UCLouvain
Institute of Mechanics,
Materials and Civil Engineering

Robust optimisation of the pathway towards a sustainable whole-energy system

A hierarchical multi-objective reinforcement-learning based approach

Doctoral dissertation presented by
Xavier RIXHON
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Thesis committee
Pr. Francesco CONTINO (supervisor, UCLouvain)
Pr. Hervé JEANMART (supervisor, UCLouvain)
Dr. Stefano MORET (ETH Zurich)
Pr. Sylvain QUOILIN (ULiège)

Abstract

This thesis will be awesome

*“Pour ce qui est de l’avenir, il ne s’agit pas de le prévoir,
mais de le rendre possible”*

– Antoine de Saint Exupéry, Citadelle, 1948

Remerciements

Thank you, thank you, far too kind

Contents

Symbols

Acronyms

BEV	battery electric vehicle
BTX	benzene, toluene and xylene
CCGT	combined cycle gas turbine
DHN	district heating network
EnergyScope TD	EnergyScope Typical Days
EUD	end-use demand
FC	fuel cell
GHG	greenhouse gases
GWP	global warming potential
HP	heat pump
HVC	high value chemicals
LCOE	levelised cost of energy
LFO	light fuel oil
LPG	liquefied petroleum gas
MMSA	Methanol Market Services Asia
MTBE	methyl tert-butyl ether
NED	non-energy demand
NG	natural gas
NRE	non-renewable energy
NSC	naphtha steam cracker
PCE	Polynomial Chaos Expansion
PV	photovoltaic
RE	renewable energy
SDGs	Sustainable Development Goals
SMR	small modular reactor

UQ	Uncertainty Quantification

Chapter 1

Case study: the Belgian energy system

As detailed by Limpens et al. [1], the analysis carried out in this work can be applied to any regional whole-energy system. As a densely-populated and highly-industrialised country with limited local renewable potentials (mainly solar and wind), the transition of Belgium from a fossil-dominated system in 2020 (Appendix A.1) to carbon-neutrality in 2050 makes it an intricate case study. Moreover, this case study and the subsequent analyses can be transferred - to some extent - to other industrialised countries highly dependent on fossil fuels with limited local renewable potentials (e.g. the Netherlands or Germany) [2]. This chapter presents the different demands to satisfy, with a particular focus on the non-energy demand, as well as the resources available and the conversion technologies to supply those. For a comprehensive understanding and detailed descriptions of the technologies, please refer to the documentation [3]. Then, the uncertainty ranges considered for some of the parameters are detailed. Finally, the CO_2-budget over the 2020-2050 transition is presented.

1.1 Contributions

First, as pointed out by Rixhon et al. [4], where most of the studies assessing whole-energy system integrate energy demands (i.e. electricity, heart and mobility), the NED is often not considered. The latter is defined as '*energy products used as raw materials in the different sectors; that is not consumed as a fuel or transformed into another fuel*' [5]. The previous analyses carried out with EnergyScope Typical Days (EnergyScope TD) considered the non-energy demand as the related primary energy needs, i.e. either natural gas or light fuel oil (LFO). To minimise the total cost of the system, the model simply selected the cheapest between the two resources (i.e. natural gas). This work goes one step further and accounts for the NED as a demand of three commodities (i.e. high value chemicals (HVC), ammonia and methanol) as well as with associated production technologies. This allows bringing the non-energy sector to a similar level of details as the other sectors. Regarding the end-use demands, keeping the same methodology to define end-use demand (EUD) in EnergyScope as Limpens et al. [6], this work considers updated values given the latest release of the "EU reference scenario 2020 : energy, transport and GHG emissions: Trends to 2050 "by the European Commission [7].

Second, given the focus of this work on the electrofuels, the case study includes a more explicit representation of e-ammonia and e-methanol (as well as their fossil-based equivalents), on top of e-hydrogen and e-methane, already included in the previous definition of the case study [8]. As detailed later on, these electrofuels are considered as renewable in the sense that their global warming potential (GWP) is zero. This more explicit representation of the molecules themselves also comes with a more exhaustive integration of the ways to produce and use them in the system.

Third, as nuclear energy could be a real game-changer in the energy transition worldwide [9], and especially in Belgium, this thesis has integrated the potential to install small modular reactor (SMR) from 2040 onward.

Fourth, where previous works considered a prescribed CO_2 trajectory to reach carbon-neutrality by 2050 [1, 8], the case study analysed in this thesis is subject to a CO_2-budget for the transition, i.e. limiting the total amount of emissions over the transition.

Finally, to a smaller extent, this work includes updated values for some parameters compared to the work of Limpens [8]. The main change concerns the cost and performance of private mobility vehicles, which is specifically a key components in the Belgian energy transition. The previous version of the case study was excessively favouring fuel cell car versus battery electric vehicle (BEV). Comparing with other works [7, 10], the CAPEX and efficiency of fuel cell cars have been increased. Regarding BEV, while the CAPEX has been kept unchanged, the efficiency and the battery capacity, i.e. the range, have been increased. As seen in the results, this change of data made BEV often more competitive than its hydrogen-based equivalent.

1.2 End-use demands

End-use demands, exogenously imposed as inputs to the model, are characterised by yearly quantities to satisfy and are also distributed over the different hours of each representative years of the transition, in order to account for their daily or seasonal variability [6, 8]. In this work, the yearly end-use demands (EUD) for all sectors are calculated from the rather slightly increasing forecast proposed by the European Commission for Belgium (Appendix 2 in report [7]).

1.2.1 Non-energy demand

Where previously published works of Rixhon et al. [4, 11] investigated more extensively the integration of the NED in the case study of Belgium, this section summarises the rationale of doing so as well as the methodology used to quantify this demand.

Definition and historical trend

The NED can be split into four main categories of final molecules [12]: (i) HVC (worldwide production of ∼365Mt/year); (ii) ammonia (∼185Mt/year); (iii) methanol (∼100Mt/year) and (iv) the other products. HVC gather the light olefins (e.g. ethylene, propylene) and aromatics (benzene, toluene, xylene – BTX), mainly for the production of plastics, synthetic fibers or rubber. Their production today relies mainly on petroleum products such as naphtha, ethane or liquified petroleum gas. Ammonia is mainly used for the production of fertilizers (∼80% of global ammonia consumption). Its production is dominated by natural gas (NG) via steam reforming to produce hydrogen, used as feedstock in the Haber-Bosch process. Methanol is mainly converted to formaldehyde (resin) but also used for the production of other chemicals (e.g. solvents and gasoline-blends). Currently, its synthesis, like ammonia, is mainly relying on natural gas via steam reforming. Finally, the other products gather all chemicals not mentioned in the other categories such as bitumen, lubricants and other heavy products from oil refineries [13].

