and H2L processes and is defined as waste heat energy per unit of energy of the main product produced.

Another enhancement dealt with the *transformers* that processes more than a single input flow with a specific ratio (e.g. biological methanation). For these technologies, a specific case was developed, where input flows are coupled with share information with respect to the total input energy. In this case, ratios are fixed and the default oemof transformer component can handle the process.

When however the ratio of input flows cannot be fixed, as for the blending option situation which will be described in Section 4.3.4, a customized *transformer* class had to be developed. The implemented solution allowed to process different inputs without fixing their input ratio.

In the model the investment optimization option described in the Section 4.1.1 was also implemented, although for the application in the work was not used.

Once the definition of all the elements of the SRES is accomplished and the interconnections between decision variables are declared, the secondary function "nodes\_from\_excel" concludes its tasks and is followed by the main function. The latter defines the model optimization, pursuing a cost minimization of the energy system, complying with constraints.

An external Python file is recalled by the main function, where the stability limit for the power system is described. The latter represents the minimum quantity of the overall power generation that has to be provided in each time-step to the system by a specific type of technology, basically conventional power generation plants (e.g. CHP, gas power plants).

To solve the linear optimization problem several solvers can be used (e.g. cbc, cplex, glpk) but in the model application of this thesis work only the default "cbc" was tested. Further developments could test and compare the results obtained from different solvers.

Once the linear optimization is completed, the last step is the selection of the main results and their print. Through the package "outpulib" from oemof, the main function returns the hourly energy system balance and the operation of the different technologies. Coupled with hourly operation of storage systems and with information of  $CO_2$  emissions, a CSV file is returned.

### 4.3.2 Assumption of single technology option for each process

Before introducing the main assumptions for the definition of the studied scenario, a number of background hypothesis are necessary.

The first main assumption that define the structure of the model regards the definition of the technology number considered for each process.

The logic background of the original model first and then of the implemented part too was to keep the system representation as simple as possible. More complex structures involve a considerable increase in computational time and optimization issue.

For this reason in all processes in which there exist more than one technology, only one solution was considered.

An example might be the choice of water electrolysis technology and fuel cell's one. In Chapter 2 the main technologies are presented, with main technological parameters reported in Tables 2.1 and 2.2. The two markets present many different solutions, each one with specific operating conditions. However, analysing the model a single aggregated node, it would have been difficult to define the market share of each technology.

For electrolyser, the chosen technology was then the LT PEMEC, thanks to its high flexibility and to the increasing market penetration [2]. Same consideration have led to select PEMFC as technology implemented for Hydrogen to Power (H2P), as described in Section 4.3.6.

Possible further implementations such as the multi-node solution (see Section 6.1) could require different considerations, enabling multiple technology option for each process.

### 4.3.3 Assumption on costs

Oemof framework, as anticipated before, allows a high degree of customization in its settings. This is true not only for technological and temporal level of detail, but also for the objective function definition, here the cost minimization.

It allows to solve the optimization problem by considering both  $C_{investment}$  and  $C_{O\&M}$



(See Section 4.1.1), returning the optimized installed capacity of the studied technology. However, oemof does not allow to consider the entire period of transition (e.g. 2020-2050) before the simulated scenario.

Investment costs for these new technologies are difficult to be predict: they depend on many factor (political, geographical) and they will decrease over time.

For this reason in the cost function (Eq. 4.6), capital expenditures are not considered yet, while for the second term  $C_{O\&M}$  only commodity costs, the ones for the supply of raw energy sources, are considered. No maintenance cost or cost of labor (e.g. employees' wage) are taken into account.

They are considered as the € necessary to supply a unit of the specific energy carrier (typically MWh), from the well to the transformation plant.

The model returned the optimized generation mix that minimize the consumption of resources (e.g. fossil NG, biomass). For each hourly time-step it evaluates the technology to produce the required amount of energy by comparing the resource available and their related cost (e.g. hydrogen use in FC compared with gas grid in GT power plant).

Results could become an helpful decision driver for policy-makers, pointing out which technologies should be target for more research and development.

After the focus on the economical hypothesis background, is then possible to introduce those assumptions that regard more the technological side of the system. In the following Sections the main background hypothesis will be presented.

#### 4.3.4 Assumptions on the gas infrastructure

Long-term projections always have a quite consistent degree of uncertainty. However, literature background leads us to make the assumption that the gas grid will be still present in the Italian energy system in 2050 [5, 34].

There will be probably a stronger switch from fossil NG to the one obtained by green  $H_2$  and captured carbon dioxide or other bio-based resources.

The existing gas grid infrastructure is then supposed to continue its transmission and distribution role. With limited investments they will manage low volume percentage hydrogen blending with methane (see Section 2.4.4).

To date, the model does not consider the possibility to separate after transmission the blended mix back to  $CH_4$  and  $H_2$ . Thus, the transported mix is destined to all the transformation processes currently fueled with methane (e.g. GT power plants). Future researches on the implementation of these separation technologies could be complemented in future.

It is important to focus on the hydrogen blending option. It is not possible to determine in advance the exact quantity of hydrogen that has to be blended in the gas transmission grid (yearly and hourly). This is because the choice of the technologies to use and at which load to run them, are all decision variables for the model.

This fact has some important consequences that have to be considered. Before to

introduce them however, it is necessary to better explain how the blending process is implemented in the model.

As introduced in Section 2.4.4, the gas transmission grid can manage low volume % hydrogen presence in the overall gas flow. In the model the maximum hydrogen share is assumed to be 20% (volume-based).

This means that if the volumetric flow in the pipelines is, for example, 1 cubic metre per second, in the case with highest  $H_2$  penetration in the grid the transported energy carrier would be  $0.2 \text{ m}^3/\text{s}$  of hydrogen and  $0.8 \text{ m}^3/\text{s}$  of gas.

It is important to notice the implications that hydrogen blending could bring. At standard condition, hydrogen has a lower energy content per cubic metre ( $10 \text{ MJ}/\text{m}^3$ ) compared to methane ( $35 \text{ MJ}/\text{m}^3$ ). This means that maintaining the same operating pressure in the grid (and therefore the same volumetric flow rate), the transported gas will have a lower energy content.

The model operates with flows that are energy-based (MWh) and for this reason an energy consumption for compression was considered in the blending process. This was necessary to keep track of the necessity to increase the flow rate of the blend gas with lower energy content to obtain the same energy transmission of the pure methane.

In the following Section 4.3.10 the assumption will be reported.

Another important consequence of the Linear Programming constraint linked to the hydrogen blending process regards the  $CO_2$  emission allocation arising from the use of the mix  $CH_4-H_2$  by the involved technologies.

Being the model free to choose the generation mix for each time-step of the simulation, it is not known which share of hydrogen will be used in the transmission grid in advance. The  $H_2$  share to be injected in the grid is a decision variable.

This means that the methane content of the resulting gas is unknown and therefore the possible  $CO_2$  related emissions.

For this reason three "blending transformers" were implemented in the model (see Fig. 4.2). Each transformer mixes methane and hydrogen with a specific ratio: 0% hydrogen volume content, 10% and 20%. For each one a specific "blend gas" bus is created, with its own properties (e.g. carbon dioxide emission related).

Except for the 0% blend, an additional energy consumption had been included in the transformation, in order to consider the necessity to compress the exit gas mix with a lower volumetric energy content with respect to the pure methane. In the Section 4.3.10 the assumptions will be presented.

The introduction of three buses requires to point out the involved implications. Carbon dioxide emissions are expressed in terms of kg of per unit of specific flow consumed, which are energy-based (MWh). They are parameter for the model.

By substituting the original gas bus with the three buses of blend gas, each one with its own properties (e.g. related emissions), the problem of carbon dioxide accounting could be considered as solved.

However, in addition to the derived higher RES complexity, there would persist the problem explained here below.

In oemof framework the default *Transformer* class needs to define inputs with a specific fixed ratio. With blending option however, it is the model to decide which mix of hydrogen and methane to use. It could prefer to use the 20%vol hydrogen blend with a small fraction of 10%vol, but the ratio between the two can change.

Thus, a potential transformer that originally consumed pure gas (e.g. a CHP plant), would then receive in input three flows, one per blend gas bus created. It would be impossible to set a ratio between the three inputs.

In order to keep linear the optimization problem, it was then required to implement a customized Transformer class.

A customized *Transformer* class was then implemented. The developed transformer allows to receive in input different flows without fixing their input ratio.

In order to limit the increase of model complexity, with 3 blend gas buses that interact with all technologies previously supplied by pure gas, a fictitious transformer of this new type, named "Blend gas unifier" (see Fig. 4.2), was implemented. Its role is to combine the buses obtained from the three blending processes ("It bus BlendGas00", "It bus BlendGas10, "It bus BlendGas20") into a single one ("It bus BlendGas unified").

The emission accounting is made upstream the mentioned transformer. The information of each blend type consumption coupled with the  $CO_2$  content known for each bus makes this operation feasible.

An additional exception has to be made for all technologies that include a system of CCU, Carbon Capture and Utilisation. A part of  $CO_2$  emission is captured and sent to other installations. A specific bus is then required to collect the generated flow of  $CO_2$ , which will finally be used as input in other transformation processes (e.g. in H2G or H2L pathways).

For these concerned technologies the information of methane absolute content in the input flows would then be necessary. It has to be remembered that the model operates with energy flows, which are converted with specific efficiency parameters. Related  $CO_2$  emissions are then expressed with input parameters. Output flow exiting from the transformer "blend gas unifier" represent the energy content of the summed three gas mixes with 0, 10 and 20%vol of hydrogen share. However, again, no information about their ratio is available in advance of the simulation.

The solution was to adapt the implemented custom transformer class for the technologies receiving in input blend gas with system of CCU at the stack. In this manner the three blend gas buses are sent directly to the custom transformer and there they are processed (e.g. burned in gas power plant). The  $CO_2$  content of each bus is known, being known the methane content present in the bus.

### 4.3.5 Multiple hydrogen storage option assumption

Some considerations have to be discussed regarding the issue of hydrogen storage. In Section 2.3 the already affirmed and the most promising options for the storage are

presented.

While other energy carriers present relatively low storage problems (physical and of economic nature), hydrogen has non-performing characteristics at ambient conditions. For these reasons, different storage options are investigated. As anticipated in the previous Section, three storage technologies are considered:

- Hydrogen compression
- Hydrogen liquefaction
- Hydrogen conversion to metal hydrides

Compressed hydrogen represents an interesting trade-off suitable for transport sector. Space requirements in private FCEVs pushed the development of high compressed  $H_2$  tanks (at  $\sim 700$  bar for small vehicles and 350 bar for heavy trucks). Hydrogen Refueling Stations HRS should then supply the energy carrier at the same operating conditions. For this reason Compressed Gaseous Hydrogen had to be investigated in the model.

The second technology regards the liquefaction process. This technology has the advantage to increase the volumetric energy density, presenting however higher energy cost.

Last option is the conversion of  $H_2$  into a metal hydride, a solution which requires low energy to store the fuel and is suitable for stationary applications.

There exist several typologies: Andersson et al. [24] suggest two promising types, magnesium-based and aluminum-based. Based on these considerations, the former, magnesium hydride ( $MgH_2$ ), was chosen for this option.

Suitable large natural storage option such as salt caverns are not present within Italian borders and for this reason they are not considered in the model. A possible further development could be the implementation of depleted oil and gas field, bearing in mind that during storage discharge a further purification would be necessary.

For the other hydrogen-based synthetic fuels only a single storage option is considered, thanks to their better suitability to be stored at non prohibitive conditions.

### 4.3.6 Hydrogen-to-Power (H2P) assumption

This sector represents the use of hydrogen to produce back electrical power. In Section 2.2.5 a description of the different possibilities is illustrated.

In the current model, however, only a single option of transformation is considered. Fuel Cell technology is an already diffused option, with significant variations between one type and another.

Literature reviews seem to indicate PEMFC technology large diffusion, sharing the market with Solid Oxide Fuel Cells. For this reason, the former is considered the only available pathway for H2P by the model.

Subsequent options, such as hydrogen turbines could be further investigated and implemented in the model. The decision driver to not include them in the model

was influenced by the zero dimension characteristic (0-D) of the model itself. The assumption made before regarding the presence of the gas transmission grid by 2050 has a first consequence in the fact that main GT systems will continue to be fed by gas, or with a blending mixture of  $H_2$  and  $CH_4$ .

With regionalization implementation, would then allow to define where specific hydrogen turbine installation could be set.

#### 4.3.7 Assumption on waste heat recovery

The model analyses the Italian energy system as a single node, being then zero-dimensional.

The installed capacities of the technologies represents aggregate values. While for power side, transmission and distribution of electricity can be easily managed, introducing transmission and distribution losses, for heat the situation changes.

While Low temperature output heat of the implemented technologies is destined to be wasted through an excess flow (see Section 4.1.2), high temperature heat produced from H2G and H2L processes, such as jet-fuel synthesis or thermochemical catalytic methanation can be recovered.

It is likely to expect that these plants will be centralized, benefiting from economies of scale. It would then be difficult to transport high amounts of heat. It is under this perspective that centralized solutions such as District Heating utilization or power generation via ORC were considered.

For Organic Rankine Cycles, there exists several different organic working fluids, each one with different operating conditions. From [54,55] and comparing with temperature ranges of heat produced from the mentioned processes the value reported in Section 5.2.3 was assumed.

In order to consider The potential use of this recoverable HT heat, a fictitious transformer was implemented, named "waste heat to DH". This was included in order to keep track of the inevitable losses that occur from the exit of the H2X plant through the district heating system to the final DH heat demand. For this reason, the same overall efficiency of the other implemented DH classes was assumed. In Section 5.2.3 the assumed data are reported.

#### 4.3.8 Assumption on hydrogen pipelines

Hydrogen transmission in a dedicated pipeline grid is not considered in the model yet. To date, this transmission system is considered for specific applications, in particular when  $H_2$  production is located close to the final-user.

Namely, the industrial sector, in the specific steel production, where a dedicated grid links the production site with the rest of the plant.

Extending this concept, hydrogen pipelines are considered in large scale power plants, where electrolyzers are connected with hydrogen storage and then with H2P systems,

Fuel Cells.

### 4.3.9 Assumption on biogas utilization

Biogas is a mixture mainly composed by methane, carbon dioxide and  $CO$ . It can be destined to different applications. In Chapter 2 three main uses are presented:

- Biogas upgrading to biomethane by means of  $CO_2$  capture
- Methane synthesis through biological methanation
- DME production from biogas

The first one does not implies chemical reactions on the process, because there is only a filtering step. All the impurities are separated from the methane content already present in the mixture.

The second one transforms the carbon molecules in the biogas into methane through the reaction with  $H_2$  and the latter converts biogas into Dimethyl Ether DME.

Biogas supply is strongly related to its production pathway, which is typically anaerobic digestion of biological residues. The bottleneck on its supply is the biomass procurement, which is limited to the nearby surround.

Furthermore, being the biogas demand from these different transformation users restricted, it seems unlikely the diffusion of a national grid infrastructure dedicated to biogas.

The size of these transformation plants will be defined by the quantity of biogas they will be allowed to process, which will amount to the supplied one to the specific installation.

For this reason in the model three different and separated pathways for biogas supply were implemented (see Figure 4.2). This was necessary in order to avoid the choice of biogas destination's switch for suitability reasons by the model.

It means that if in a specific time-step, biogas conversion into methane through biological methanation would not be convenient, while upgrading would be cheaper even than its storage, the model should not allocate that biogas quantity to upgrading. Translating the problem to a real example it would mean that biogas supplied to a biological methanation plant sited in, for example, Turin, should be transported to a different upgrading plant, located in Milan. This barely happens, due to transportation cost and issue. Moreover, it must be remembered that the model analyses a single node energy system, the overall Italy.