The NED currently represents around 20% of the final energy consumption in Belgium [14]. Over the recent history, there has been a relatively constant evolution of three main categories of the final consumption for non-energy use in Belgium, [15]: (i) naphtha and liquefied petroleum gas (LPG) (between 59% and 67% of the total final consumption, around 59.4 TWh in 2019), (ii) NG (between 9% and 14%, 11.8 TWh in

2019), and (iii) others (i.e. bitumen, coal tar and other oil products) (between 21% and 28%). Naphtha and LPG are consumed in a naphtha cracker, which results in ethylene and propylene, what will be considered as HVC in the rest of this work. Similarly, NG, as non-energy carrier, is used in steam methane reformer to produce the required hydrogen to the synthesis process of ammonia. The small shares of bitumen and coal tar are respectively used for roadworks and to produce synthetic gas through gasification. Finally “other oil products"take into account, indistinguishably, tar and sulphur as well as by-products of the refineries (e.g. benzene, toluene and xylene (BTX)). About methanol, there is currently no production plant in Belgium even if the country plays a role in trading this commodity between its neighbouring countries and consumes part of what it imports.

Methodology of quantification

The non-energy demand studied in this analysis focuses on the chemical industry (more than 90% of the non-energy use in Belgium) and, similarly to other studies [12, 13], is split between the three aforementioned main groups of products (i.e. HVC, ammonia and methanol). Before describing these three demands, this study excludes bitumen, coal tar and “other oil products". The first two represent marginal shares of the current non-energy use in such a way that they should not affect the big trends provided by this study. As described previously, the latest are mostly by-products from refineries that the system uses because they are available. However, in a perspective of defossilisation, since the future of fossil-based refineries is unclear, they have not be implemented in this study nor their by-products.

Regarding HVC, the future of their production is highly uncertain. One of the reasons is new regulations and strategies promoting recycling and limitation of single-use plastics [16]. Besides this uncertainty, Belgium stays a major exporter as approximately 2/3 of plastic raw materials produced locally are exported abroad [17]. Even if a significant part of HVC produced in Belgium is not locally consumed, this demand has been set based on the assumption that Belgium will keep its industrial activity in this sector. This assumption does not consider the net imports of HVC, unlike ammonia and methanol, which will be more traded commodities in the future (as energy carriers and non-energy products). Therefore, the actual demand of HVC is inferred from the consumption of naphtha and LPG as non-energy use as well as energy-carrier in the chemical and petrochemical industries [15]. This assumption is based on the fact that, in the conversion processes to produce HVC from naphtha or LPG, these fuels also serve as energy-carrier to supply the process itself. Then, given the respective efficiencies ($1.83t_{naphtha}/t_{HVC}$ and $1.67t_{LPG}/t_{HVC}$) [12], the current demand of HVC is estimated equal to 3069 kt, without making distinctions between the different chemicals (i.e. ethylene, propylene and BTX).

The ammonia sector in Belgium is quite different: the country locally produces and imports ammonia much more than it exports it. Thanks to a database from the United Nations [18] and the National Bank of Belgium, it has been identified that, over the last ten years, Belgium has imported, exported and locally produced, on average, respectively, 1010 kt, 105 kt and 990 kt of ammonia. Therefore, on top of the local production, the net import (i.e. import minus export) is also included in this non-energy demand. This gives a current demand of 1895 kt of ammonia.

Concerning the demand of methanol, similarly to ammonia, this work solely considers the net imports as there is no local production in Belgium. To define the actual non-energy demand of methanol, only a 51%-share of this net import is kept since, according to the Methanol Institute and Methanol Market Services Asia (MMSA), this share is used for formaldehyde production in Belgium [19]. The rest of the methanol is used for energy purposes, mostly as methyl tert-butyl ether (MTBE) in gasoline blending. This methodology gives a current non-energy demand of methanol of 269 kt.

Finally, after converting these masses of products into energy content (i.e. LHV: HVC - 47 MJ/kg, ammonia - 18.8 MJ/kg and methanol - 19.9 MJ/kg), this work assumed constant shares between the three categories within the NED and the same growing rate as presented by Capros et al. [20].

1.2.2 Forecast of the demands over the transition

Although, given a significant and unsubstantiated discrepancy in the non-energy use forecasts compared to their previous report (i.e. +80% over the 2020-2030 time window), the evolution trend of the NED of the current work has been inferred from the previous edition, published in 2016, [20]. Looking at Figure 1.1, between 2020 and 2050, one observes a noteworthy increase of the electricity (+40%), passenger (+45%) and freight mobility (+35%) demands. The rise of the non-energy demand is more limited, i.e. +6%, whereas the heating demands is forecast to decrease: -11% and -3% respectively for the low and high-temperature heat demands. Regarding the center graph of Figure 1.1, it is the aggregation of the same data as in the left graph but per category, rather than per sector, with the non-energy demand being associated with the industry. This illustrates how industrialised is Belgium, compared to households and services, and, consequently, highly energy-intensive. The right graph of Figure 1.1 gives the passenger and the freight mobility. The sharp increase from 2020 to 2025 is due the COVID-crisis that has significantly reduced these demands in 2020. As far as the hourly discretisation of these demands is concerned, time series are based on historical values of 2015 for parts of electricity and low-temperature heating demands [6]. A daily time series is used for the passenger mobility and applied similarly to every typical days. Finally, for the other demands, the yearly demand is distributed uniformly over the different hours of the year.