The 0-D model is required to analyse aggregated data, but it is important to prevent possible solutions that would deviate from a real feasible situation, like the previous example.

### 4.3.10 Technological data assumptions

Once the definition of the main background hypothesis has been completed, it is necessary to analyse the implemented technologies for the different *P2H* and *Hydrogen-to-X (H2X)* pathways.

As the technological review provided in Chapter 2, the data assumption presented below will follow the same schematic division.

#### Main technical data assumed in Power to Hydrogen (P2H)

Regarding the hydrogen generation, main water electrolysis technologies were presented in Section 2.1. Literature reviews suggest an increasing role of Low Temperature Proton Exchange Membrane electrolyzer system (LT PEMEC).

As introduced in the background hypothesis, for computational issue there is the necessity to choose a single technology option for a specific process. For these reasons, LT PEMEC was chosen to describe the P2H pathway.

In the subsequent Table 4.1 are presented the main technological parameters.

Table 4.1. Main technical parameters assumptions for Power to Hydrogen (P2H) pathway

	$H_2$ efficiency (LHV)	Thermal efficiency	$H_2O$ consumption [kg/ $MWh_{H_2}$ ]	Ref.
LT PEMEC	0.74	0.1	270	[2, 4]

The first efficiency term represents the unit of  $H_2$  obtained per one unit of input electricity in a LHV energy basis, while the thermal efficiency defines the Low Temperature heat that can be recovered per input unit.

Third column was added to keep track on water requirement to be destined exclusively for power generation. Being the analysis zero dimensional the only useful information that can be obtained is the overall consumption.

However, in a multi-regional model characterization, resource allocation like water management would become crucial in order to determine long term strategies. We will come back on the possible implications in Chapter 6.

#### Main technical data assumed in Hydrogen to Gas (H2G)

In table 4.2 the technical values assumed for the hydrogen to gas (H2G) pathway are presented. The two processes described in Chapter 2 are biological methanation and catalytic thermochemical one.

In the model a third process that returns synthetic methane was implemented: biogas upgrading. Even if it does not join the H2G category, it produces the same output, methane. For this reason its main assumptions are reported below.

For biological methanation and for the biogas upgrading is used biogas, whose composition is assumed to be 60%vol of  $CH_4$  and 40%vol of  $CO_2$ . This assumption is required in order to calculate the hydrogen quantity that is theoretically necessary to react with the carbon dioxide contained in the biogas mix. With Equation 2.7 is possible to define the quantity of hydrogen required in the biological methanation reactor. In [6] is reported the additional power consumption that is necessary to stir the  $H_2$  and the biogas in the reactor. The three inputs in biological methanation are then biogas, hydrogen and electrical power. Collected all the needed information, it is possible to estimate the amount of each input flow, expressed as a share of energy required on the total energy input. For 1 MWh of synthetic methane exiting the reactor, the input biogas flow represents the 42.6% of the total energy that enters the reactor, with a power demand of 7.8% of the total and a hydrogen stream that covers the remaining 49.6%. All energy requirements are calculated referring to the Lower Heating Value (LHV) of the specie. No recoverable waste heat is assumed from the biological methanation, because of its low operating temperature range (see Section 2.2.2).

As introduced in Section 2.2.4, biogas upgrading allows to separate and purify the methane content present in the mix from the other impurities, that for the previous assumption consist in carbon dioxide. In the model after Author's calculations, is estimated a  $CO_2$  production of approximately 100 kg per MWh of produced methane, 95% of which is then captured and used as source for other hydrogen-based synthetic fuel. Finally, a methane slip of roughly 2% of the entering biogas flow occurs in the biogas upgrading plant [4].

Table 4.2. Main technical parameters assumptions for methane synthesis processes in hydrogen to Gas (H2G) pathway

Process	Overall efficiency	Output heat [ $MWh/MWh_{CH_4}$ ]	$CO_2$ used [ $kg/MWh_{CH_4}$ ]	Ref.
Catalytic methanation	0.79	0.245 <sup>a</sup>	200	[6, 69, 70]
Biological methanation	0.72	-	-	[6]
Biogas upgrading	0.98	-	-	[4]

<sup>a</sup> the value does not include the heat required to self-sustain the process, which has already been subtracted.

### Main technical data assumed in Hydrogen to Liquid (H2L)

Once the hypothesis for the hydrogen generation and its first possible conversion in H2G had been clarified, the next step is to describe the assumptions behind *Hydrogen to Liquid* pathway.



Several new technologies were implemented in the model, some of which currently are still at a low Technology Readiness Level (TRL $\sim$  5), mainly because the necessary process steps are already available, but the global pathway still requires technical approvals. An example might be the synthesis of jet-fuel from methanol [12].

For this reason, a higher level of uncertainty was experienced in the research of technical information for some of H2L pathways. The main parameters are presented in Table 4.3.

In Section 2.2.3 different processes were presented. The main hydrogen-based synthetic fuels analysed were jet-fuel, Dimethyl Ether (DME), methanol and finally ammonia. As for H2G with biogas upgrading, in the model a bio-based pathway, named *Biomass to Liquid* to synthesize jet-fuel was implemented.

This additional bio jet-fuel synthesis from used cooking oils and fats process was included in the model in order to best represent the heterogeneity of the energy system.

As anticipated before, very few information were available especially in the different jet-fuel synthesis pathways from renewable resources. Complete energy balances were presented for the bio-based jet-fuel obtained from waste oils and fats.

For this reason some assumptions were necessary to be able to implement all the promising processes in the model. They are presented in the following lines.

The first important assumption made in the model regarded the outputs of the jet-fuel synthesis. As reported in Section 2.2.3, jet-fuel synthesis is currently obtained from coal gassification and from gas. The output stream is a mix of different products, in which  $\sim$  50-60% by energy is suitable for jet-fuel use. The remaining part is typically composed by liquified Petroleum Gas (LPG) and Naphtha.

In the model these two streams are not considered and thus represented in the SRES. The process efficiency takes into account the only jet-fuel part produced.

The second main assumption regards the jet-fuel synthesis via Fischer-Tropsch. As described in Section 2.2.3, the input stream is syngas, a gaseous mixture of mainly carbon monoxide and hydrogen. The model aims to return a single year simulation of the Italian energy system in the long term, namely 2050, where fossil based resources like coal and oil will be banned.

Jet-fuel synthesis via Fischer-Tropsch will be still possible providing that the input syngas stream would be obtained from renewable sources. Hydrogen would be produced via water electrolysis, while carbon molecule would be obtained from  $CO_2$  capture.

Jet fuel is a mixture of a variety of hydrocarbons. Its exact composition is strongly related to the used source, it is then difficult to define the specific hydrocarbon share. The range of molecular mass between hydrocarbons depends on the properties requirement for the product (e.g. freezing point). Typically jet-fuel has a carbon number distribution between about 8 and 16 (carbon atoms per molecule).

In order to estimate the carbon dioxide requirements reported in Table 4.3, a mean carbon molecule of  $C_{12}H_{26}$  was assumed.

Table 4.3. Main technical parameters assumptions for Hydrogen to Liquid (H2L) pathways

	Overall efficiency	Output heat	CO <sub>2</sub> used	Inputs	Ref.
	$[MWh/MWh_{product}]$	$[kg/MWh_{product}]$	$[MWh/MWh_{tot\ in}]$		
methanol synthesis	0.58	0.560	251	H <sub>2</sub> = 1      Heat <sup>c</sup>	[4, 14]
jet-fuel from MeOH	0.9	0.266 <sup>a</sup>	-	MeOH = 0.91      H <sub>2</sub> = 0.09 <sup>a</sup> Heat <sup>c</sup>	[13]
jet-fuel from FT	0.53	0.266 <sup>a</sup>	254 <sup>a</sup>	H <sub>2</sub> = 1      Heat <sup>c</sup>	[13, 70]
bio jet-fuel from fats & oils	0.665	0.266	-	biomass = 0.79      H <sub>2</sub> = 0.09      gas = 0.12	[4]
DME from MeOH	0.607	-	-	MeOH = 0.897      Heat = 0.102	[71]
DME from biogas	0.624	0.417	-	biogas = 1      Electricity <sup>b</sup>	[71, 72]
Ammonia synthesis	0.67	-	-	H <sub>2</sub> = 1      Electricity <sup>b</sup>	[20]

<sup>a</sup> from Author's calculations;

<sup>b</sup> required electricity is internally produced using unconverted reactants

<sup>c</sup> required heat is internally produced thanks to the exothermicity of the process

Jet-fuel synthesis requires a pure hydrogen stream for the last process steps in order to improve its cold properties (see Section 2.2.3). However, being the technologies that produce it from renewable sources still at an early development stage, information about energy balances are very scarce and uncertain.

The synthesis processes start from different compounds, although they are cracked in order to obtain a mixture of carbon and hydrogen molecules. For this reason pure  $H_2$  stream required in hydrocracking and isomerization steps was assumed to be the same to the one in jet-fuel synthesis from biomass, which is known.

Last assumption made in the jet-fuel pathway follows the same logic of the previous one. Being the required steps to obtain the final product similar, the heat produced by the overall reaction was assumed to coincide to the one required in the *Biomass to Liquid* pathway, which is known.

### Main technical data assumed in Hydrogen to Power (H2P)

The third possible utilization pathway for the hydrogen is to be reconverted back to power. As mentioned in previous Section 4.3.6, only Fuel Cell technology was considered within the H2P category. However, in the model also Fuel Cell technology from ammonia was implemented.

As for water electrolysis there already exist different FC technologies, which are presented in Section 2.2.5, each one with different operating conditions and properties. To date, the most diffused technology are PEMFC, with an increasing interest for Solid Oxide ones. The former were then chosen as representative for the process in the model.

Table 4.4. Main technical parameters assumptions for Hydrogen to Power (H2P) pathways

	Electrical efficiency (LHV)	Thermal efficiency	Input	Ref.
LT PEMFC	0.6	0.2	$H_2$	[2, 8]
$NH_3$ Fuel Cell	0.394	0.265	Ammonia ( $NH_3$ )	[73]

Due to the generation of heat during the reaction, in the model was useful to distinguish the quantity of heat produced from the main output. It is under this logic that two efficiencies are defined: a thermal and an electrical one.

The former expresses the power generation compared with the total input flow, while the latter defines the heat quantity over the input energy.

Ammonia Fuel Cells are composed by a  $NH_3$  cracker, which separates back nitrogen from hydrogen and a subsequent Alkaline Fuel Cell (AFC), which produces electrical power. Assuming a complete conversion of ammonia back to its original reactants, coupling the technical data provided by [73], the electrical and thermal efficiencies of the overall process were calculated. Values are reported in Table 4.4.

### Main technical data assumed in Hydrogen storage

Hydrogen has non-performing characteristics at ambient conditions, with very low volumetric energy densities compared to different fuels. While for other processes only a single option was implemented in the model, as introduced in Section 4.3.5, for  $H_2$  storage three options were investigated: hydrogen compression, liquefaction and transformation into metal hydride.

Each one however requires an energy penalty. In order to keep track of the power requirements, three transformers were determined. Main technical values are reported in Table 4.5.

Table 4.5. Main technical parameters assumptions for hydrogen storage transformation process

	Overall efficiency (LHV)	Inputs [MWh/ $MWh_{tot\ in}$ ]		Ref.
$H_2$ compression	0.96	$H_2$ , 0.96	Electricity, 0.04	[24]
$H_2$ liquefaction	0.847	$H_2$ , 0.85	Electricity, 0.15	[24]
$H_2$ to metal hydride	0.979	$H_2$ , 0.98	Electricity, 0.02	[24, 27]

The logic behind these transformers is to return in output the  $H_2$  with the characteristics to be stored. For compression ( $CGH_2$ ), it is assumed to use steel vessels with a pressure of 350 bar.

In the model hydrogen is assumed to supply mainly the heavy transport (buses and trucks) and to cover the  $H_2$  demand in industry, namely the steel production. Being the transport demand the dominant part of the overall hydrogen demand, the operating pressure for heavy transport applications will be assumed as the reference one in  $CGH_2$  storage tanks.

In Section 5.1, the main assumption on  $H_2$  demand will be better described.

For liquefaction ( $LH_2$ ), Andersson et al [24] report an energy cost of 6 kWh per kg of liquified hydrogen, which explains the second row of the Table 4.5.

Lastly, for  $H_2$  storage through metal hydrides, there exist several possibilities. After a literature review, the most promising and commercially diffused metal hydride seemed to be the magnesium hydride ( $MgH_2$ ), which was taken as reference in the model.

Possible different setups could be developed in future, introducing different options simultaneously and comparing them. For Further developments, please refer to Section 6.1.

From Table 4.5 it looks that for storage via metal hydride the lowest energy cost is demanded. However, this information is not sufficient to completely describe the storage options.

Here below the main characteristics of the storage options themselves are then reported.

Table 4.6. Main technical parameters assumptions for hydrogen storage

	Charge efficiency <sup>a</sup>	Capacity loss [% per time-step]	Discharge efficiency <sup>b</sup>	Ref.
<i>CGH<sub>2</sub></i> (350 bar)	1	0	1	[24]
<i>LH<sub>2</sub></i>	1	0.0042 <sup>c</sup>	0.95	[24, 28]
Magnesium hydride	1	0	0.76	[24]

<sup>a</sup> it reports unitary efficiency because energy cost are already accounted in Table 4.5;

<sup>b</sup> it considers energy costs (heat) required in metal hydride storage to release hydrogen and the losses due to phase change from liquid to gaseous in *LH<sub>2</sub>*;

<sup>c</sup> it express the % losses on the contained capacity due to boil-off action that occur in liquified *H<sub>2</sub>* tanks. The time-step is hourly

### Main technical data assumptions for the remaining processes and storages

In this last Section the hypothesis made for the technical data that describe the remaining processes and storages are presented. Table 4.7 reports the main values for the remaining storages.

Table 4.7. Main technical parameters assumptions for storage of remaining synthetic fuels

	Charge efficiency	Capacity loss [% per time-step]	Discharge efficiency
DME storage	1	0	1
jet-fuel storage	1	0	1
methanol storage	1	0	1
gas storage	1	0	1
biogas storage <sup>a</sup>	1	0	1
<i>CO<sub>2</sub></i> for CCU <sup>b</sup>	1	0	1

<sup>a</sup> in Section 4.3.9 different applications for biogas are presented. Each one has a specific bus and a specific storage. They present the same characteristics and for simplicity, only a general biogas storage class is reported;

<sup>b</sup> the storage for *CO<sub>2</sub>* and its transmission are not deepened in the thesis work. Ideal values for efficiency are then assumed

While hydrogen storage presents some criticisms and requires challenging storing operative conditions (e.g. liquefaction at -253°C), the other synthetic fuels implemented in the model are much easier to store.

Most of them are liquid at ambient (or nearby ambient) conditions. Simple metal vessels or pipelines are efficient solutions to store those energy carriers.

Gaseous fluids such as gas and biogas are then stored in geological storage sites,

storage tanks or pipelines at non-prohibitive pressures (typically  $< 75$  bar).

All these considerations led us to assume auxiliary energy cost for the remaining storage technologies as counted in the final power demand. In Table 4.7 the synthetic fuels storages implemented in the model are then presented, with unitary efficiencies during both charge and discharge.

In Table 4.7 the options of Carbon Capture and Utilization (CCU) is also presented. CCS had also been implemented in the model, but it has not been used in the scenario analyzed in the following Chapter. The combination of the two Carbon Capture typologies would be subject for future developments.

Last processes that still need to be presented are the carbon dioxide capture from air, through the Direct Air Capture (DAC) technology and the  $H_2$ - $CH_4$  blending transformers. They are presented in Table 4.8.