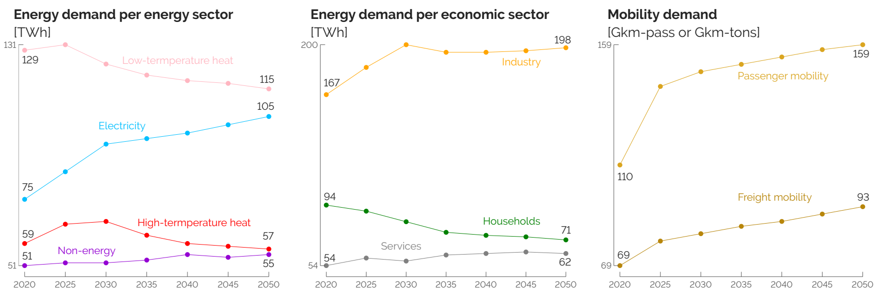

Figure 1.1. EnergyScope splits the whole-energy system end-use demands (EUD) into two sets: (non)-energy and transport-related. This figure presents the nominal values of each of these demands. In the center graph, the non-energy demand has been fully associated with the industrial demand. As detailed previously, the non-energy demand is expressed in tons of physical products (i.e. high value chemicals (HVC), ammonia and methanol) and then translated into their respective energy equivalent, in TWh. Graphs have been adapted from [1].

1.3 Resources

To supply the aforementioned demands, EnergyScope Pathway implements a variety of resources defined by their cost of purchasing, c_{op}, their global warming potential, gwp_{op}, as well as their availability, as detailed by Limpens et al. [1]. Figure 1.2 depicts the evolution the respective costs of purchasing. Regarding “renewable electrofuels”, these are in line with the recent study of Genge et al. [21] who carried out an extensive review and “meta-analysis[22, 23] of 30 studies on the supply costs of chemical energy carriers”. Then, besides their cost, the resources are either limited or unlimited in terms of availability and either renewable or not. The limitation in terms of availability can be direct or indirect. On the one hand, woody (23.4 TWh) and wet biomass (38.9 TWh) are limited by their local potentials and the consumption of waste (17.8 TWh) and coal (33.4 TWh) is assumed not to exceed the current use. On the other hand, wind, solar, hydro and uranium are limited by the technical potentials respectively, of photovoltaic (PV) panels (59.2 GW), onshore (10 GW) and offshore (6 GW) wind turbines, run-of-the-river power plants (0.1 GW) and nuclear power plants (6 GW). As SMR are foreseen, if installed, to be around the same locations (i.e. Thiange and Doel) as the conventional nuclear power plants and using the same area in kW/ha, the same 6 GW are assumed to be the maximum capacity for SMR. This is even without considering the potential limit due to the local availability, in terms of volume and flow rate, of enough water that would be a more socially-accepted solution than cooling towers exhausting a dense plume. Imported electricity is limited in two ways: the potential of instantaneous capacity of interconnection with neighbouring countries (i.e. 11.9 GW by 2050 [24]) and a limitation to 30% of the yearly electricity end-use demand (i.e. 32.4 TWh by 2050). In the current work, the electrofuels (i.e. e-methane, e-hydrogen, e-methanol and e-ammonia) are assumed to be "sustainable" in the sense that they do not increase the concentration of CO_2 in the atmosphere [25]. In practice, it means that their GWP is assumed to be zero in the model. Regarding specifically these electrofuels, the Hydrogen Import Coalition [26] has carried out an extensive techno-economic analysis to estimate their respective cost of purchasing, after having identified some key locations from which importing these energy carriers (e.g. Chile, Australia or Morocco). As the amount to import from each of these locations is hard to forecast, the current work considers the average cost between the different locations. Besides these, every other resource has its specific GWP like coal ($gwp_{\text{op,coal}} = 0.40\,\text{kt}_{\text{CO}_2\text{,eq}}/\text{GWh}$), natural gas ($gwp_{\text{op,NG}} = 0.27\,\text{kt}_{\text{CO}_2\text{,eq}}/\text{GWh}$) or the fossil-based molecules equivalent to the electrofuels (e.g. $gwp_{\text{op,ammonia}} = 0.46\,\text{kt}_{\text{CO}_2\text{,eq}}/\text{GWh}$ or $gwp_{\text{op,methanol}} = 0.41\,\text{kt}_{\text{CO}_2\text{,eq}}/\text{GWh}$).

1.4 Conversion technologies: SMR, NED-related and others

As the end-use demands are defined as energy (and non-energy with the NED) services rather than a certain quantity of oil or solar irradiance, for instance, technologies are implemented to convert these resources into the end-use demands. Besides their CAPEX, OPEX and lifetime defined in Section **??**, production and conversion technologies (i.e. combined cycle gas turbine (CCGT), car or boiler) have a conversion efficiency whereas storage technologies (i.e. thermal storage, battery or molecule storage) exhibit their own charge/discharge losses. Eventually, there are also infrastructure technologies like the grid or the district heating network (DHN) that allow to account

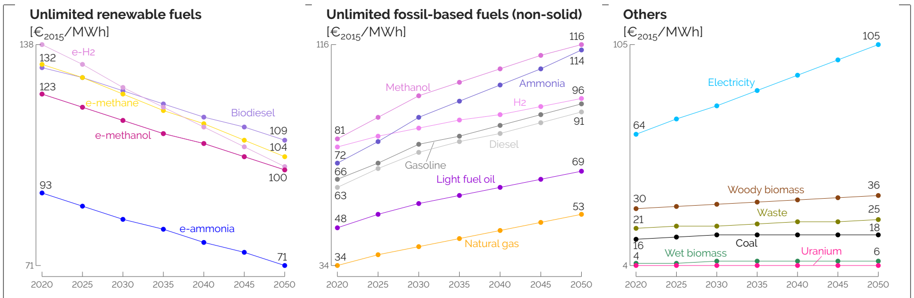

Figure 1.2. Cost of purchasing the different resources. Besides the free local renewables (i.e. sun, wind and hydro) limited by technical potentials, EnergyScope accounts for renewable energy carriers and their respective fossil counterparts (left and center graphs). These fuels can be imported from abroad without limitation on their availability. Other carriers are limited either by their local potentials (i.e. biomass and waste) or other considerations like the power grid interconnections or the capacity of nuclear power plants.

for the investment necessary, respectively, to integrate more intermittent renewables in the power sector and the expand the use of centralised heating systems. The exhaustive list of these technologies have already been presented in previous works [8].

A specific attention is to put on the implementation of small modular reactor (SMR) whereas the 6 GW of conventional nuclear are assumed to drop to 2 GW in 2025 and total phase-out by 2035. Similarly to the analysis of EnergyVille [27], a Belgian consortium for energy research, and in line with the Belgian Nuclear Research Centre (SCK-CEN) [28], SMR are implemented with the features listed in Table 1.1. Where most of the features are similar to conventional nuclear power plants, it differs from these on two main points: their potential year start, 2040, and their flexibility. Indeed, unlike the current nuclear power plants, constrained in the model to produce a constant power output at every hour of the year (i.e. baseload production as it is actually the case in Belgium), SMRs, are flexible in the sense that their production can vary between 0 and their full capacity independently at any hour of each representative year. Here, we simplify SMRs as only producing electricity and assume that the after-heat is lost to the atmosphere anyway.

For the sake of comparison, Figure 1.3 gives the levelised cost of energy (LCOE) of the principal technologies to produce electricity, based on the computation used by Limpens [8]. Compared to the other flexible generation units, SMR is significantly

Table 1.1. Nominal features of the SMRs in EnergyScope. SMR exhibits the advantage to have a fully flexible production (i.e. between 0 to the full capacity) unlike conventional nuclear that is constrained to produce a constant baseload at every hour of the year. [(a)] This annual availability accounts for yearly maintenance where the reactors might not operate or, at least, not at their maximum capacity. [(b)] 2040 is the soonest year at which SMR could be available, optimistically assuming industrial prototypes being completed by 2035 and 5 additional years for their commercial installation.

Feature	**Value**	**Unit**	**Similarity with conventional nuclear**
CAPEX	4850	€/kW	✓
Annual OPEX	103	€/kW/year	✓
Lifetime	60	year	✓
Efficiency	40%	-	✓
Maximum capacity	6	GW	✓
Annual availability	85%[(a)]	-	✓
Operational year	2040[(b)]	-	✗
Flexibility	Full	-	✗

more cost-effective. In addition, we see that CCGT supplied by e-ammonia outcompetes its e-methane equivalent, unlike their respective fossil-based equivalent.

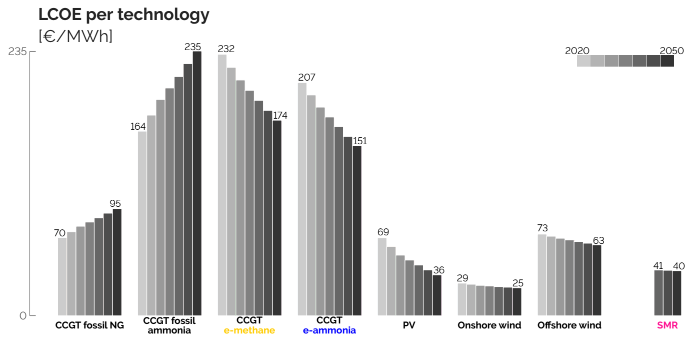

Figure 1.3. Levelised cost of energy (LCOE) for the main technologies in the power sector. Where SMR is cheaper than the other flexible options, CCGT running on e-ammonia is, a priori, cheaper than its e-methane alternative.

Figure 1.4 illustrates the different paths to produce the final molecules of the NED integrated within the model. Similarly to [29], naphtha, here considered as LFO, resulting from refinery operation is modeled as an imported commodity. Presented here for the specific year of 2035, all data and related references can be found in [30]. To keep the same level of details with other sectors of the model, the implementation of the conversion technologies consists of a single kind of technology per type of resource to produce a certain product. For instance, in the model, there is only one technology to produce HVC either from naphtha or from LPG, two liquid fossil hydrocarbons, i.e. naphtha steam cracker (NSC). For ammonia and methanol, the molecules can either be produced locally from other resources or directly imported (with distinction between non-renewable and renewable molecules). Some other technologies included in the model (not represented here for the sake of clarity), are able to turn some resources presented here into others (e.g. NG to hydrogen, woody biomass to hydrogen or to synthetic natural gas, more information in [6]).

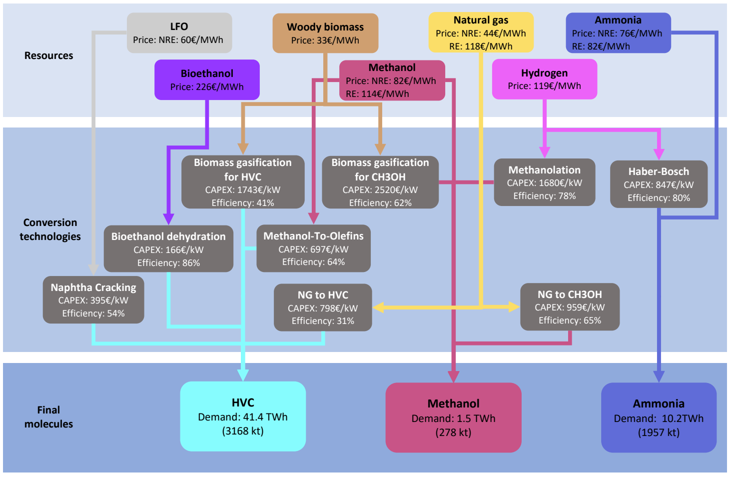

Figure 1.4. Schematic view of the different resources able to produce HVC, ammonia and methanol with their related conversion technologies (including energy efficiency and their CAPEX - in €/kW of final molecules). Values stand for 2035. Graph from [11]

1.5 Uncertainty ranges

Table 1.2 gives the uncertainty ranges of some key parameters. Like other works [31, 32], the uncertain parameters are assumed to be independent and uniformly distributed between their respective lower and upper bounds. A particular attention is to pay to the potential installation of SMR, at the bottom of Table 1.2. As detailed before, the commercial availability of such a technology is uncertain but would not be before

2040. Consequently, for SMR, the parameter $f_{\text{max,SMR}}$ influences the maximum capacity to install to translate somehow the readiness of this technology. As SMRs are foreseen, if installed, to be around the same locations (i.e. Tihange and Doel) as the conventional nuclear power plants and using the same area in kW/ha, the same 6 GW are assumed to be the maximum capacity for SMRs. If it is (i) smaller than 0.6, there is no possibility to install SMR during the transition; (ii) between 0.6 and 0.8, these 6 GW can be installed only in 2050; (iii) between 0.8 and 0.9, these can be installed from 2045 onward and; (iv) higher than 0.9, the prescribed maximum capacity can be installed from 2040 onward. Based on the local sensitivity analysis carried out by EnergyVille [27], the current work also considers a [-40%; +44%] range on the CAPEX of SMR, on top of the uncertainty about the availability. Finally, the the cost of purchasing renewable electrofuels presents a wide range, [-64.3%; +179.8%], like the other imported commodities.