The former consumes power to capture  $CO_2$  and two possible categories exist: low temperature DAC and high temperature ones. In the model the second one was implemented, which has an overall consumption of electrical power of 1.75 MWh per tonne of carbon dioxide captured [2].

Table 4.8. Main technical parameters assumptions for DAC and blending option

	<b>Overall efficiency</b>	<b>Inputs</b> [MWh/MWh <sub>tot in</sub> ]		<b>Ref.</b>
DAC	571.4 <sup>a</sup>	Electricity = 1		[2]
blending process (0%vol $H_2$ )	1	$CH_4 = 1$		[2]
blending process (10%vol $H_2$ )	0.9997 <sup>b</sup>	$CH_4 = 0.969$	$H_2 = 0.031$	[2]
blending process (20%vol $H_2$ )	0.9993 <sup>b</sup>	$CH_4 = 0.933$	$H_2 = 0.067$	[2]

<sup>a</sup> for the DAC, the efficiency expresses the total mass of  $CO_2$  (kg) that is captured by using a unit of electrical power (MWh). For this case it has to be intended not as an energy efficiency, while as the ratio of the produced output divided by the required input, that is energy-based;

<sup>b</sup> from Author's calculations

For the blending option, discussed in Sections 2.4.4 and 4.3.4, several considerations have to be mentioned. As indicated above, three different ratio were implemented in the model, depending on the hydrogen content in a volume basis in the gas grid injected mix: 0, 10 and 20%vol of  $H_2$  were considered.

Except for the pure methane case, where no real mixing occurs, the other two mixing processes have to take into account the volumetric energy density reduction of the output mixed gas.

While methane has a volumetric energy density of 35 MJ per cubic metre, hydrogen gas has a lower value, 10 MJ/ $m^3$ . This means that while a cubic metre of pure gas

would transport 35 MJ, a cubic metre with 20%vol of hydrogen would contain only 30 MJ.

The model operates with flows that are energy-based (MWh). For this reason an energy cost for compression was necessary to increase the flow rate of the blend gas with lower energy content, obtaining the same energy transmission of the pure gas.

However, this problem has to be counter-balanced with the pressures in play. As will be described in the next Chapter, the main hydrogen demand covers heavy transport applications, where a compressed gaseous  $H_2$  is supplied at 350 bar. Water electrolysis technology is assumed to be LT PEMEC, with current operating pressure range of 30-80 bar. gas grid infrastructure today operates with pressure below 75 bar. Having available compressed hydrogen, a conservative 1% of the energy content of the mixed  $H_2$  was considered as the energy penalty required to transport in the grid the same energy amount of pure gas case.





# Chapter 5

## Model application

### 5.1 Scenario definition

The aim of the thesis is to provide a model that can assess the role of hydrogen in the Italian energy system in a long-term scenario. For this reason, the tested time horizon was set to 2050.

The analysed scenario is set-up with the aim to reduce  $CO_2$  emission of the national energy system by minimizing the fossil resources utilization. A strong decarbonisation is requested not only in the power generation sector, but also all the final energy sectors (i.e. transportation, residential and tertiary buildings, industry, agriculture). In this perspective, the rationale behind the scenario construction is the following.

- 1) In all end-use sectors, energy service demand reductions should be realized as much as possible (i.e. less space heating demand in buildings through better thermal insulation, less power demand through the use of more efficient motors and appliances, a shift from private to public transport in the mobility sector).
- 2) The fossil fuels that today are used in final energy sectors have to be substituted with zero-carbon alternatives as much as possible.
- 3) These zero-carbon alternatives should be, in sequential order: electricity,  $H_2$ , synthetic methane or other e-fuels<sup>1</sup>. As long as it is reasonable, electrification should be preferred over  $H_2$  in order to avoid the energy penalty of the electrolysis. At the same time,  $H_2$  should be preferred over synthetic fuels to avoid the energy penalty related to the conversion processes, as well as to minimize the demand for neutral  $CO_2$  sources.
- 4) If there is enough  $H_2$  available in the system, it can be blended into the gas grid (up to 20%vol) to contribute to the decarbonisation of the residual gas consumption.

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<sup>1</sup>As described in Chapter 2,  $H_2$  can be used to produce synthetic methane or other synthetic fuels (e-fuels). The acronym e-fuel means literally "electric fuel", a synthetic product obtained with the use of  $H_2$  from renewable power and captured  $CO_2$ . Examples of e-fuels can be methanol (MeOH), dimethyl ether (DME), jet-fuel and ammonia obtained through the combination of green hydrogen with carbon molecules.

5. 5) RE in the power generation sector should be deployed as much as possible.
6. 6) Coal is phased-out in the power generation sectors.
7. 7) Costs are assigned to natural gas and biomass, i.e. to the remaining commodities that can be used by the model to cover the energy demand in each time step.
8. 8) Other assumptions and constraints are entered (e.g. installed capacity of storage systems and conversion technologies).

Finally, when the scenario is set-up, the model is run and it returns the optimized supply-demand combination that is able to cover all the annual and hourly demands without shortages.

The manufacturing industry is excluded from the analysis, except for the elements that interact directly with the power sector, i.e. final  $H_2$  consumption for steel production and NG consumption in industrial CHP plants. The use of other fossil fuels in the industry sector (e.g. coal in cement plants, NG in industrial boilers) is considered out-of-scope and could be a matter of future works.

It is important to notice that, to pursue the first point of the rationale list, in-depth evaluations should be made through external analyses (e.g. simulation of an average yearly renovation rate in buildings), as well as through external policy indications (e.g. plans to achieve a shift from road to rail, and from the private to the public transport). All these assessments are clearly out of the scope of this thesis. In fact, the aim of the work is not to formulate a proper national decarbonisation strategy, but to provide a model to assess the potential role of hydrogen and  $H_2$ -based fuels in possible low carbon futures. As a consequence, reasonable assumptions regarding energy demand values have been made taking advantages of the knowledge that the RELAB research team has developed in the last 5 years [30–32] and during its on-going research activities.

Having said that, in the following sections it is described how the above rationale has been implemented and translated into input data.

### 5.1.1 Hydrogen demand in industry

In this scenario, it is assumed a direct use of  $H_2$  in the steel industry.

To date, hydrogen utilization as a pure product is mainly in the chemical sector and hydrogen is currently obtained with the methane steam reforming reaction (Eq.2.6). Looking at 2050, hydrogen could be consumed also to produce primary steel (i.e. steel from iron ore deposits).

In Italy, the primary steel industry has an important role, having in operation one of the biggest integrated steel plants in Europe. Today, the production is based on a blast-furnace (BF) in which the iron ore is smelted into iron by using coke as reducing agent. The molten iron is then converted into steel in the Basic Oxygen Furnaces

(BOF).

There are two promising routes to decarbonise steel production: applying CCS to the existing BF-BOF steel plant or avoiding  $CO_2$  emissions through the use of hydrogen. In the second case, the BF-BOF steel plant should be dismantled and substituted with a direct reduced iron (DRI) plant. The DRI is a commercial process in which natural gas is used as reducing agent. However, in the long term,  $H_2$  from electrolysis could be used instead of natural gas with the same function. The DRI- $H_2$  process is still in the R&D phase, but there are interesting pilot plants in construction in Europe [37, 74].

In this scenario, hydrogen demand for steel-making was estimated with the following hypothesis:

- 5 Mt of primary steel are produced in Italy in 2050 (annual average of the period 2015-2018)
- 50% of this production will be based on the DRI- $H_2$  process
- The assumed specific  $H_2$  demand of the DRI- $H_2$  process is 1,7 MWh  $H_2$ /t steel (based on data from [75])

The green hydrogen demand in 2050 is therefore = 4,2 TWh.

Typically, steel plants operates continuously during the year at full load. In the scenario, hydrogen demand for industry application is then assumed to be constant each (i.e. equal values for each hour of the year).

### 5.1.2 Energy demand in the transport sector

Assumptions regarding the transport sector should be made considering different sub-sectors:

- Road transport: heavy duty vehicles and buses
- Road transport: cars and light duty vehicles
- Aviation
- Navigation

Here below the main hypothesis made to replace the use of fossil fuels in the transport sector are presented.

#### **Road transport: electrification, $H_2$ and DME**

In the definition of the scenario, the heavy transport sector was assumed to be fueled with hydrogen.

To date there are already strong interests and consistent investments in development hydrogen technology for automotive applications.

Asiatic motor companies have already placed on the market some light vehicles fueled

by hydrogen. However, the current main limits of this technology spread are economically based.

Fuel Cell stacks and compact on-board hydrogen storage tanks still present very high production costs, which makes light FCEVs not competitive with current fossil-based or hybrid alternatives yet.

The main criticism for light vehicles is the space available for fuel storage. Range requirements and limits in space for the  $H_2$  tank impose to compress the gaseous fuel up to 700 bar. This requires to use very expensive metal alloys to guarantee safety parameters of the car and respect space limits.

A different situation occurs with heavy trucks and buses. They offer higher space availability for the on-board tank, enabling to use lower pressure level and ensuring longer ranges. Common pressure value is 350 bar.

To date only few hundreds of hydrogen fueled buses and trucks are in operation at a global level, mainly thanks to some pilot projects [2, 25, 38], as presented in Section 2.2.1.

Hydrogen can represent an attractive option for long-distance and heavy duty transport, where battery-based solutions are unlikely to become competitive. Following this reasoning, in a zero-dimensional representation of the Italian energy system it resulted easier to assume the total heavy transportation fuel demand covered by hydrogen.

Freight transport is mainly along highways, where centralized hydrogen refuelling stations can be installed. The latter can better describe the aggregation imposed by the single node hypothesis. Furthermore, public transportation fueled by  $H_2$  can describe as well the need for centralized refueling station. They could be built nearby the motor pool, taking advance of economies of scale.

Light transportation is instead a more unpredictable market. In the more recent period a consistent step change in the private automotive sector started. Major companies started to introduce electrified vehicles, in addition to the hybrid classes currently on the market.

Several projections [2, 5, 7] suggest the increasing diffusion of hydrogen in this market, with however an important role of the Battery Electric Vehicles (BEV). It is for this reason that, in the scenario, light vehicles are assumed to be electrified for the majority, with a fraction of e-fuels (Dimethyl Ether, DME) for the remaining part.

### **Aviation and navigation: synthetic jet fuel, ammonia and methanol**

In aviation and naval sectors, oil-derived fuels are difficult to replace. For this reason current R&D are investigating sustainable ways to synthesize them. Different solution of the H<sub>2</sub>L pathway were presented in Chapter 2. This lead to the reasonably assumption that fossil oil will be banned in 2050 Italian energy system.

In the aviation sector, full electrification is considered unlikely, as well as a complete supply with hydrogen. Long range requirements and weight limits are strong drawbacks in aviation sector. From this perspective, the presence of e-jet fuel was assumed in the scenario.

Another interesting transport subsector is the naval transportation. Currently naval engines are fueled mostly with diesel, with less than the 1% fueled with liquefied Natural Gas (LNG) and methanol [16].

liquefied hydrogen or compressed one are not suitable due to low volumetric energy densities compared with the common fossil fuels, being in the naval sector space optimization crucial to maximize the freight transport.

For this reason, a growing interest is emerging for ammonia and methanol as possible alternatives. To date there are no marine engines fueled with  $NH_3$ , but few methanol pilot projects describe the change on course [16].

From this perspective, the presence of ammonia and methanol were assumed in the model. An important aspect to be underlined on maritime and aviation sector is the difficulty on consumption and emission's allocation. Being both of them two routes for the international trading, it was necessary to separate national from international traffic.

### **Estimation of the annual demands in the transport sector**

Once that all  $H_2$  and synthetic fuel destinations are clarified, it is possible to estimate their demand.

The rationale adopted was to start from international transport consumption estimation [2, 16, 36, 40] for the future and then to extrapolate the weighted contribution of the Italian country.

Being the available projection at global level, no information are found on the separation between national and international transports within the same reference. It was then assumed the national contribution starting from the international value.

Defined these background assumptions, an overall annual value of 12 Mtoe was then obtained for the overall national transport sector that has to be further divided into the subsectors that were discussed above.

The first strong assumption concerns the definition of the road transportation share from the naval and aviation one. The latter as mentioned before, suffer from the uncertainty on national/international consumption. While in the international transport they have a major role, within national border the leading position belongs to the road transport.

From this perspective, the Author assumed that the 90% of the overall consumption belonged to the road transport, with a split almost equal between light vehicles and heavy trucks/buses.

Remaining 10% of the transport sector demand was assumed to supply aviation (5%) and naval transport (2.5%) and the non-electrified road vehicles with DME (2.5%).

The high uncertainty behind this method was related to the difficulty to separate national from international travels. A possible further implementation on the model might be a study on the national transportation sector and its relationships with border countries.

### Demand hourly profiling for the various energy carriers

Once the annual values of the e-fuels demands were estimated, the following step was to define their hourly profile during the year.

Hydrogen demand was assumed to have a constant profile when heavy transport is allowed, and zero in the forbidden moments. In order to define the period of time when heavy trucks are allowed to operate, the calendar for the Italian highways was taken as reference. It was reported the days where freight transport was permitted with hourly indication [76] actualized with the data. During holidays or on Sunday heavy transport are forbidden.

The profile was then normalized. When the heavy transport is allowed, the normalized hourly value is equal to the maximum, 1. When instead freight transport was forbidden on the highways, the trucks should be remain shut down, with no needs of eventual refueling. It should remain only the constant part of the hydrogen consumption due to the steel production, the 4.5%.

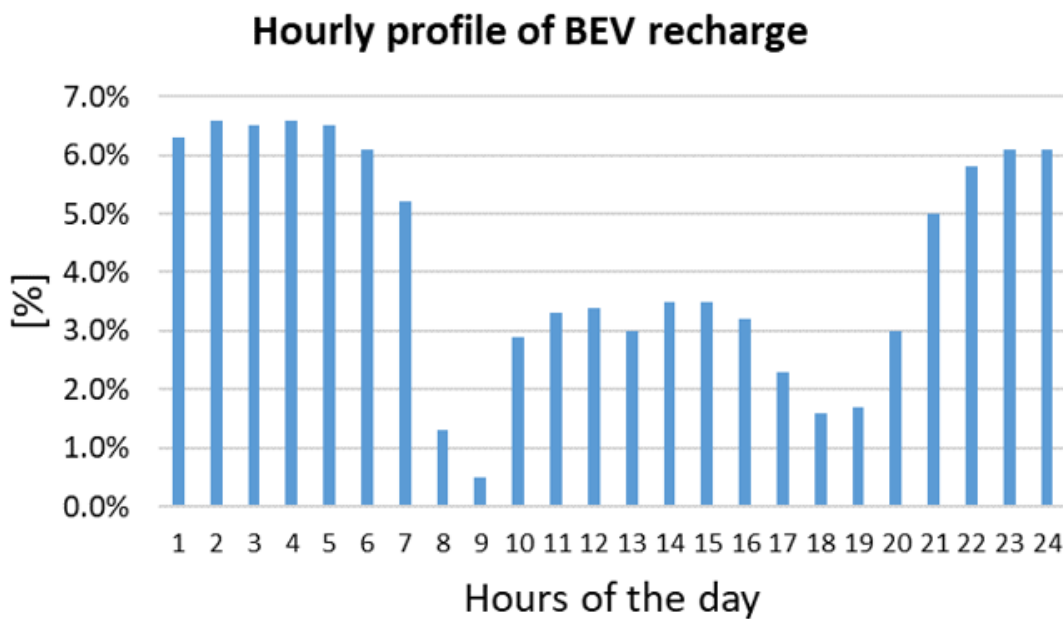


Figure 5.1. Hourly profile of recharge for BEVs; on the X-axis the hours of the day are presented, while on the Y-axis the percentage of the daily power consumption used in BEVs recharge used in the specific hour. It follows a smart management of the recharging infrastructure, without concentrating the recharge period during evening/early night

However, the fixed base profile is assumed to be the 10%. This can be explained with the fact that the main trucks driving ban has validity only on the highways and not on the smaller roads. Furthermore, urban public transports are not influenced by this dynamic and there is the additional possibility of refueling off the clock by freight trucks. With more detailed information it would then be possible to estimate

more accurate profiles. This could be an interesting further development.