The exhaustive list of the parameters accounted in this work is presented in Appendix A.3.

Table 1.2. Illustration of the uncertainty characterisation for different parameters for the year 2025. $^{(a)}$ Per [33], "I: investment-type, II: operation-type (constant uncertainty over time), III: operation-type (uncertainty increasing over time)". $^{(b)}$ The nominal value of each parameter is 0, meaning no variation compared to the nominal values of the impacted parameter in the model. $^{(c)}$ This range has been inferred from the local sensitivity analysis performed by EnergyVille [27].

Category	Parameter	Meaning	Type$^{(a)}$	Relative variation$^{(b)}$ min	Relative variation$^{(b)}$ max
Cost of purchasing	$c_{\text{op,fossil}}$	Purchase fossil fuels	II	-64.3%	179.8%
	$\boldsymbol{c_{\text{op,electrofuels}}}$	**Purchase electrofuels**	**II**	**-64.3%**	**179.8%**
Investment cost	$c_{\text{inv,car}}$	CAPEX car	I	-21.6%	25.0%
	$c_{\text{inv,e\_prop}}$	CAPEX electric motor	I	-39.6%	39.6%
	$c_{\text{inv,fc\_prop}}$	CAPEX fuel cell engine	I	-39.6%	39.6%
	$c_{\text{inv,PV}}$	CAPEX PV	I	-39.6%	39.6%
	$\boldsymbol{c_{\text{inv,nuclear\_SMR}}}$	**CAPEX SMR$^{(c)}$**	**I**	**-40.0%**	**44.0%**
Consumption	$\eta_{\text{e\_prop}}$	Consumption electric vehicles	I	-28.7%	28.7%
Potential installed capacity	$f_{\text{max,PV}}$	Max capacity PV	I	-24.1%	24.1%
	$f_{\text{max,windon}}$	Max capacity onshore wind	I	-24.1%	24.1%
Hourly load factor	$c_{\text{p,t,PV}}$	Hourly load factor PV	II	-22.1%	22.1%
	$c_{\text{p,t,winds}}$	Hourly load factor wind turbines	II	-22.1%	22.1%
Resource availability	$avail_{\text{elec}}$	Available electricity import	I	-32.1%	32.1%
	$avail_{\text{biomass}}$	Available local biomass	I	-32.1%	32.1%
End-use demand	$pass\_EUD$	Passenger mobility EUD	III	-7.5%	7.5%
	$industry\_EUD$	Industry EUD	III	-20.5%	16.0%
Miscellaneous	i_{rate}	Interest rate	I	-46.2%	46.2%
	$\Delta_{\text{change,freight}}$	Modal share change freight mobility	-	-30%	30%
	$\Delta_{\text{change,pass}}$	Modal share change passenger mobility	-	-30%	30%
	$\boldsymbol{f_{\text{max,SMR}}}$	**Potential capacity SMR**	**-**	**0**	**1**

1.6 CO_2-budget for the transition

In most of the studies carried out on the pathway optimisation of a whole-energy system, a CO_2-trajectory is *a priori* set to reach carbon-neutrality by 2050. Nerini et al. [34] used the emission trajectory indicated by the UK's Committee on Climate Change in their analysis of the impact of limited foresight to achieve the target of 80% reduction of greenhouse gases (GHG) by 2050 in the United Kingdom. In their assessment of the impacts of economy-wide emissions policies in the water-energy-land nexus, Licandeo et al. [35] analysed different CO_2-trajectories considering more or less severe water scarcity for the US. Poncelet et al. [36] with LUSYM (Leuven University SYstem Model) and EnergyVille [27] with TIMES-BE also set decreasing emission trajectories in their analysis of respectively the Belgian power sector and whole-energy system. Others only set the objective as the carbon-neutrality by 2050. For instance, Heuberger et al. [37] investigated the impact of different factors (e.g. limit of the foresight in the future, availability of “unicorn technologies"or committed versus market-driven decarbonisation strategies) to reach this ultimate objective in the UK system.

In this work, the effect of greenhouse gases is cumulative over time and a constraint is set on the overall emissions of the transition—a CO_2-budget for the transition. The arbitrarily chosen way of attributing emissions-budget to Belgium is usually called “grandfathering". Even though this approach has his pros and cons out of discussion within the scope of this work, it consists in “maintaining that prior emissions increase future emission entitlements"[38]. This budget ($1.2\,Gt_{CO_2,eq}$) corresponds to the proportion of Belgium's emissions in the world emissions in 2020 ($34.8\,Gt_{CO_2,eq}$ [39]) applied to the global budget to have a 66% chance of limiting warming to 1.5°C of $420\,Gt_{CO_2,eq}$ [40]. Therefore, in this work, a limit has been put on $gwp_{lim,trans} = 1.2\,Gt_{CO_2,eq}$ in Eq. (**??**). This is another sign of the urgency to act to mitigate climate change as this 30-year budget represents only 10 years of the current emissions.

Compared to a linear decrease from the current emissions, as done by Limpens et al. [1], this budget represents a 60% reduction of the cumulative emissions over the transition. Appendix A.2 compares the emissions trajectory between the REF case and a case (without SMR) where the linear decrease is imposed between 2020 and carbon-neutrality in 2050.

Bibliography

[1] G. Limpens, X. Rixhon, F. Contino, H. Jeanmart, Energyscope pathway: an open-source model to optimise the energy transition pathways of a regional whole-energy system, Elsevier in Applied Energy (2024).

[2] J. Dommisse, J.-L. Tychon, Modelling of Low Carbon Energy Systems for 26 European Countries with EnergyScopeTD : Can European Energy Systems Reach Carbon Neutrality Independently?, Master's thesis, UCLouvain, 2020. URL: `http://hdl.handle.net/2078.1/thesis:25202`.

[3] G. Limpens, EnergyScope Pathway documentation, ???? URL: `https://energyscope-pathway.readthedocs.io/en/v1.1/`.

[4] X. Rixhon, D. Tonelli, M. Colla, K. Verleysen, G. Limpens, H. Jeanmart, F. Contino, Integration of non-energy among the end-use demands of bottom-up whole-energy system models, Frontiers in Energy Research-Process and Energy Systems Engineering 10 (2022).

[5] Eurostat, Energy, Transport and environment statistics, 2019 edition, 2019.

[6] G. Limpens, H. Jeanmart, F. Maréchal, Belgian energy transition: What are the options?, Energies 13 (2020) 261.

[7] E. Commission, D.-G. for Climate Action, D.-G. for Energy, D.-G. for Mobility, Transport, A. De Vita, P. Capros, L. Paroussos, K. Fragkiadakis, P. Karkatsoulis, L. Höglund-Isaksson, W. Winiwarter, P. Purohit, A. Gómez-Sanabria, P. Rafaj, L. Warnecke, A. Deppermann, M. Gusti, S. Frank, P. Lauri, F. Fulvio, A. Florou, M. Kannavou, N. Forsell, T. Fotiou, P. Siskos, P. Havlík, I. Tsiropoulos, S. Evangelopoulou, P. Witzke, M. Kesting, N. Katoufa, I. Mitsios, G. Asimakopoulou, T. Kalokyris, EU reference scenario 2020 : energy, transport and GHG emissions : trends to 2050, Publications Office, 2021. doi:`doi/10.2833/35750`.

[8] G. Limpens, Generating energy transition pathways: application to Belgium, Ph.D. thesis, Université Catholique de Louvain, 2021.

[9] IEA, Nuclear Power and Secure Energy Transitions, Technical Report, IEA, Paris, 2022. https://www.iea.org/reports/nuclear-power-and-secure-energy-transitions, License: CC BY 4.0.

[10] J. Schnidrig, T.-V. Nguyen, X. Li, F. Maréchal, A modelling framework for assessing the impact of green mobility technologies on energy systems, Technical Report, EPFL, 2021.

[11] X. Rixhon, M. Colla, D. Tonelli, K. Verleysen, G. Limpens, H. Jeanmart, F. Contino, Comprehensive integration of the non-energy demand within a whole-energy system: towards a defossilisation of the chemical industry in belgium, in: 34th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems (ECOS 2021). Taormina, Italy, 2021, pp. 152–163.

[12] IEA, The Future of Petrochemicals – Analysis, https://www.iea.org/reports/the-future-of-petrochemicals, 2018.

[13] V. Daioglou, A. P. Faaij, D. Saygin, M. K. Patel, B. Wicke, D. P. van Vuuren, Energy demand and emissions of the non-energy sector, Energy & Environmental Science 7 (2014) 482–498.

[14] FPS Economy, ENERGY Key Data (2021).

[15] Statbel, Energy statistics by economic sector and by energy source, https://statbel.fgov.be/en/themes/energy/energy-statistics-economic-sector-and-energy-source, (Accessed February 11, 2021).

[16] European Commission, European strategy for plastics, https://ec.europa.eu/environment/waste/plastic_waste.htm, (Accessed February 16, 2021).

[17] Agoria & essenscia, The belgian plastics industry and the circular economy, https://www.essenscia.be/wp-content/uploads/2019/11/Plast_BROCH_A5_HR.pdf, (Accessed February 16, 2021).

[18] United Nations - Climate change, National inventory submissions 2020, https://unfccc.int/ghg-inventories-annex-i-parties/2020, (Accessed February 16, 2021).

[19] M. M. S. Asia), Mmsa supply and demand forecast, https://www.methanolmsa.com/additional-mmsa-services/temp-price-forecasts/, (Accessed February 16, 2021).

[20] P. Capros, A. De Vita, N. Tasios, P. Siskos, M. Kannavou, A. Petropoulos, S. Evangelopoulou, M. Zampara, D. Papadopoulos, C. Nakos, et al., Eu reference scenario 2016-energy, transport and ghg emissions trends to 2050., European Commission Directorate-General for Energy (2016). doi:10.2833/9127.

[21] L. Genge, F. Scheller, F. Müsgens, Supply costs of green chemical energy carriers at the european border: A meta-analysis, International Journal of Hydrogen Energy (2023).

[22] M. J. Grant, A. Booth, A typology of reviews: an analysis of 14 review types and associated methodologies, Health information & libraries journal 26 (2009) 91–108.

[23] M. J. Page, J. E. McKenzie, P. M. Bossuyt, I. Boutron, T. C. Hoffmann, C. D. Mulrow, L. Shamseer, J. M. Tetzlaff, E. A. Akl, S. E. Brennan, et al., The prisma 2020 statement: an updated guideline for reporting systematic reviews, International journal of surgery 88 (2021) 105906.

[24] ELIA, Electricity scenarios for Belgium towards 2050, Technical Report, 2017.

[25] X. Rixhon, G. Limpens, F. Contino, H. Jeanmart, Taxonomy of the fuels in a whole-energy system, Frontiers in Energy Research - Sustainable Energy Systems and Policies (2021). doi:10.3389/fenrg.2021.660073.

[26] Hydrogen Import Coalition, Shipping sun and wind to belgium is key in climate neutral economy, https://www.portofantwerp.com/sites/default/files/Hydrogen%20Import%20Coalition.pdf, 2021.

[27] EnergyVille, Paths2050 - the power of perspective, https://perspective2050.energyville.be/, 2022 (accessed December 2022).

[28] SCK-CEN, Small modular reactor (smr), https://www.sckcen.be/en/expertises/nuclear-systems/small-modular-reactor-smr, (Accessed July 2023).

[29] I. Tsiropoulos, R. Hoefnagels, S. de Jong, M. van den Broek, M. Patel, A. Faaij, Emerging bioeconomy sectors in energy systems modeling–integrated systems

analysis of electricity, heat, road transport, aviation, and chemicals: a case study for the netherlands, Biofuels, Bioproducts and Biorefining 12 (2018) 665–693.

[30] https://github.com/xrixhon/Non_energy_demand/tree/NED, March 2021.

[31] X. Li, S. Moret, F. Baldi, F. Maréchal, Are renewables really that expensive? the impact of uncertainty on the cost of the energy transition, in: Computer Aided Chemical Engineering, volume 46, Elsevier, 2019, pp. 1753–1758.