For the light transport that is electrified, a recent study [77] of the Italian RSE, whose acronym means "Ricerca sul Sistema Energetico", analysed the possibility of electrification for light vehicles.

Here useful information are reported, such as a mean daily load profile with hourly characterization for vehicle recharge. The combination of the daily profile (reported in Figure 5.1) with the assumed annual consumption allowed to determine the final light vehicle power demand value and profile.

For the remaining e-fuels, no information were available for aviation and naval consumption's partition during the year. For this reason, demand profile for the remaining synthetic fuels present in the scenario was assumed to be constant for each of them. As mentioned before, a possible future development reported in Section 6.1 could be the study of final demands.

### 5.1.3 Natural Gas constraints

Once the synthetic fuel demands had been determined, the next step is to define the resource availability.

Fossil fuel resources are expected to be banned in the next years, with the exclusion of Natural Gas. Coal phase-out is already occurring and is expected to be completely abandoned in the medium term.

The only remaining fossil fuel available is expected to be fossil Natural Gas. Currently more than 90% of the national gas demand is supplied by import. Being the national production expected not to increase in next years, fossil import is likely to be still present in the future.

The Italian gas Transmission System Operator (TSO) SNAM in collaboration with the power TSO Terna provided useful long-term projections for the evolution of gas sector [34]. Historical annual gas consumption series are reported with collateral information on daily peaks and storage availability.

Collecting the mentioned information, it was then possible to assume an initial value of the available fossil NG for the scenario under consideration.

2018 total consumption of gas was nearly 72.7 billion  $m^3$  (or  $\sim 707$  TWh), which correspond to a mean consumption of 200 million of cubic metres per day.

The report contains also the historical maximum daily gas consumption, from which the mean value of  $380 * 10^6 \frac{m^3}{day}$  was obtained .

Having the model an hourly time-step resolution, the last value divided per 24 hours was assumed as the maximum quantity of gas that may have to be supplied to the grid ( $\sim 154$  GW).

In the model the role of fossil NG is confirmed to be the same of the current one. Thus, the maximum available fossil NG was estimated to coincide with the 707 TWh mentioned above.

This quantity should considerably overestimate the effective gas consumption that are expected by 2050. Energy efficiency and electrification of heating system will play an important role in the next years. This trend was already reported in the projections contained in the Italian 2030 "Piano Nazionale Integrato per l'Energia e il Clima" (PNIEC) [35].

It is then likely to expect a decreasing Natural Gas consumption. The value assumed before (707 TWh) of available fossil NG was the initial one. First run of simulations will confirm the mentioned expectations, as will be described in Section 5.3.

#### 5.1.4 Assumption on total storage capacities for $H_2$ , $H_2$ -based products and $CO_2$

The next baseline assumption concerns the storage availability.

In order to minimize the utilization of fossil fuel resources with the collateral effect of net  $CO_2$  emissions reduction, the other alternatives to fossil NG have to be produced and stored when the conditions are favourable.

Storages of alternative solutions have been then assumed to be able to store high capacities.

The increasing penetration of renewable energy in the system determines not only unbalance problems between demand and supply during the day. This problem management had already been raised in 2030 projections, where a lower REs share (32% of the final energy consumption) is assumed with respect to 2050 targets.

Full decarbonisation would result in much higher REs penetration. This issue would then become crucial, with seasonal unbalances expected between summer, where over-generation problem occurs, and winter, with possible energy shortages. Electrification of the system would not be enough, unless to decide of increment battery storage to an unrealistic amount.

From this perspective the *Power to Hydrogen* first and then the H2X pathways represent a very interesting solution. The over-generation occurring in the summer, when higher availability of Photovoltaic (PV) produce more power than the required by the system, could be exploited via water electrolysis.

The large amount of hydrogen utilization pathways would lead to the synthesis of many compounds, namely SNG and e-fuels. Those quantity however should be stored in large quantities, in order to guarantee the existence of reserves during shortage periods.

An initial very large value of maximum allowed stored capacity was assumed for the three options of hydrogen storage and for its by-products. Except for gas storage, for which the national storage capacity is available, the other storages were sized in the following manner.

Each of the three option for hydrogen storage capacity was defined as the required one to store the entire  $H_2$  production for 1000 consecutive hours (or  $\sim 40$  days). The 3 contributions together allowed a store for 120 days at maximum production and no



consumption.

For the other e-fuels, the same logic was followed, ensuring per each a storage of 60 days at maximum production and no consumption. These very high amounts were set to allow the model to analyse all the possible generation mixes pursuing fossil usage minimization without too strict constraints.

Lastly, the  $CO_2$  storage. As anticipated in the model both CCU and CCS are implemented, although the latter has not been implemented in this scenario analysis. Its exclusion was defined in order to promote carbon combination with hydrogen and a wiser generation mix. The CCS availability would be used only as a last decarbonization resource.

In the model the maximum feasible storage capacity was assumed, as the captured carbon dioxide of the processes where CCU is enabled as if they run at maximum load the entire year. Currently in the model CCU was implemented for exhaust gas treatment in all GT plants, biogas upgrading plants as at the output of DAC units. The obtained annual maximum storage capacity was on the order of magnitude of 70 Mton of  $CO_2$ . In Italy the underground  $CO_2$  geological storage capacity is estimated to be around 20-40 Gt  $CO_2$ , partly in aquifers and partly in exhausted oil and gas wells [33]. A further extension would be to the industrial CHP that produce heat and power for self consumption.

## 5.2 Input data description

In this Section the main input data will be presented. Starting from the definition of the overall Gross Inland Consumption a focus of the main demand values and the available resources will be provided.

Subsequently, evaluations on installed capacity for main Power to Hydrogen and Hydrogen to X pathways will be reported, to finally introduce the main simulation results.

### 5.2.1 Final energy demand

The first class of parameters that have to be estimated are the overall consumption. They are grouped in three main categories, which together form the Final Energy Consumption. This represents the total energy demand consumed by end users of a country. It excludes the energy consumed by the energy sector itself and this important peculiarity will be called back in results analysis.

As introduced, final demands were grouped in three categories:

- Power demand
- Heat demand
- Hydrogen and  $H_2$ -based fuels demand

The former covers the net electric load, the cooling demand in residential and tertiary sector that occurs during hot season plus the assumed demand for BEVs in transportation.

Heat demand is inclusive of all the required heat in residential and tertiary sector plus the required heat for industrial applications covered by industrial CHPs. A further characterization of heat for residential and tertiary sector was then already developed in the original version of the model, and was then confirmed in the version presented in the thesis.

In the specific a focus on Domestic Hot Water (DHW) and on District Heating (DH) was conducted.

The third demand class regards hydrogen and all the e-fuels that covers the demands in transportation presented in the previous Section 5.1.2. They all are presented in Table 5.1.

Table 5.1. Assumed annual values for the main demands in the model

Demand class	Demand	Annual demand [TWh]
Power demand	Net electrical load	254.73
	Cooling electrical demand in residential sector	22.83
	Cooling electrical demand in tertiary sector	10.60
	Electrical demand for BEVs recharge	59.2
Heat demand	Heat load in residential sector	158.99
	DH in residential sector	9.99
	DH in tertiary sector	0.48
	DHW in residential & tertiary sector	60.29
	DHW demand covered by DH	1.15
	Heat demand in tertiary sector	54.29
	Heat demand in industry <sup>a</sup>	51.2
	Heat losses in DH network	2.33
$H_2$ and e-fuels demand	Hydrogen demand (trucks & steel)	68.27
	Jet-fuel demand	6.34
	Methanol demand	1.16
	DME demand	3.17
	Ammonia demand	3.17

<sup>a</sup> It represents the only part that is covered by industrial CHPs

BEVs recharge power demand were estimated as for the previous transportation sector by comparing the information available in the 2030 PNIEC, the international long-term projections for 2050.

The energy demand values presented in Table 5.1 were estimated by combining estimation previously introduced (e.g. BEV recharge demand) with assumptions made in Section 5.1.

Heat demand shows a wider characterization, with a focus on District Heating. In order to maintain the same level of detail for the 2050 simulation, a literature review on the current DH systems situation in Italy [78, 79] was demanded. Coupling these information with the estimations of Section 5.1, it was then possible to estimate the value reported in Table 5.1.

### 5.2.2 Available resources

After the definition of the Final Energy Consumption presented in the previous Section, the following step was to determine the available resources.

In oemof framework the class of *Source* is used to express where a raw energy carrier comes from (e.g. import of fossil NG, power production from PV). In the Table 5.2 presented below the main renewable sources, bio-based ones and fossil NG are reported.

Starting from the fossil fuels sources, as described in Section 4.3.4, the only available fuel is assumed to be Natural Gas. The annual maximum availability is the obtained number of the assumptions previously presented. This number is expected to be a considerable overestimation of the required amount of methane and will be the parameter on which the simulations will focus.

As introduced in the Section 5.1, the aim of the simulation is to reduce  $CO_2$  emission of the system by minimizing the fossil resources utilization to the limit condition without shortages. The model has to return the optimized generation mix that is able to cover the complete demands without any shortage.

In order to do the reduction, first attempt simulations must be conducted to estimate the mean current gas requirement by the model. The latter represents the quantity of energy that on average is supplied to the system. Reducing the fossil NG availability, the required quantity must be overcome by alternatives, namely synthetic methane from H<sub>2</sub>G pathways and with blending option in the transmission grid. This logic is followed during all the simulations.

Concerning the REs sources, here below the main assumptions are reported. Hydroelectric, which in the model is divided into two components to separate uncontrollable flowing river from the water reservoirs, had been already exploited at its maximum. It is unlikely to expect a consistent increase in its capacity. Same consideration can be made for geothermal heat and power generation.

For biogas availability, 2030 projections suggest a potential role of roughly 100 TWh [80]. Being biogas strictly limited by the amount of biomass that can be gasified, it is assumed to maintain the same overall value for the 2050 simulation. Different uses of biogas imposed different pathways, as described in Section 4.3.9. To date, most of the biogas treatment is to remove toxic impurities. Another further possibility would

Table 5.2. Assumed values for import, renewable and bio-based sources

Source	Capacity [MW]	Annual max [TWh]	Variable cost [€/MWh] <sup>a</sup>
Coal	0	0	15.24
Fossil NG	153 935.18	707	41.10
Oil	0	0	68.53
Ligneous biomass	None <sup>b</sup>	None <sup>b</sup>	90.00
Biogas <sup>g</sup>	372.1	3.26	16.00
Biofuels <sup>f</sup>	0	0	77.00
Urban waste	None <sup>b</sup>	None <sup>i</sup>	0.00
Hydro (reservoir) <sup>h</sup>	6 895.1	27.7	0.00
Solar thermal heat indiv <sup>c</sup>	6 638	6.97	0.00
Solar thermal heat plant <sup>d</sup>	0.693	0.0007	0.00
Industry heat recovery destined to DH	41.0	0.32	0.00
Geothermal heat to DH	135.0	1.06	0.00
Net electricity import	8 539.1	26.1	0.00
PV	300 000	471.12	0.00
Wind	47 000	128.91	0.00
Hydro (river) <sup>h</sup>	5 625.3	22.61	0.00
Geothermal power	1 600	11.71	0.00
Waste oils and animal fats to H2L	879.9	7.71	0.00
Biogas for upgrading	8 071.61	70.7	16.00
Biogas for biological methanation	3 106.64	27.21	16.00
Biogas for DME	0	0	16.00
H <sub>2</sub> O for electrolysis <sup>e</sup>	32.4 * 10 <sup>3</sup>	283.82 * 10 <sup>6</sup>	0

<sup>a</sup> it expresses only the commodity cost

<sup>b</sup> it means that the capacity is not significant

<sup>c</sup> Heat generation via solar thermal panels individual buildings

<sup>d</sup> Heat generation via centralised solar thermal plants

<sup>e</sup> maximal water requirement for hydrogen synthesis via water electrolysis. Measure in cubic metres of liquid water

<sup>f</sup> biofuels destined to power production, banned from 2030 [35]

<sup>g</sup> biogas destined to power production

<sup>h</sup> reservoir means hydroelectric power from water basin; river means hydroelectric power from non-adjustable rivers

<sup>i</sup> urban waste annual max value is implicitly fixed by the thermal and power demands that it has to supply

be the upgrading, the separation of methane from the carbon content (i.e. carbon dioxide) and then injected to the grid.

Biological methanation is at R&D level, although some pilot projects are already on operation. A considerably increasing interest is growing around the technology and for this reason is likely to expect wider application in long-term. While upgrading technology simply filter the carbon content, with biological methanation the  $CO_2$  presence could then react with hydrogen in a reactor (see Section 2.2.2).

The author then assumed a persistent major role of upgrading plants (70%) and the remaining part to be destined to biological methanation. A 3% of the total available biogas was left for power generation, representing the existing small CHP direct application of biogas, which are unlikely to be decommissioned.

Biogas transformation into DME has been implemented in the model, although it is not used in this scenario. Literature review [19] reports the possibility to have direct DME synthesis from biogas instead of the current 2 step process with methanol synthesis (see Section 2.2.3). However, no existing plants are current operating in the Italian system. For the presented simulations, it was assumed not to use this possible pathway.

For waste oil and animal fats, the Author estimated the value from [42].

The remaining REs sources are wind and Photovoltaics (PV). 2030 PNIEC assumes a capacity of 17.5 GW for wind power generation capacity and 50 GW for PV. Today, current values are roughly 9.8 GW for wind and 19.7 GW for photovoltaics. In order to cover the 30% of the total final consumption with REs in 2030, the two mentioned sources had to more than double their installed capacity in the current national projections [35].

The estimation becomes more critical for a farther time-horizon like 2050, where full decarbonisation target imposes a much stronger REs penetration in the energy system. It is in this perspective that the value for wind power of generation was assumed to be 47 GW.

The assumed installed capacity for PV was more difficult to be determined. This mainly because in the developed scenario a full decarbonization imposes a wider REs penetration on the overall power generation. However, the collateral effect of decarbonisation is the availability reduction in fossil NG, whose energy content the system continues to require.

The energy originally provided by the fossil NG has to be then overcome by different alternatives, mainly with synthetic methane obtained with H<sub>2</sub>G.

It is then clear that high green  $H_2$  requirements, to satisfy the pure demand and the demand in its by-products, a high power availability in over-generation situations was necessary.

For this reason, the value of PV installed capacity was assumed to be 300 GW. This value is compatible with the results of previous research activities carried out by the RELAB group on the national context [31].

### 5.2.3 Technical parameters of $H_2$ and $H_2$ -based fuels synthesis technologies

Last class of data that the model required was composed by information of the main implemented processes.

The three Tables (A.1, A.4, A.2), listed in Appendix A, report the assumptions on installed capacity of the main processes of P2H, *Hydrogen to X* pathways and for power and heat generation. They were divided into three classes because of the different input parameters inserted.

For the existing CHP and *Power to Heat* technologies, already present in the original version of the model, the followed logic was the same for heat demand estimation. The same level of characterization was confirmed, starting from the provided 2013 data and comparing with the 2030 projections in order to determine the ratio of each category with respect to the overall demand.

Starting from the initial demand, the supply share of each technology was determined. This share was assumed to remain constant. After the estimation of the 2050 final demands, it was then possible to adjust the expected installed capacity for the Heat generation. The new capacities had to be able to cover the estimated demands keeping the share previously determined.

Further implementations could concern the study to assess a stronger electrification of the heat generation sector.

For *Power to Hydrogen* first and its utilization pathways then, a different approach was required. The main issue was the fact that to date these technologies are at initial diffusion on the market in a national perspective. In Italy a well-established green hydrogen framework does not exist yet as in the case of gas infrastructure.

The pursued logic was to determine an output installed capacity for each introduced technology that was able to process the required quantities without constituting critical bottlenecks. It is under this assumption that transformers such as the ones bounded to the  $H_2$ -methane blending or to consider the power requirement for hydrogen storage were set with large capacities.

Installed capacity for the main *Hydrogen to X* processes were estimated after a first attempt simulation set. Defining a load duration curve for each process, useful information could be obtained.

Load duration curves returns the production flows during every hourly time-step in descending order. Figure 5.2 reports an example where in the X-axis the operating time is presented, while in the Y-axis the used capacity for each time-step is indicated.

Using this concept it was then possible to obtain a first order of magnitude for the used capacity of main implemented processes to cover the final demands.

This reasoning was particularly crucial in the definition of installed capacity for hydrogen synthesis via water electrolysis. The definition of this capacity had tickle-down consequences for all the  $H_2$  utilization pathways. Currently it could represent the most important bottleneck of the model.

After some simulations, through the analysis of the load duration curve, the value of

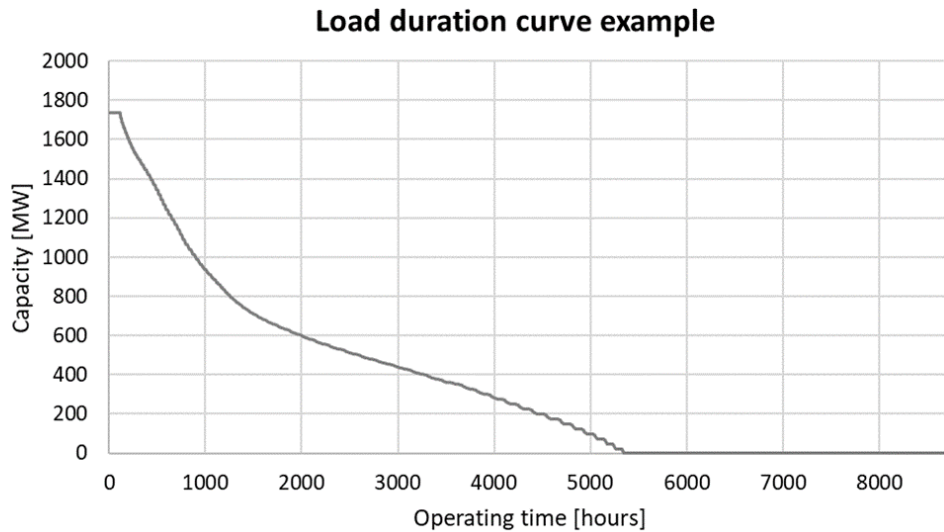


Figure 5.2. Load duration curve example

120 GW for output  $H_2$  installed capacity was then determined. The load duration curve showed a period of roughly 700 hours at nominal capacity. This number balanced the installed quantity and the operating time in which all the electrolyzers are being used with the amount of over-generation present.

A subsequent required assumption was related to those technologies that can directly consume pure hydrogen to produce back power, up to now only Fuel Cell technology. Its sizing was assumed to be able to completely transform all the produced hydrogen as if it was entirely destined to H2P pathway.

In the model currently it was overestimated, being inserted a value of output power capacity coincident with the hydrogen capacity of the electrolyzers. However, load duration curves has outlined that the peak capacity in H2P was never reached.

In the definition of *Hydrogen to Gas* and *Hydrogen to Liquid*, literature review outlined some technologies that produce some recoverable heat as output product. Although the high uncertainty level in some H2L processes presented in Section 4.3.10, due to the lackness of complete and homogeneous data on energy balance (e.g. jet-fuel synthesis technologies), in the model was implemented the possibility to recover a part of this heat.

Last step required to completely describe the input data given to the model regarded the load variation of the technologies. There exist some technologies that are more flexible, while some others are not. Again, the system describes a single node situation, with aggregate production capacities and demands.

Some technologies, such as methanol synthesis or catalytic thermochemical methanation do not allow much flexibility in operating load. Their minimum load is very high, roughly the 90% of the nominal capacity, below which it is more convenient to avoid production.

However, in the model aggregate capacities are assumed. In thermochemical catalytic methanation, current sizes are in the range of hundred  $MW_{CH_4}$ . In the model it is then assumed to reach lower minimum aggregate load by turning off several plants, while maintaining the remaining ones at nominal load. This can be seen as the analogy of nuclear power plants in France. Each plant has very limited flexibility, but, acting on the overall number, it is possible to obtain a very high global flexibility.

For this reason, also these not flexible technologies were assumed to reach minimum load.

Finally, some consideration on the assumed storage capacities are presented below. Main values are reported in Table A.3.

As introduced in Section 5.1.4, storage total capacity was generally obtained by multiplying the production capacity of a synthesis process to a determined amount of hours. This was estimated in order to ensure the possibility of long period storage, enabling seasonal storage possibility.

With the hypothesis assumed in the previous section and the main *Hydrogen to X* technology installed capacity defined, the total storage capacity is then calculated. Charge capacity and discharge one represent the maximum charge and discharge time-step quantity that can enter or exit the storage. Input flow is assumed to coincide with the total production capacity of the energy carrier that is going to be stored. Discharge flows instead are assumed bigger when there are no particular constraints. An example could be the Pumped Hydroelectric Energy Storage (PHES), where water is pumped back to the upstream basin when there are over-generation periods with excess electricity. Here the maximum charge and discharge capacity are limited by the pump-turbine system, that have a maximum volumetric flow rate.

Initial capacity represents the initial stored capacity at the beginning of the year simulation. By default, the model is obliged to reach the same initial stored value given by this parameter. This means that if at the beginning of the simulated year a stage is 10% full, at the end of the year will have to reach the same value.

Initial capacity values were confirmed for the classes already existing in the original NEMeSI version.

For the implemented ones, an initial empty condition was assumed for the first round of simulations. Subsequent reasoning will be described in the following result section. The values of classes pre-existing the H2X implementation were adjusted with the long-term projections for 2050, keeping fixed the original ratio with respect to the power & heat generation sector.



## 5.3 Results

In this Section the main results of the scenario analysis are presented. Previously some consideration regarding the several rounds of simulation to reach the minimum fossil NG availability under which there are shortages. Then a focus on the power generation and consumption allocation is presented, followed by a detailed analysis on hydrogen production and utilization.

Lastly, some consideration about Hydrogen to X pathways are mentioned.

### 5.3.1 Energy required by the system from the gas grid

The main decision driver is the minimization of the consumption of fossil Natural Gas, with a focus on the decarbonization goal. As presented in Section 4.3.4, reducing the availability of fossil sources, it is demanded to the model to determine a generation mix capable to overcome the energy cap linked to fossil NG reduction. There would be produced alternatives such as synthetic methane from renewable pathways or with an higher  $H_2$  penetration in the grid through the blending option. The sum of these alternatives will have beneficial effects on the overall decarbonization.

Several rounds of simulation were then run in order to proceed with the fossil NG availability. In Table 5.3 the main rounds are reported, with a brief description of their goal and the results obtained.

Table 5.3. Description of the aim of the main different rounds of simulation and the obtained major results; each round provided useful information that were used to set the subsequent round in a progressive point of view

Round	Aim	Results
Setup	To evaluate the initial installed capacity for P2H	120 GW
I	To determine the amount of energy required to the gas grid	~370 TWh (181 TWh from fossil NG)
II	To evaluate the minimum quantity of NG fossil used without shortages	177 TWh of fossil NG; seasonal storage behaviour for $H_2$ and gas
III	To evaluate the initial storage level for $H_2$ and gas that overcome shortage problem	~12 TWh both
IV	To evaluate the minimum quantity of NG fossil used without shortages (with initial level of $H_2$ and gas storages)	166 TWh of fossil NG

For this reason the first round of simulations was conducted in order to determine the total amount of energy from gas grid required by the system. This was obtained

observing the demand that had to be supplied with processes that used gas. In this operation, it is helpful to look at Figure 4.1 and 4.2 to determine which are the fixed demands that consume methane energy and the ones that consume it without fixed profiles.

In a right-to-left logic on the mentioned SRES schemes and applying the conversion factors for each transformation backward, the total required energy from methane pathway was obtained.

However, during this process two important consideration had to be kept in mind. As introduced in Section 2.4.4, hydrogen blending in the gas grid is implemented. This means that the energy flows that supply CHPs technology or gas plants could contain up to the 20%vol of hydrogen.

The second point to stress is that an uncertainty on the estimation of the minimum methane requirement is due to the presence of unfixed demands. While for fixed profile demand the model is obliged to use a specific technology (e.g. small CHPs in residential and tertiary sector), this doesn't necessarily happen with free profile technologies.

In these situations the model might consider less expensive to use methane to generate power, using for example a gas power plant instead of using hydrogen FC.

Bearing in mind the two mentioned arguments, a mean value of 370 TWh of energy was required from gas grid, of which  $\sim 304$  TWh came from fixed profile demands and 66 TWh from free profile ones.

The first important information that can be extrapolated from the data is the maximum amount of methane that the model could consume. As described in Section 4.3.4, the first NG fossil availability of 707 TWh was considerably an overestimation, as expected. Energy efficiency improvement on the demand side (including electrification of heat in building), and increasing REs penetration in the generation mix outlined in the long-term projections have the main consequence of fossil consumption reduction.

The next step required to proceed with the analysis was to determine the origin of the methane used in a scenario with an overestimated NG fossil availability. This can clarify how much fossil methane might be reduced without other variations.

In the model four possible methane supply are implemented:

- Fossil NG
- methane synthesis via thermochemical catalytic methanation
- methane synthesis via biological methanation
- methane from biogas upgrading

The first round of simulations, with more NG availability than the required one, returned an utilization of imported fossil natural gas of roughly 181 TWh, with contribution of synthetic methane from renewable H<sub>2</sub>G and biogas upgrade of 173 TWh and 15 TWh from hydrogen injected in the grid. The second term was composed

by  $\sim 66$  TWh of  $CH_4$  coming from thermochemical catalytic methanation, 68 TWh from biogas upgrading and the remaining 39 TWh from biological methanation.

Once the mean utilization of energy from gas grid was estimated, and then the quantity of imported NG, it was possible to pursue the fossil resource minimization target until the lowest quantity consumed that does not present any electrical or thermal shortage.

Maintaining the same nominal capacity estimated in Section 4.3.4 for fossil methane (153.93 GW), to supply 181 TWh of NG the import process should operate for a some amount of hours. It is useful to introduce the concept of Equivalent Operating Hour (EOH).

EOH represents the hours required to a technology with a given nominal capacity to produce the overall measured quantity at its maximum load. It expresses the hours of operation at nominal conditions to produce the investigated value.

It can be expressed as follow:

$$\text{Equivalent Operating Hours [h]} = \frac{\text{Annual produced quantity [MWh]}}{\text{Nominal installed capacity [MW]}} \quad (5.1)$$

Traducing the previous NG fossil data, to supply 181 TWh during the year, import should work at its nominal capacity for 1175 equivalent operating hours.

Collected all these consideration, a second round of simulation was then launched. The followed logic was a gradual reduction of the overall fossil NG annual availability, starting from the determined 181 TWh.

The fossil NG reduction stopped almost immediately below 177 TWh, presenting some electrical shortages in the resulting generation mix. In the beginning it seemed that there were no room for manoeuvre in the resources' balancing.

Thermal demand presented a better situation, with no thermal shortages, even with much lower fossil NG availability. This meant that the energy system was able to entirely cover all the thermal demands.

Analysing better the annual profile of the shortages, it emerged a full concentration of hourly power deficit in the first period of the year, namely the first month. By keeping to reduce the fossil NG availability, the hours presenting shortages increase in number and in absolute power deficit values, from January to propagate themselves to the spring first and then to the entire year. Figure 5.3 shows the concentration of shortages at decreasing NG fossil availability. On the Y-axis the share of total demand that is not supplied is reported, while on the X-axis represents the period of the simulated year.

By reducing the fossil NG availability, electrical shortages occur during the first period of the year. In this period the REs availability is low (e.g. low solar irradiation for PV), while gas requirements for heating are high. The combination of the two factors obliges the model to synthesise renewable methane or produce  $H_2$  for blending

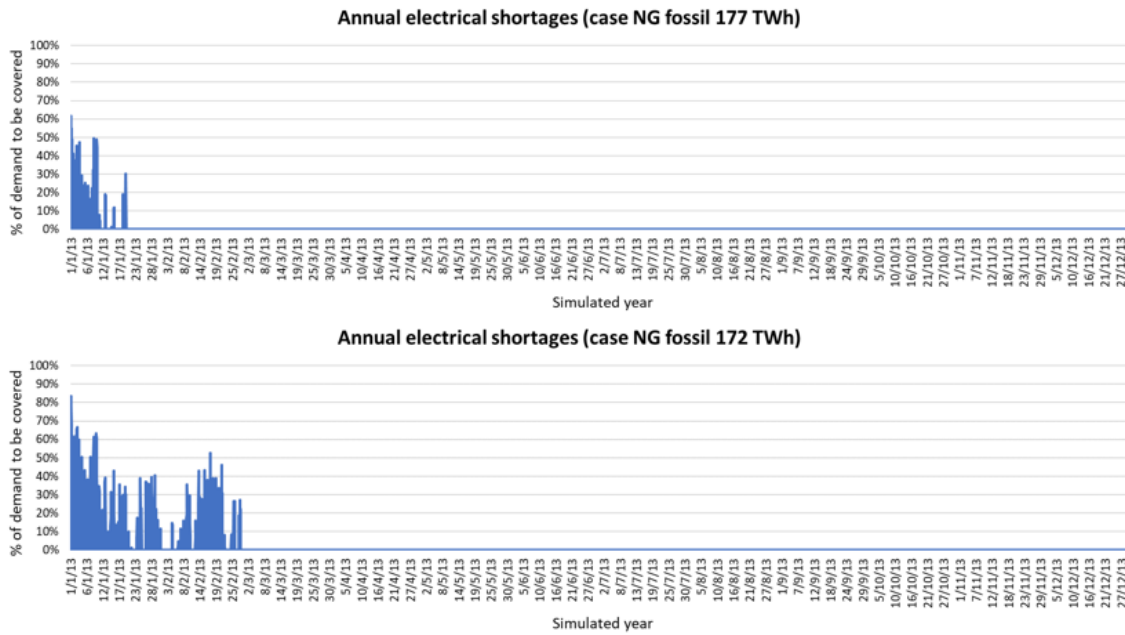


Figure 5.3. Annual electrical shortage profile; the graph shows the share of the total power demand that had to be covered by fictitious shortage flow created by the model (see Section 4.1.2). Two cases are presented to outline the increase in shortage's number by reducing fossil NG availability

option to cover the deficiency of methane available by resorting to electrical shortages.

At the same time, other consideration emerged by the result analysis. As illustrated in the previous Section, initial storage levels of the implemented *Hydrogen to X* part were assumed null. The model starts with empty storage level and then it begins to use them if they are advantageous. By default however, at the end of the year it is set up to bring back them at their initial value. This setting could be customized in oemof framework, but for the current setup it was decided the default setting. In future developments a revision of the time horizon could be then implemented, starting simulation of more than one year to better study seasonal behaviours.

Focusing back up on the mentioned consideration, it emerged that during the year a  $H_2$  seasonal storage occurred from summer to winter. Its trend depicts a gradual growth till the end of September, from when a turnaround starts, in order to arrive at empty condition at the end of December.