[32] D. Coppitters, W. De Paepe, F. Contino, Robust design optimization of a photovoltaic-battery-heat pump system with thermal storage under aleatory and epistemic uncertainty, Energy 229 (2021) 120692.

[33] S. Moret, Strategic energy planning under uncertainty, Ph.D. thesis, EPFL, 2017.

[34] F. F. Nerini, I. Keppo, N. Strachan, Myopic decision making in energy system decarbonisation pathways. a uk case study, Energy strategy reviews 17 (2017) 19–26.

[35] F. Licandeo, F. Flores, F. Feijoo, Assessing the impacts of economy-wide emissions policies in the water, energy, and land systems considering water scarcity scenarios, Applied Energy 342 (2023) 121115.

[36] K. Poncelet, E. Delarue, D. Six, W. D'haeseleer, Myopic optimization models for simulation of investment decisions in the electric power sector, in: 2016 13th International Conference on the European Energy Market (EEM), IEEE, 2016, pp. 1–9.

[37] C. F. Heuberger, I. Staffell, N. Shah, N. Mac Dowell, Impact of myopic decision-making and disruptive events in power systems planning, Nature Energy 3 (2018) 634–640.

[38] C. Knight, What is grandfathering?, Environmental Politics 22 (2013) 410–427.

[39] Our World in Data, Global co2 emissions from fossil fuels, https://ourworldindata.org/co2-emissions, (Accessed July 2023).

[40] Intergovernmental Pael on Climate Change (IPCC), Global Warming of 1.5°C. An IPCC Special Report on the impacts of global warming of 1.5°C above pre-industrial levels and related global greenhouse gas emission pathways, in the context of strengthening the global response to the threat of climate change, sustainable development, and efforts to eradicate poverty, Technical Report, 2018.

[41] SPF Economie, Energy - key data - edition february 2022, Brussels, Februrary 2022.

[42] S. Moret, V. Codina Gironès, M. Bierlaire, F. Maréchal, Characterization of input uncertainties in strategic energy planning models, Applied Energy 202 (2017) 597–617.

[43] X. Rixhon, G. Limpens, D. Coppitters, H. Jeanmart, F. Contino, The role of electrofuels under uncertainties for the belgian energy transition, Energies 14 (2021) 4027.

Appendix A

Case study: the Belgian energy system

A.1 Belgian energy system in 2020

The Belgian whole-energy system of 2020 was largely based (88.6% of the primary energy mix) on “conventional fuels"(i.e. oil and oil products (38.2%), natural gas (29.5%), uranium (16.3%) and solid fossil fuels (4.6%) while the rest mainly accounts for 26.7 TWh of lignocellulosic and wet biomass, 12.8 TWh of wind and 5.1 TWh of solar [41]. Given the data available in the literature (mostly for the power sector) and, when not available, following the assumptions made by Limpens et al. [6], Table A.1 gives the major technologies used in 2020 to supply the different demands of Figure 1.1.

A.2 CO_2-budget versus linear decrease of emissions

Figure A.1 shows the yearly emissions attributed for each sector in the REF case (i.e. imposed CO_2-budget) and a case where the CO_2-trajectory is constrained instead. Interestingly, these two transition pathways end up in a similar carbon-neutral whole-energy system in 2050. The two main sectors that significantly reduce their emissions in the REF case are the production of HVC and the high-temperature heat. In the former, this is linked to the extended use of oil products through naphtha-cracking. The latter is produced by industrial coal boilers for longer, until 2040. Overall, ending up to the same level of emissions in 2050, the REF case represents a 60% reduction of the cumulative emissions compared to the linear decrease, for a 7.5% more expensive transition.

Table A.1. Major technologies used to supply the 2020-demands of Figure 1.1 in terms of share of production and installed capacity. [(a)] The decentralised heating units provide 98% of the low-temperature heat demand. [(b)] The private mobility accounts for 80% of the passengers mobility.

End-use demand	Major technologies	Share of supply	Installed capacity
Electricity	Nuclear	39%	5.9 GW
	CCGT	21%	3.9 GW
	Wind turbines	14%	5.0 GW
Heat High-Temp.	Gas boiler	36%	3.3 GW
	Coal boiler	30%	2.3 GW
	Oil boiler	20%	1.5 GW
Heat Low-Temp. (DEC)[(a)]	Oil boiler	48%	21.4 GW
	Gas boiler	40%	17.5 GW
	Wood boiler	10%	4.4 GW
Heat Low-Temp. (DHN)	Gas CHP	59%	0.3 GW
	Gas boiler	15%	0.3 GW
	Waste CHP	15%	0.1 GW
Private mobility[(b)]	Diesel car	49%	93.5 Mpass.-km/h
	Gasoline car	49%	94.7 Mpass.-km/h
	HEV	2%	5.9 Mpass.-km/h
Public mobility	Diesel bus	43%	3.6 Mpass.-km/h
	Train	43%	3.9 Mpass.-km/h
	CNG bus	5%	0.8 Mpass.-km/h
Freight mobility	Diesel truck	74%	62.7 Mt.-km/h
	Diesel boat	15%	10.8 Mt.-km/h
	Train	11%	2.5 Mt.-km/h
HVC	Naphtha/LPG cracking	100%	4.6 GW
Ammonia	Haber-Bosch	100%	1 GW
Methanol	Import	100%	-

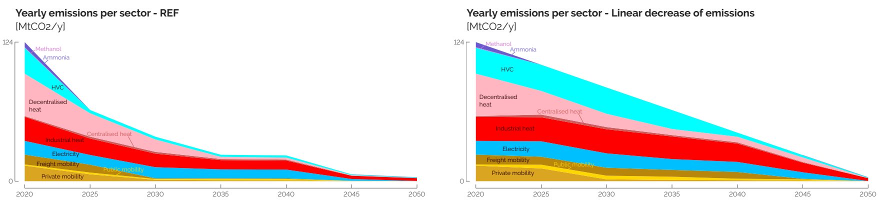

Figure A.1. Respecting the CO_2-budget imposed in the REF case drastically cuts the emissions of the system, especially in the production of high value chemicals (HVC) and the high-temperature heating sector.

A.3 Uncertainty characterisation for the 5-year steps transition

Table A.2 summarises the uncertainty ranges for the different groups of technologies and resources, for the year 2025. Refer to [33, 42] for the methodology and sources. As the model optimises the system every 5 years, $N = 5$ has been selected to get the final ranges of uncertainties of type II and III, based on the work of Moret [33]. For type III uncertainties (i.e. uncertainty ranges increasing with time), a 50% increase has been set arbitrarily between the ranges for 2025 and these same ranges for 2050. In other words, for these specific uncertainties, the ranges for 2050 are 50% larger than for 2025.

Rixhon et al. [43] analysed the impact of these parameters on the total cost of the snapshot Belgian whole-energy system in 2050 subject to different GWP limits. Based on this work, we have selected a subset of impacting uncertainties, added others due to the pathway formulation (e.g. $\Delta_{\text{change,pass}}$), and listed them in Table A.2. The uncertainty characterisation gives the uncertainty ranges per parameter or group of parameters (category).

This work considers nine groups of uncertain parameters: (i) the cost of purchasing imported energy carriers; (ii) the investment cost (i.e. CAPEX) of some technologies, mostly related to the mobility sector and the integration of renewables; (iii) the maintenance cost (i.e. OPEX) of every technology; (iv) the consumption of electric and fuel cells vehicles in the mobility sector; (v) the potential installed capacity of renewables; (vi) the hourly load factor of renewables accounting for variability of solar irradiance or wind speed; (vii) the availability of resources considered as limited (i.e. biomass and electricity); (viii) the end-use-demands split per sector of activities (i.e. households, services, passenger mobility and industry) and (ix) other parameters like the interest rate or the modal share change in different key sectors. For the specific case of SMR, the parameter $f_{\text{max,SMR}}$ will influence the maximum capacity (i.e. 6 GW) to install to translate somehow the readiness of this technology. If it is (i) smaller than 0.6, there is no possibility to install SMR during the transition; (ii) between 0.6 and 0.8, these 6 GW can be installed only in 2050; (iii) between 0.8 and 0.9, these can be installed from 2045 onward and; (iv) higher than 0.9, the prescribed maximum capacity can be installed from 2040 onward.

Table A.2. Application of the uncertainty characterization method to the EnergyScope Pathway model for the year 2025. [(a)] Per [33], “I: investment-type, II: operation-type (constant uncertainty over time), III: operation-type (uncertainty increasing over time)". [(b)] The nominal values of each of the parameters is 0, meaning no variation compared to the nominal values of the impacted parameter in the model. [(c)] This range has been inferred from the local sensitivity analysis performed by EnergyVille [27].

Category	**Parameter**	**Meaning**	**Type**[(a)]	**Relative variation**[(b)] min	max
Cost of purchasing	$c_{\text{op,fossil}}$	Purchase fossil fuels	II	-64.3%	179.8%
	$c_{\text{op,elec}}$	Purchase electricity	II	-64.3%	179.8%
	$\boldsymbol{c_{\text{op,electrofuels}}}$	**Purchase electrofuels**	**II**	**-64.3%**	**179.8%**
	$c_{\text{op,biofuels}}$	Purchase biofuels	II	-64.3%	179.8%
Investment cost	$c_{\text{inv,car}}$	CAPEX car	I	-21.6%	25.0%
	$c_{\text{inv,bus}}$	CAPEX bus	I	-21.6%	25.0%
	$c_{\text{inv,ic\_prop}}$	CAPEX ICE	I	-21.6%	25.0%
	$c_{\text{inv,e\_prop}}$	CAPEX electric motor	I	-39.6%	39.6%
	$c_{\text{inv,fc\_prop}}$	CAPEX fuel cell engine	I	-39.6%	39.6%
	$c_{\text{inv,efficiency}}$	CAPEX efficiency measures	I	-39.3%	39.3%
	$c_{\text{inv,PV}}$	CAPEX PV	I	-39.6%	39.6%
	$c_{\text{inv,grid}}$	CAPEX power grid	I	-39.3%	39.3%
	$c_{\text{inv,grid\_enforce}}$	CAPEX grid reinforcement	I	-39.3%	39.3%
	$\boldsymbol{c_{\text{inv,nuclear\_SMR}}}$	**CAPEX SMR**[(c)]	**I**	**-40.0%**	**44.0%**
Maintenance cost	$c_{\text{maint,var}}$	Variable OPEX of technologies	I	-48.2%	35.7%
Consumption	$\eta_{\text{e\_prop}}$	Consumption electric vehicles	I	-28.7%	28.7%
	$\eta_{\text{fc\_prop}}$	Consumption fuel cell vehicles	I	-28.7%	28.7%
Potential installed capacity	$f_{\text{max,PV}}$	Max capacity PV	I	-24.1%	24.1%
	$f_{\text{max,windon}}$	Max capacity onshore wind	I	-24.1%	24.1%
	$f_{\text{max,windoff}}$	Max capacity offshore wind	I	-24.1%	24.1%
Hourly load factor	$c_{\text{p,t,PV}}$	Hourly load factor PV	II	-22.1%	22.1%
	$c_{\text{p,t,winds}}$	Hourly load factor wind turbines	II	-22.1%	22.1%
Resource availability	$avail_{\text{elec}}$	Available electricity import	I	-32.1%	32.1%
	$avail_{\text{biomass}}$	Available local biomass	I	-32.1%	32.1%
End-use demand	HH_EUD	Households EUD	III	-13.8%	11.2%
	$services\_EUD$	Services EUD	III	-14.3%	11%
	$pass\_EUD$	Passenger mobility EUD	III	-7.5%	7.5%
	$industry\_EUD$	Industry EUD	III	-20.5%	16.0%
Miscellaneous	i_{rate}	Interest rate	I	-46.2%	46.2%
	$\%_{\text{pub,max}}$	Max share of public transport	I	-10%	10%
	$\Delta_{\text{change,freight}}$	Modal share change freight mobility	-	-30%	30%
	$\Delta_{\text{change,pass}}$	Modal share change passenger mobility	-	-30%	30%
	$\Delta_{\text{change,LT\_heat}}$	Modal share change LT-heat	-	-30%	30%
	$\boldsymbol{f_{\text{max,SMR}}}$	**Potential capacity SMR**	**-**	**0**	**1**