A similar behaviour was observed, although on a smaller scale, for methane storage. This latter tends to considerably reduce with the NG fossil reduction, as can be expected. Reports on gas grid infrastructure [3, 34] indeed confirm the necessity to rely on methane storages to cover the winter peaks in demand, that cannot be covered through the nominal supply chain of import and national production.

In Figure 5.4, the trend of hydrogen and methane storage are reported. Especially for  $H_2$ , an important storage can be observed. On the Y-axis the current stored capacity of the energy carrier is showed, with the X-axis representing the period of the year.

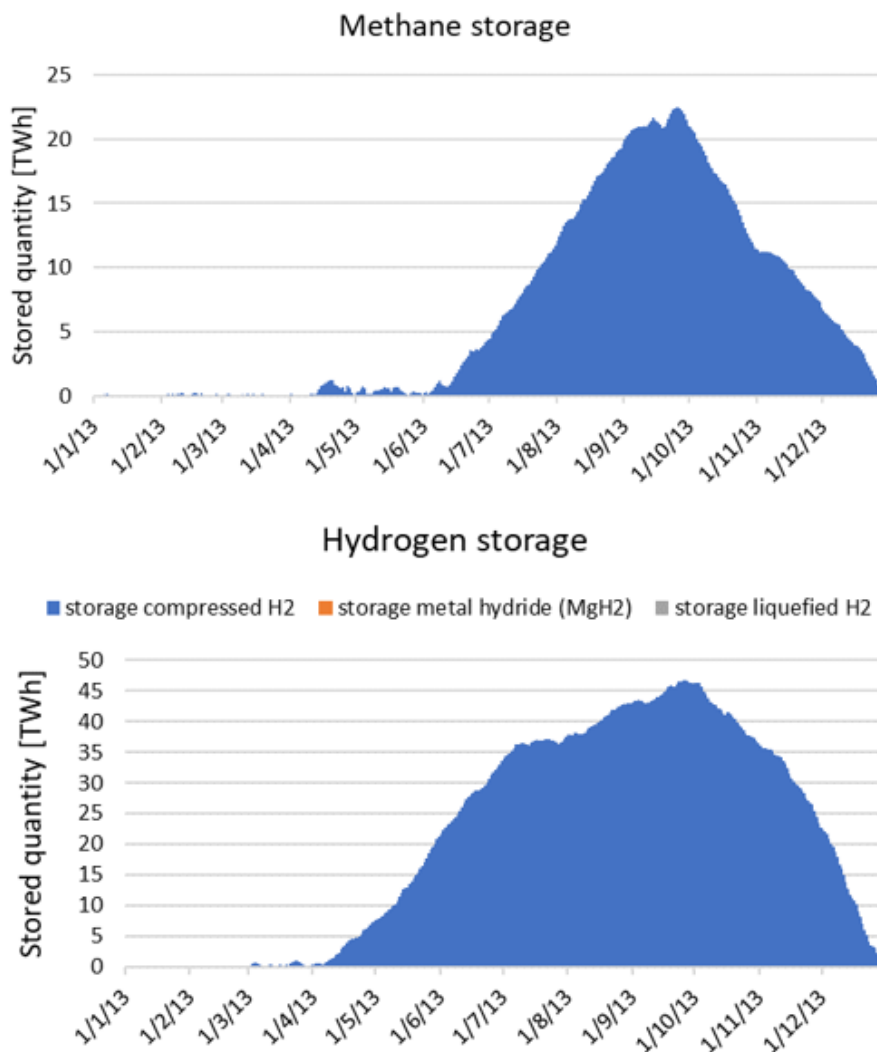


Figure 5.4. Storage of hydrogen and methane during the year simulation

For these reasons a correction on the scenario setup was made and a third round of simulations was performed (see Table 5.3). The reasoning followed was to assume an initial value for hydrogen and gas storage. In the specific, for hydrogen was assumed to start with a level that was experienced at the beginning of the last month of the simulated year, namely  $\sim 12$  TWh. The logic was to assume the discharge to start one month later, in order to have available a residual amount of green  $H_2$  at the beginning of the subsequent year.

However, the limit of this simulation is that current version of the model is set to return a single year simulation, where the seasonal storage behaviour cannot be completely studied.

For gas initial storage level the same logic was first assessed, assuming as initial level the one reached at the beginning of the December, roughly 6 TWh. Three different evaluation were made. First with only hydrogen initial storage, then with

only gas and lastly with the two together.

The three combinations presented all shortages, although lower in number and absolute values, with the same concentrated trend in the first period of the year. The presence of initial gas stored quantity returned a better impact on shortage reduction with respect to the only hydrogen initial storage option. The simultaneous presence of initial level for both allowed the system to obtain the lowest level of shortages at last. The shortage problem was not solved with the first initial level assumed. Annual gas demand and supply profile provided by [34] outlines a longer period of dependence from storage by the Italian grid, requiring bigger stocks.

Under this perspective, gas initial stock was increased. The same initial storage level (12 TWh) for both hydrogen and methane was assumed and the same simulations' sequence was repeated. Results showed no more presence of electrical shortages at the current NG availability level (177 TWh), enabling the possibility to continue its reduction.

With the previous adjustments it was then possible to pursue the NG fossil dependence reduction goal.

The new round of simulation arrived at the minimal imported fossil availability of 166 TWh. Below this value even increasing initial stocks the shortage problem was not solved. Although power deficiencies during the first period of the year were compensated by storage, there was not enough gas available during the remaining part of the year to cover the demand and to fill up the storage, without resorting to shortages.

### 5.3.2 Power generation and consumption

In the following an analysis of the main consumption will be presented. The focus will be on the power side, being the thermal demands always covered even at lower fossil NG availability levels.

In Table 5.4 the classes of power production are listed. The first consideration that can be made regards the share of renewable energy sources on the total power generation. The total amount obtained from RE is equal to 690 TWh, which means  $\sim 86\%$  of the total power generation. The remaining part is provided by gas use in power plants and CHPs (10.9%) and import of electricity (3.2%). In Figure 5.5 the power production allocation and consumption are presented.

This information however is not complete. In fact, the reduction of available fossil methane imposed the necessity to counterbalance with the synthesis of renewable one or by using the blending option with injection of hydrogen in the grid.

It is then required to analyse the composition of the gas burned in these power plants, to determine the real fossil source share on the total power production.

To generate the power and heat required by the energy system, an overall amount of 371 TWh of energy was required. This is composed by the contribution of fossil NG, methane deriving from biogas upgrading and the two methanation process plus an injection in the grid of hydrogen, as reported in Table 5.5.

Table 5.4. Annual power generation from the different sources

Source	Annual power generation [TWh]	Share on total [%]
Hydroelectric	47.6	5.9%
Electricity import	26.1	3.2%
Wind	128.9	16.0%
PV	470.7	58.4%
H2P (Fuel Cell)	13.2	1.6%
Geothermal	11.7	1.5%
Coal & oil	0	0%
Gas <sup>a</sup>	87.5	10.9%
Urban waste	12.9	1.6%
Power from waste heat recovery (ORC)	3.1	0.4%
Bioenergy	4.4	0.5%
<b>Total</b>	<b>806</b>	

<sup>a</sup> It comprises the total amount of energy provided by gas grid, meaning NG, synthetic methane and  $H_2$  injected with the blending option. Fossil NG contribution is investigated in Table 5.5

Table 5.5. Energy provided by the gas grid

Gas grid energy supply	Total energy provided [TWh]	Share on total energy provided
Fossil NG	166.6	44.9%
Methane from biogas upgrading	69.3	18.7%
Methane from biological methanation	38.7	10.4%
Methane from catalytic methanation	73.8	19.9%
$H_2$ injected into the grid	22.3	6.0%
<b>Total</b>	<b>370.7</b>	

It has to be underlined that energy carrier's composition in the gas grid is not the same during all the simulated year. Although the hydrogen injected in the grid is the maximum possible during almost of the year (20%vol content), there are small periods

where blending option injects a mix with the 10%vol content of  $H_2$ . Thus, power and heat generation fed by energy that comes from the gas grid are not obtained from a flow with the same energy composition. Making an approximation, the share of energy composition reported in Table 5.5 was assumed as the one of the grid during the simulated year.

With this information, of the 87.5 TWh of power produced by gas power plants and CHPs, only the 45% can be assigned to fossil NG. This translates the effective share of fossil methane only on the 4.8% of the total power generation.

Once the power production side had been analysed, the next step was to focus on the power consumption one. In Figure 5.5 the power production and consumption are presented.

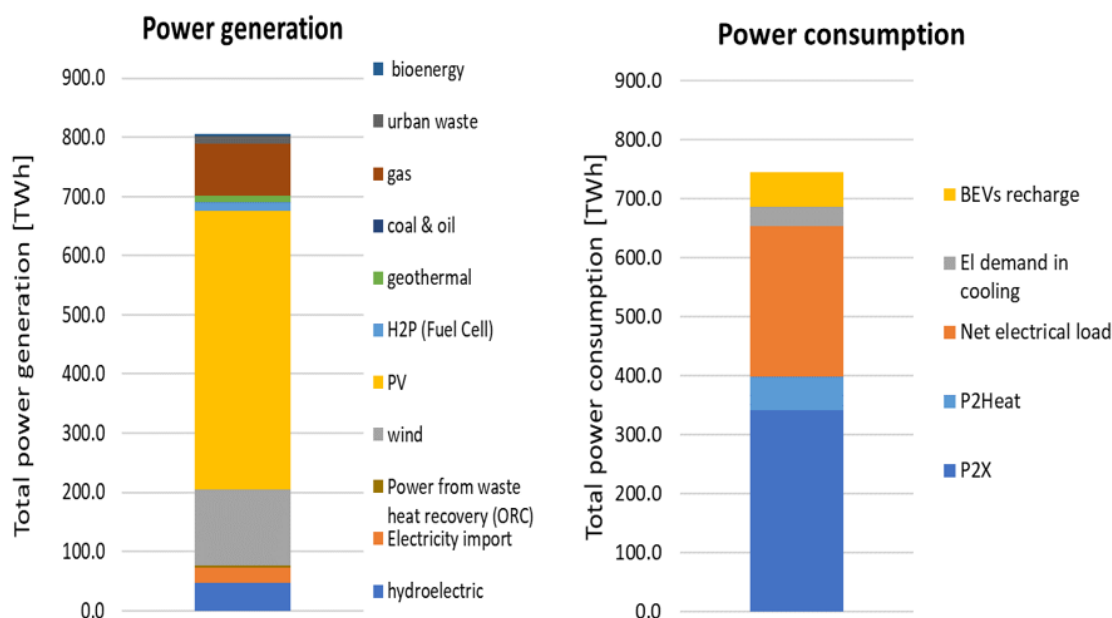


Figure 5.5. Annual power generation divided by source (left) and annual power consumption (right)

Again, it is useful to start from the annual power consumption, defining the final uses. In Table 5.6 the direct and indirect consumption of power are presented.

The first point to be reported is the very large amount of indirect consumption on the overall power demand. The final demand covers nearly the 47% of the total power consumption, but the remaining part is to be destined to other transformation within the energy system.

The indirect use are grouped mainly into two groups: *Power to Heat* and a more general *Power to X*. The former represents the use of electrical power for heat generation. The latter describes instead all the power uses to synthesise other energy carriers, namely hydrogen and its by-products.



Table 5.6. Direct and indirect power consumption

	<b>Power destination</b>	<b>Total energy provided [TWh]</b>	<b>Share on total energy supplied</b>
Power to X	P2X	341.2	45.7%
	DAC	0.9	0.1%
Final demand	net electrical load	254.7	34.1%
	cooling demand	33.4	4.5%
	BEVs recharge	59.2	7.9%
Power to Heat <sup>a</sup>	P2Heat	56.7	7.6%
<b>Total</b>		<b>746.2</b>	

<sup>a</sup> it includes electrical heat pumps and the over-generation that is destined to Thermal Energy Storage

The two groups can be additionally divided with higher level of detail. Starting from the Power to Heat, three main contributions are described in Table 5.7.

Table 5.7. Indirect power consumption: focus on Power to Heat

<b>Power destination</b>	<b>Total energy provided [TWh]</b>	<b>Share on total energy supplied</b>
DHW	19.2	33.9%
District Heating	2.2	3.8%
Space Heating	35.3	62.3%
<b>Total</b>	<b>56.7</b>	

Here three main power destinations are presented. The former indicates the electrical consumption of Air-Source Heat Pump technology to produce Domestic Hot Water. The second term represents the over-generation power that is destined to Thermal Energy Storage (TES) systems in District Heating (DH) applications and for electrical heat pumps coupled with them.

Last contribution regards the Air-source and the Air-to-Air heat pumps used to cover space heating in buildings.

The second class of indirect power consumption destined to the *Power to X* pathways is presented in Table 5.8 below.

As it can be expected, almost the totality of indirect consumption measured in Power to X are destined to  $H_2$  synthesis via water electrolysis. It is the main source for all the hydrogen utilization pathways described in Chapter 2.

Secondary terms are the power consumption in H2G (e.g.  $H_2$  stirring in biological methanation) or in hydrogen storage, with the transformation processes previously

Table 5.8. Indirect power consumption: focus on Power to X

<b>Power destination</b>	<b>Total energy provided [TWh]</b>	<b>Share on total energy supplied</b>
Power to Hydrogen	332.51	97.2%
Hydrogen to Gas	4.99	1.5%
Hydrogen storage	3.7	1.1%
DAC	0.89	0.3%
<b>Total</b>	<b>342.10</b>	

mentioned. In the same group also power consumption for  $CO_2$  capture via DAC is included, being a resource used in the synthesis of hydrogen-based fuels.

### 5.3.3 Hydrogen production and utilization

Once the overall power generation and consumption had been analysed, it is useful to focus on hydrogen production and utilization. As described in Chapter 2, there are basically four possible applications: it can be destined to direct use, to e-fuels synthesis (H2L), to methane synthesis (H2G) or lastly to produce back power (H2P). In direct utilization it was useful to distinguish between the final  $H_2$  demand and hydrogen use in blending option in the gas grid. The following Table 5.9 shows the distribution of produced green hydrogen.

The first fact that emerges from the hydrogen allocation is its use in the H2G pathway. As presented in Figure 5.6, almost the half of the produced  $H_2$  is destined to synthesise the methane that is required by the system. Furthermore, almost another 9% is used for the same purpose, through its injection to the grid. This results in 56% of green hydrogen production to compensate the limitation in fossil NG availability.

Another interesting consideration regards its reconversion to produce back power via Fuel Cell technology. Less than the 10% of the overall production is directly used to direct power generation.

Finally, one third of the total amount is destined to direct uses in heavy transportation and industrial sector (e.g. steel production) and the remaining part is consumed as source for H2L.

In Figure 5.7 two daily power generation and consumption profiles are presented. The curves represent an average day power generation and consumption in winter (left side) and during summer (right side). The first visible difference is the contribution given by PV generation.

During winter the contribution of solar irradiation is lower, requiring the intervention of H2P (via Fuel Cell) combined with storage technologies such as batteries discharge or Pumped Hydroelectric Energy Storage (PHES).

From consumption side, it can be noticed that during the central part of the day power

Table 5.9. Hydrogen consumption in different utilization pathways and total amount of final products obtained

$H_2$ destination	Total [TWh]	Specific destination [TWh]	Total final product obtained [TWh]
Final $H_2$ demand	68.3	-	-
Gas grid injection	22.3	To blending $H_2$ 10%vol = 1.97	Blended gas ( $H_2$ 10%vol) = 63.9 <sup>a</sup>
		To blending $H_2$ 20%vol = 20.37	Blended gas ( $H_2$ 20%vol) = 302.5 <sup>a</sup>
H2Gas	115.7	To biological methanation = 21.76	Synthetic methane = 38.7 <sup>a</sup>
		To catalytic methanation = 93.9	Synthetic methane = 73.8
H2Liquid	16.6	To methanol synthesis = 10.96	Methanol = 6.4
		To e-jetfuel (via MeOH <sup>b</sup> ) = 0	E-jetfuel (via MeOH <sup>b</sup> ) = 0
		To e-jetfuel (via FT) = 0	E-jetfuel (via FT) = 0
		To bio-jetfuel (via waste oil) = 0.94	Bio-jetfuel (via waste oil) = 6.3 <sup>a</sup>
		To ammonia synthesis = 4.73	Ammonia = 3.2
H2Power	21.9	-	Electricity = 13.2

<sup>a</sup> Final product is greater than energy provided by  $H_2$  because of contributions of external energy carriers (e.g. methane, biogas and waste oils)

<sup>b</sup> MeOH = methanol

generation exceeds the normal demand, entering in the situation of over-generation. In these hours two other demands are supplied, namely the Power to Heat and Power to X. Here in Power to Heat demand is included only the power that is used in Thermal Energy Storage, while for Power to X all the consumption for P2H and Hydrogen to X are included.

As discussed before, they convert power in excess to different energy carriers that can be directly used or stored.

Another important information that can be obtained by looking at the graph regards the summer daily curve. Here it can be noticed that in the central part of the day, summing all the direct and indirect consumption, plus the possibility to charge batteries and pump back water to upstream basin (PHES), a quantity of unused power

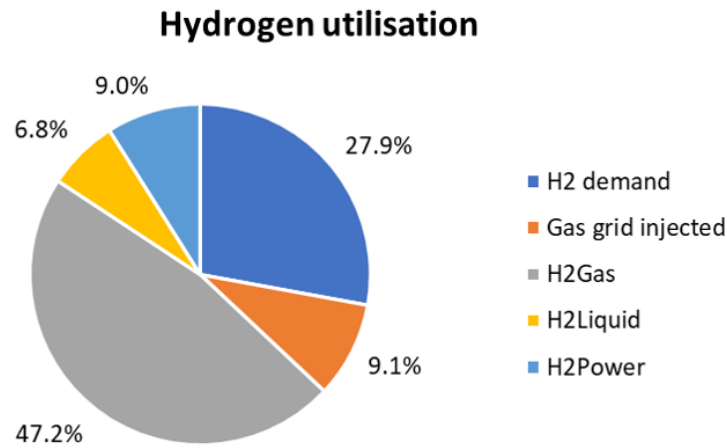


Figure 5.6. Hydrogen allocation in different uses

generated remains. This cannot be stored and is then wasted by the model, through the oemof *excess* class (see Section 4.1.2).

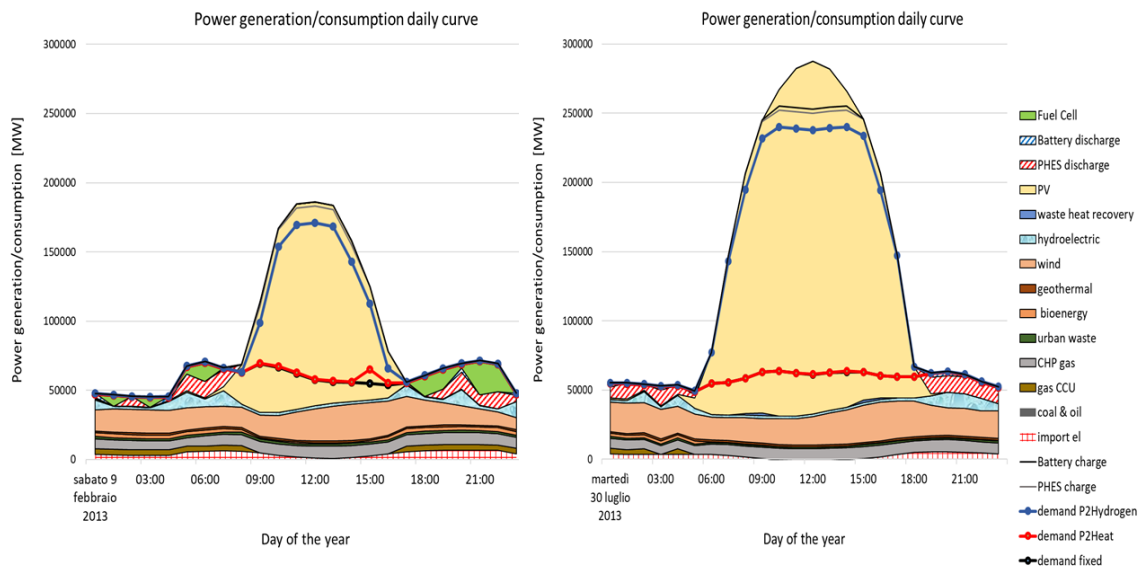


Figure 5.7. Daily power generation and consumption curve; left graph shows an average day of winter, while right one shows a typical summer day. Cumulative area describes production side, while cumulative curves show the demand side

This last consideration introduces another important aspect of the optimized energy system mix returned by the model: the presence of electrical excesses. Excess flows represent a fictitious solution that allows the model to waste a specific energy quantity that NEMeSI does not know where to allocate. In power sector, electrical

excesses represent the situation of over-generation, periods in which generation exceeds the consumption.

They are fully-fledged an energy waste, that justifies the importance to assess the potential role of hydrogen in the energy system. In the model a total amount of 6.25 TWh of power is wasted, with over-generation occurring 350 hours in a year. The maximum hourly peak is  $\sim 68$  GW and this provides helpful consideration.

As introduced in previous Section 5.2, high uncertainty was related to the sizing of the new technologies of Power to Hydrogen and Hydrogen to X implemented in the model. In particular, a potential role of bottleneck was identified in water electrolysis technology.

As discussed before, hydrogen can represent an important resource for multiple utilization. After a first round of simulation, a value of 120 GW of installed capacity was assumed.

The maximum hourly power peak of 68 GW means that through electrolysis, an additional amount of 50 GW of hydrogen could be obtained int that time-step. Some additional simulations were made increasing the installed capacity of electrolysis technology up to 160 GW. In Figure 5.8 is represented the obtained load duration curve for the PEMEC technology.

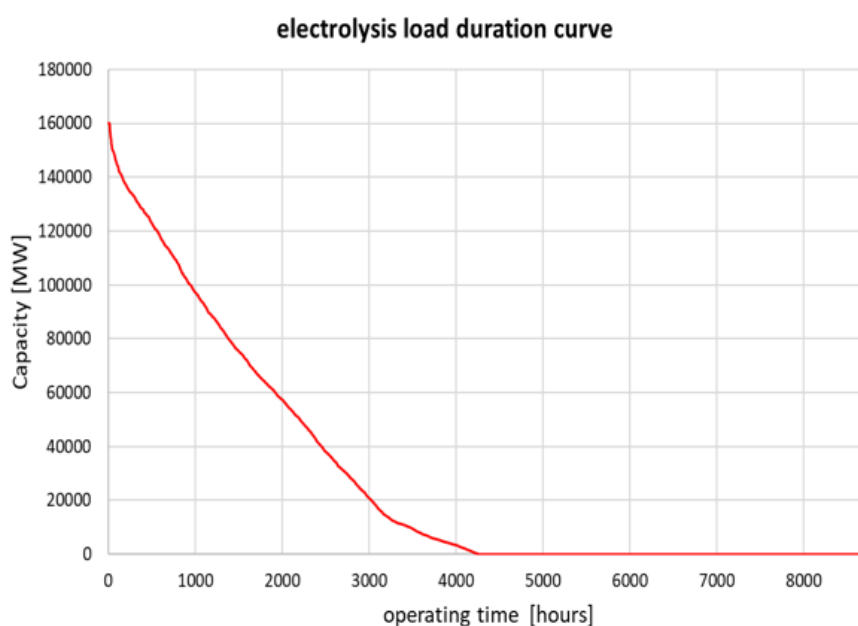


Figure 5.8. Water electrolysis load duration curve; on the Y-axis is represented the used capacity of the electrolyzer technology, while on the X-axis the operating hours during which this capacity was used are presented

Results on this simulation showed a reduction of the overall power excess of only 0.07 TWh during 7 hours. Looking at the load duration curve of Figure 5.8 it can be noticed that PEMEC are used at nominal capacity only 20 hours over a year. In order to completely eliminate over-generation situation, an additional capacity

of 10 GW of electrolyzers should be installed, that would be totally used only one hour on the entire year. With electrolysis installed capacity above 120 GW, a wider amount of PEMECs would not be used unless few hours, without legitimating their installation.

Finally, a possible future implementation could be the study of sizing technologies' capacity pursuing an investment optimization, in coordination with the current simulation setup. In Chapter 6 we will come back on the topic.

Lastly, an overall panoramic view of the optimised energy system returned by the model is presented. Through the help of Table 5.10 the main used technologies are compared.

Some information that can immediately be drawn regard the H2L pathways. In the specific the jet-fuel synthesis. In the model the totality of jet-fuel is obtained via biomass pathways, using waste oils and animal fats. It seems to be less energy demanding, although the high availability of hydrogen to produce electric jet-fuel. This confirms the literature review made on the technology, under which to date current renewable processes of jet-fuel production are more energy-intensive than the alternatives [40].

Regarding H2G and H2L pathways, the developed model allows to estimate the recoverable heat. Assessing its use in District Heating system or in power generation via ORC, an significant value of 31 TWh of recoverable heat is returned. The analysis underlines a preference in power generation via ORC with 23 TWh of heat used (roughly the 72% of the recovered heat). A possible explanation might be the power scarcity derived by low fossil NG availability. Roughly 7 TWh are destined to District Heating purposes while the remaining part is wasted through oemof's *excess flow*. This can be relevant, being the total final heat demand for DH  $\sim 11.6$  TWh, meaning that recoverable heat from H2G and H2L processes should be further investigated in future.

Another useful information already outlined was the low utilization of hydrogen FC technology to convert it directly to power, as for the same process for ammonia, which is not used.

Renewable methane processes are used at their maximum installed capacity only for few hours. The main bottleneck seems to be the resource availability, namely hydrogen. The latter however is produced at its maximum for more than 700 hours, with more than 2000 equivalent operating hours.

For blending option, as expected the reduction of fossil NG availability imposes to maximize the synthetic methane production and the injection of hydrogen into the gas grid. No pure methane is destined to CHP and gas plants. Furthermore, the overestimated installed capacity for these processes were confirmed to be much greater than the real demand. However, they never present isolated peak uses and this allows to exclude abnormal concentration of gas mix to be injected in a single time-step.

Last word on hydrogen storage utilization. The scenario setup had the main hypothesis to allow very large amounts of storage capacity for all hydrogen and its by-products. Especially for hydrogen, the results seems to prefer the  $H_2$  compression

at 350 bar instead of its conversion to metal hydride or liquefaction. The latter can be excluded due to its loss rate (e.g. boil-off issue), that weakens this solution for long seasonal storage.

$MgH_2$  metal hydride seems promising especially for stationary applications, but however it still presents high energy consumption during its transformation process (e.g. energy to release the trapped hydrogen). The other e-fuel storages do not present seasonal accumulations.

However, in this model choice it has to be stressed that the model does not consider investment costs for these technologies and in order to provide a more complete description of the scenario, a further integration with investment optimization could lead to deeply different results. This further implementation would be object of the next Chapter.

Table 5.10. Annual production and equivalent operating hours of the main implemented process in the model

Process	Annual output production [TWh]	EOH [h]	Installed capacity [GW]	Max used capacity [GW]	Share used/installed capacity [%]
Electrolysis	246.1	2050.5	120	120	100.0%
Fuel cell	13.2	109.6	120	41.69	34.7%
Methanol synthesis	6.4	2129.1	3	3	100.0%
Bio-jetfuel synthesis	6.3	1056.4	6	0.74	12.5%
E-jetfuel (via MeOH)	0.0	0.0	6	0	0.0%
E-jetfuel (via FT)	0.0	0.0	5	0	0.0%
Catalytic methanation	73.8	1152.8	64	50.28	78.6%
Biogas upgrading	69.3	2309.8	30	30	100.0%
Biologic methanation	38.7	968.6	40	40	100.0%
Fossil NG	166.6	1082.0	153.93	153.93	100.0%
DME synthesis	3.2	452.7	7	1.74	24.8%
Ammonia synthesis	0.0	7929.1	0.4	0.4	100.0%
$NH_3$ fuel cell	0	0	0.4	0	0.0%
it_BlendGas_unifier <sup>a</sup>	50.7	2.0	25 000	20.34	0.1%
it_blending_process_00 <sup>a</sup>	0.0	0.0	10 000	0	0.0%
it_blending_process_10 <sup>a</sup>	63.9	6.4	10 000	58.84	0.6%
it_blending_process_20 <sup>a</sup>	302.5	30.3	10 000	57.60	0.6%
$H_2$ compression	119.3	2386.9	50	50	100.0%
$H_2$ liquefaction	0.1	1.7	50	13.69	27.4%
$H_2$ to metal hydride	5.1	102.9	50	43.02	86.0%
Power from waste heat	3.1	207.8	15	2.57	17.1%
DAC <sup>b</sup>	$510.6 * 10^6$	510.6	$1 * 10^6$	$1 * 10^6$	100.0%

<sup>a</sup> Name of the processes implemented in the model that mix  $CH_4-H_2$  with 3 ratios and unify the them into a single stream (see Section 4.3.4)

<sup>b</sup> Direct Air Capture output capacity represents the kg of  $CO_2$  captured, as the annual output production



# Chapter 6

## Conclusions

In the thesis a new energy system model is provided, which is able to analyse a wider and more heterogeneous national energy system, with the addition of the promising technologies related to *Power to Hydrogen* and *Hydrogen to X* pathways.

Here below the main addition of the work are summarised. The main consideration from the model application are then summarized, concluding by pointing out the possible future developments to further enhance the analysis and reduce current uncertainties.

The existing model was able to simulate the Italian energy system, limiting the analysis to the generation and use of electricity and thermal services adopting current and soon-to-market technologies. Hence, it does not take into account sector integration with the technologies that could exploit over-generation electricity coming from a higher REs penetration in the energy system.

After a literature review of the main technologies related to hydrogen and  $H_2$ -based synthetic fuels production, the most promising processes were selected.

With the implemented additional pathways, the model version developed in this work enables to provide information on a wider and more heterogeneous national energy system, assessing the role that hydrogen-based technologies could have in a 2050 scenario and estimating their potential recoverable heat.

Hydrogen synthesis via water electrolysis and its reconversion into power (H2P) via Fuel Cell are implemented. Several different uses of green- $H_2$  are assessed, including a blending option in the gas grid infrastructure. Information about specific pathways in H2G or H2L are returned, with a comparison with potential bio-based alternatives. Several synthetic e-fuels are modelled, namely methanol, DME, jet-fuel and ammonia that represent the current most promising utilization of the produced green hydrogen. Multiple technologies for hydrogen storage have been implemented in order to compare physical storage like compression and liquefaction with material-based one, through the transformation of  $H_2$  into metal hydride.

Information of the potential recovery of waste heat from High Temperature H2G and H2L processes are reported with possible applications in District Heating (DH) or in power generation via ORC.

The model application analyses the Italian energy system in a long-term scenario

with a single year simulation, assuming 2050 time-horizon. With an aggregated national spatial resolution and an hourly time-step, the model faces the consequences of a huge REs penetration that is expected to get closer to zero  $CO_2$  emission target. This profound modification of the energy system determines several challenges, one for all the issue of summer over-generation combined with supply shortages during winter due to high REs variability.

From this perspective, the model provides some consideration regarding the benefits that hydrogen generation would bring to the system balancing, returning the optimised energy system mix that would be necessary to reduce at minimum the fossil dependence.

A focus of the model application was the analysis of the alternatives to fossil Natural Gas, assessing the consequences of its gradual reduction. From this perspective, the model returns a generation mix with a minimum quantity of used fossil NG (166 TWh) with respect to the total energy that is required from the gas grid (roughly 370 TWh). A considerable part of this energy can be supplied with hydrogen generation coupled with carbon capture and biomethane production from biogas upgrading. This has the consequence of higher power generation requirement, due to a consistent part of indirect uses on the total power consumption ( $\sim 46\%$  of the total generation) that is destined to Power to Hydrogen. Another 46% of the total generation is destined to final power demands (e.g. net electrical load), while last 8% is destined to Power to Heat.

The obtained green  $H_2$  is destined for more than an half to H2G, in order to compensate the lack of energy supply required to the gas grid due to the fossil NG availability reduction. Methane synthesis from biological and catalytic methanation is pushed to the maximum allowed by resources availability, as well as for the methane production from the biogas upgrading.

Furthermore, blending option is favored. For most period of the year (84%) the quantity of hydrogen injected into the gas grid is the maximum allowed (20%vol), while for the remaining time a 10%vol of hydrogen is injected. The two solution are preferred to minimize the amount of energy of gas grid that has to be supplied by fossil NG.

H2P seems to be exploited as backup resource during periods in which conventional power generation plants, storages and REs are not enough to cover the demand. Typically the period of early morning and evening in fall and winter. During the remaining part of the year, REs availability (mainly PV) can overcome the power demand, by exploiting over-generation periods to produce hydrogen.

Regarding  $H_2$  storage, a seasonal behaviour is observed. With the assumption of very large amounts of storage capacities, it emerges a preference for hydrogen compression at 350 bar. The long period of storage de facto excludes the  $H_2$  liquefaction, where boil-off issue determines a loss rate that does not justify its utilisation.

$MgH_2$  metal hydride seems promising especially for stationary applications, but it still has high energy consumption during the transformation process back to hydrogen. Moreover, if their cost is taken into account, their presence is unfavoured.

Lastly, the developed model allows to estimate the recoverable heat from the main processes of H2G and H2L pathways. Assessing its use in District Heating system or

in power generation via ORC, an significant value of  $\sim 31$  TWh of recoverable heat is returned. The analysis underlines a preference in power generation use via ORC (roughly the 72% of the recovered heat) due to the power scarcity derived by low fossil NG availability, plus another 23% destined to District Heating.

Further researches could be continued on this topic, in order to better study and characterize the potential of recoverable heat.

## 6.1 Areas of improvement

The developed model analyses the Italian energy system as as a single node. The zero-dimensional property translates that all the data provided and returned by the model are aggregated. Like other single node model, there is a lack of detail when results have to be applied to a physical representation of the system. A solution would be to implement the multi-node characterization in the model. Tthis addition would allow to describe n-nodes and their interconnections. For the Italian case, a possibility might be to implement a six-node representation, as for the current six bidding-zone division determined for the power system, determined by the current transmission bottlenecks, that in future might change.

This solution would allow a more precise characterization of the different part of the country. For example, heat demand during the winter could be better described by differentiating the North Italy node from Sicily one. Or it would be possible to better allocate power generation by REs (e.g. PV in Sardinia v. hydroelectric in the North region).

Another future development, to be balanced with the complexity that would arise, would be the broadening of the range of options for each process. The model would be enabled to choose between different technologies for the same process, ensuring a more complete analysis on energy allocation. An example might regard the different technologies for *Hydrogen to Power* via Fuel Cell process. This however, should be weighted with the investment cost of each technology that should be considered in the optimization problem.

Since the time horizon for the simulated scenario is 2050, high uncertainty levels characterize all the estimations. An improvement could derive from further enhancements of input data. For example an additional detailed study for the specific final demands (e.g. transport sector) in a long-term scenario could be coupled with the current model version. The simulation would benefit from better estimations.

A further possible implementation regards the possibility to add import option for hydrogen and e-fuels. Literature review for aviation suggests that internal production of jet-fuel will probably not be enough to cover the demand, even combining bio-based with electric one [12, 40].

For this reason import options for hydrogen and its by-product were implemented in the model, although not considered in the tested scenario. Coupled with regionalization, a further study of the interconnections with border countries would then allow

to determine the quantities of fuel and other energy carriers that could be exchanged. For example, periods of over-generation in the Italian energy system could coincide with some shortage of border countries, allowing potential international trading of power and synthetic fuels, with several economical benefits and energy savings.

Lastly, a further possible way of improvement would be the share of output data between different energy system model classes. NEMeSI is a *Bottom-Up* model, enabling an high technological resolution of the system. However, it suffers from not considering macro-economics effects, that would instead be deepened by a *Top-down* model (see Section 3.1.1).

The combination of the two would strengthen the scenario results, returning a more complete description of the studied energy system.

# Appendix A

## Input data tables

To ease the graphic representation in Chapter 5, where hypothesis and input data description are reported, here the main tables with the main technical parameters are presented.

Table A.1. Main technical values assumed for System Heating and Domestic Hot Water technologies

Destination	Technology	Overall efficiency <sup>a</sup>	Share <sup>b</sup>	Description
for SH	ASHP	3.36	0.28	air-source heat pumps
	A2AHP	4.18	0.38	air-to-air heat pumps
	GAHP	1.60	0.19	gas heat pumps
	gas_boiler	0.90	0.00	gas boilers
	oil_boiler	0.85	0.00	oil boilers
	biomass_boiler	0.84	0.16	biomass boilers
for DHW	GAHP	1.60	0.17	gas heat pumps
	gas_boiler	0.90	0.00	gas boilers
	oil_boiler	0.85	0.00	oil boilers
	biomass_boiler	0.84	0.00	biomass boilers
	ASHP	3.36	0.83	air-source heat pumps

<sup>a</sup> efficiencies are adjusted with a profile during the simulated year

<sup>b</sup> it represents the share of the overall individual heat demand covered by each technology

Table A.2. Main technological parameters assumed for the processes

Process name in the model	Output capacity [MW]	efficiency <sup>a</sup>	max <sup>b</sup>	min <sup>b</sup>
it_urban_waste_pp	800	0.42	1	0
it_coal_pp	0	0.35	1	0
it_oil_pp	0	0.31	1	0
it_bio_l_pp	368.7	0.35	1	0
it_bio_g_pp	500	0.41	1	0
it_bio_f_pp	622.5	0.25	1	0
it_PV_feed_in	300 000	1	1	0
it_el_boilers_ resid+ter_conv	2 509.6	1	1	0
it_biomass_boiler_dh	581.3	0.81	1	0
it_biogas_to_CH4	30 000	0.98	1	0
it_DAC	1 000 000	571.4 <sup>c</sup>	1	0
it_WasteHeat_to_DH	15 000	0.9	1	0
it_ORC	15 000	0.136	1	0
it_MeOH_to_DME	7 000	0.607	1	0
it_H2_to_NH3	400	0.67	1	0
it_gas_pp	4 024.2	0.45	1	0
it_H2_to_CH4	64 000	0.79	1	0
It_H2_to_MeOH	3 000	0.58	1	0
FT_to_jet_fuel	5 000	0.53	1	0
it_BlendGas_unifier	25 000 000	1	1	0
it_res/int_boiler1	1 600	0.9	1	0
it_res/int_boiler2	204.7	0.9	1	0
it_res/int_boiler3	176	0.9	1	0
it_res/int_boiler4	2 106.2	0.9	1	0
it_res/int_boiler5	0	0.9	1	0
it_res/int_boiler6	5 212.9	0.9	1	0
it_res/int_boiler7	581.3	0.9	1	0
biologic_methanation	40 000	0.72	1	0
it_blending_process_00	10 000 000	1	1	0
it_blending_process_10	10 000 000	0.999	1	0
it_blending_process_20	10 000 000	0.99	1	0
it_fats_to_jet_fuel	6 000	0.665	1	0
It_H2_compression	50 000	0.960	1	0
It_H2_liquefaction	50 000	0.847	1	0
It_H2_to_metal_hydride	50 000	0.979	1	0
MeOH_to_jet_fuel	6 000	0.91	1	0

<sup>a</sup> efficiency LHV basis

<sup>b</sup> it represent the maximum/minimum load of the plant, range [0-1]

<sup>c</sup> DAC efficiency represents the total kg of captured  $CO_2$  per an input energy unit (MWh)

Table A.3. Main technological parameters assumed for the storage technologies

Process name in the model	Capacity storage [MWh]	Charge capacity [MW]	Discharge capacity [MW]	Initial capacity <sup>a</sup>
it_stor_(+boil_elc)1	12 800	1 600	1 600	0
it_stor_(+boil_elc)2	1 637	205	205	0
it_stor_(+boil_elc)3	1 408	176	176	0
it_stor_(+boil_elc)4	16 849	2 106	2 106	0
it_stor_(+boil_elc)5	0	0	0	0
it_stor_(+boil_elc)6	0	0	0	0
it_stor_(+boil_elc)7	0	0	0	0
it_hydro_dammed	57 782	9 630	9 630	0.1
it_PV_stor	6 429	804	804	0
it_seas_stor_dh	0	0	0	0
it_el_boilers_resid+ter_int	0	0	0	0
it_compr_hp	0	47	47	0
it_storage_phs	61 352	7 669	7 669	0.2
it_storage_phs_new	45 000	4 500	4 500	0.2
it_storage_bat	24 000	3 000	3 000	0.2
it_storage_H2_compressed	120 000 000	120 000	120 000 000	0
it_storage_H2_liquefied	120 000 000	120 000	120 000 000	0
it_storage_H2_metal_hydride	120 000 000	120 000	120 000 000	0
it_CO2_temp_storage <sup>b</sup>	$70.08 * 10^9$	8 000 000	29 648 665	0
it_CH4_storage	126 388 889	287 935	194 444	0
it_jet_fuel_storage	10 000 000	6 000	6 000	0
it_MeOH_storage	4 320 000	3 000	3 000	0
it_biogas_temp_storage	178 602	372	178 602	0
it_biogas_upgr_temp_storage	3 874 373	8 072	3 874 373	0
it_biogas_methan_temp_storage	1 491 189	3 107	1 491 189	0
it_DME_storage	7 200 000	5 000	5 000	0
it_biogas_DME_temp_storage <sup>c</sup>	250 000	5 000	5 000	0

<sup>a</sup> it represents the initial stored capacity at the beginning of the year simulation, with a range [0-1]

<sup>b</sup>  $CO_2$  storage is measured in [kg]

<sup>c</sup> technology that was implemented in the model but not used yet

Table A.4. Main technological parameters assumed for the processes with power and thermal outputs

Process name in the model	Power capacity [MW]	Electrical efficiency <sup>a</sup>	max <sup>b</sup>	min <sup>b</sup>	Thermal capacity [MW]	Thermal efficiency <sup>a</sup>	max2 <sup>b</sup>	min2 <sup>b</sup>
it_chp_dh	1 566.9	0.40	1	0	2 106.2	0.40	1	0
it_chp_dh_oil	0	0.40	1	0	0	0.40	1	0
it_pp_excess	2 214.8	0.50	1	0	204.7	0.05	1	0
it_pp_excess_oil	0.0	0.50	1	0	0	1	1	0
it_chp_industry_pro	7 887.6	0.40	1	0	3 746.6	0.19	1	fixed <sup>c</sup>
it_chp_dh_bio	1 806.9	0.23	1	0	5 212.9	0.67	1	0
it_urban_waste_chp	800	0.30	1	0	1 600	0.60	1	0
It_chp_resid+ter	8.5	0.25	1	0	20.5	0.60	1	0
it_chp+hp	0	0.30	1	0	0	1.00	1	0
it_non_disp_chp	0	0.25	1	0	0	0.60	1	0
it_fuel_cell	120 000	0.6	1	0	40 000	0.20	1	0
it_NH3_fuel_cell	400	0.394	1	0	80 710.7	0.265	1	0
it_electrolysis	120 000	0.74	1	0	16 216.2	0.1	1	0
it_chp_industry_self	7 607.7	0.27	1	0	11 270.7	0.40	1	0
it_bio_g_to_d	500 000	0.624	1	0	208 448.3	0.26	1	0

<sup>a</sup> efficiencies are LHV basis. Thermal efficiency represent the total heat produced per energy input

<sup>b</sup> it represent the maximum/minimum load of the plant, range [0-1]. First columns are for power generation, last columns for heat generation

<sup>c</sup> the minimum load follows a specific profile during the year

<sup>d</sup> technology that was implemented but not used yet



# Acronyms

<b>AEC</b>	Alkaline Electrolyzer Cell
<b>AFC</b>	Alkaline Fuel Cell
<b>AEMEC</b>	Anion Exchange Membrane Electrolyzer Cell
<b>B2L</b>	Biomass to Liquid
<b>C2L</b>	Coal to Liquid
<b>CAPEX</b>	Capital Expenditure
<b>CCGT</b>	Combined Cycle Gas Turbine
<b>CCU</b>	Carbon Capture and Utilisation
<b>CGE</b>	Computable General Equilibrium
<b>CHP</b>	Combined Heat and Power plant
<b>CSP</b>	Concentrated Solar Power
<b>DAC</b>	Direct Air Capture
<b>DEA</b>	Danish Energy Agency
<b>DH</b>	District Heating
<b>DHW</b>	Domestic Hot Water
<b>DME</b>	Dimethyl Ether
<b>DRI</b>	Direct Reduction of Iron
<b>EOH</b>	Equivalent Operating Hour
<b>EPC</b>	Equivalent Periodical Cost of the investment
<b>FC</b>	Fuel Cell
<b>FCEV</b>	Fuel Cell Electric Vehicle
<b>FT</b>	Fischer-Tropsch
<b>G2L</b>	Gas to Liquid

<b>GHG</b>	Green-House Gas
<b>GT</b>	Gas Turbine
<b>H2G</b>	Hydrogen to Gas
<b>H2L</b>	Hydrogen to Liquid
<b>H2P</b>	Hydrogen to Power
<b>H2X</b>	Hydrogen to X
<b>HRS</b>	Hydrogen Refueling Station
<b>ICE</b>	Internal Combustion Engine
<b>IEA</b>	International Energy Agency
<b>LHV</b>	Lower Heating Value
<b>LOHC</b>	Liquid Organic Hydrogen Carrier
<b>LP</b>	Linear Programming optimization problem
<b>LPG</b>	Liquefied Petroleum Gas
<b>MCFC</b>	Molten Carbonate Fuel Cell
<b>MeOH</b>	Methanol
<b>NG</b>	Natural Gas
<b>ORC</b>	Organic Rankine Cycle
<b>P2G</b>	Power to Gas
<b>P2H</b>	Power to Hydrogen
<b>P2X</b>	Power to X
<b>PAFC</b>	Phoshoric Acid Fuel Cell
<b>PE</b>	Partial Equilibrium
<b>PEMEC</b>	Proton Exchange Membrane Electrolyzer Cell
<b>PEMFC</b>	Polymer Electrolyte Membrane Fuel Cell
<b>PHES</b>	Pumped Hydroelectric Energy Storage
<b>PSA</b>	Pressure Swing Adsorption
<b>PV</b>	Photovoltaics
<b>RE</b>	Renewable Energy

<b>SDG</b>	Sustainable Development Goal
<b>SH</b>	Space Heating
<b>SOEC</b>	Solid Oxyde Electrolyzer Cell
<b>SOFC</b>	Solid Oxide Fuel Cell
<b>SRC</b>	Steam Rankine Cycle
<b>SRES</b>	Scheme of the Reference Energy System
<b>TES</b>	Thermal Energy Storage
<b>TRL</b>	Technology Readiness Level
<b>TSO</b>	Transmission System Operator
<b>WACC</b>	Weighted Average Cost of Capital
<b>WGS</b>	Water-Gas Shift



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