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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

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in partial fulfillment of the requirements for
the degree of Doctor in Engineering Sciences

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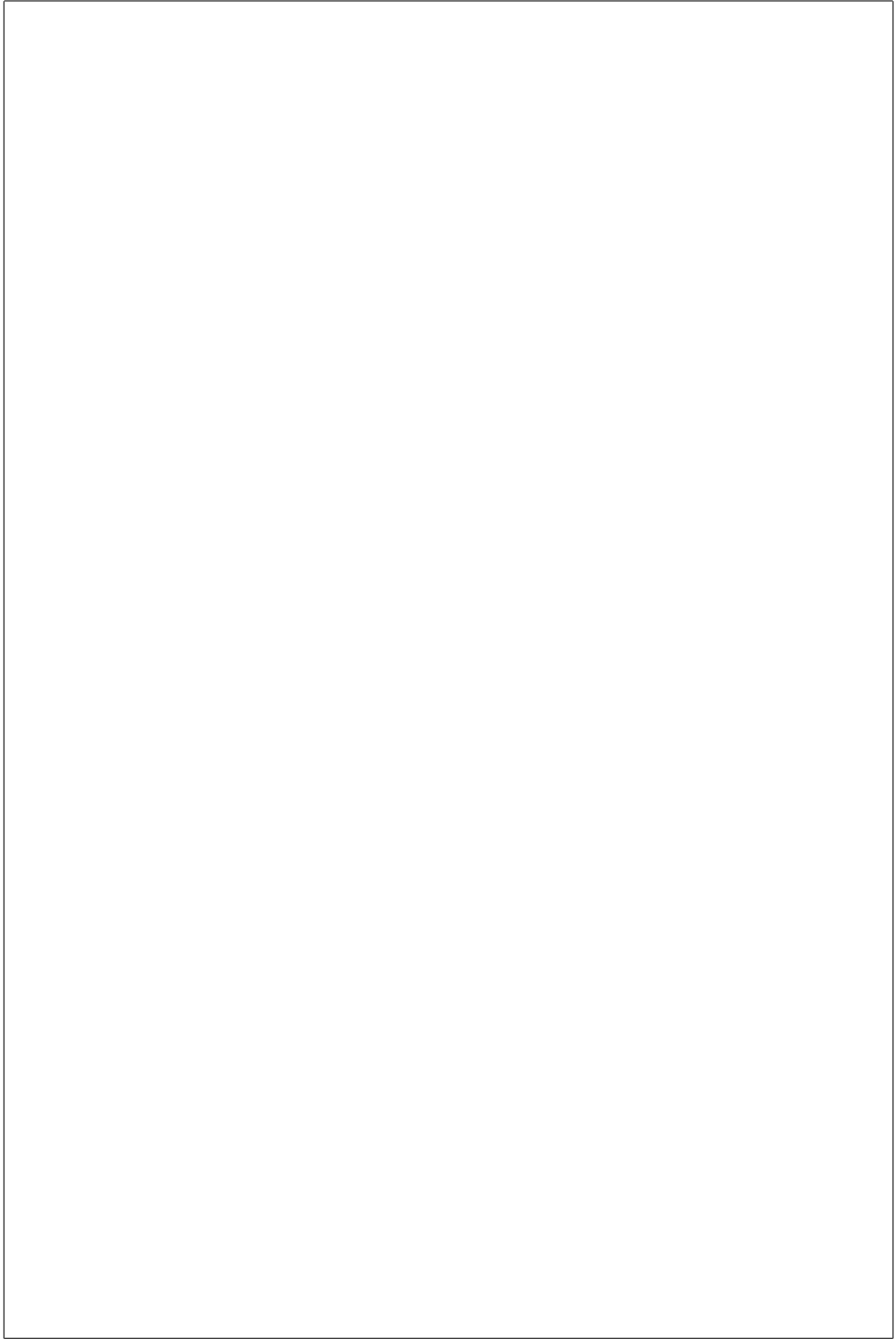
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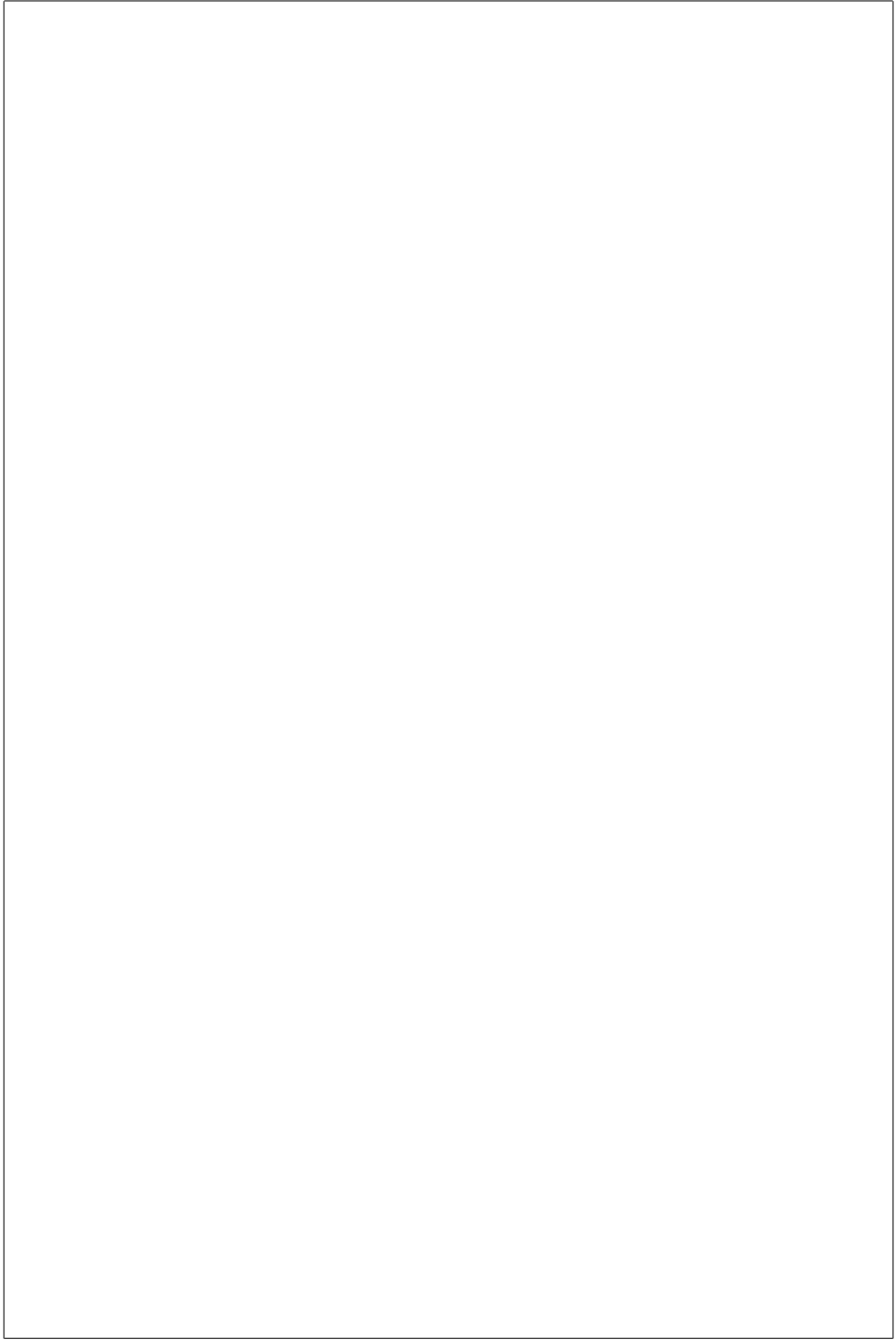
Abstract

This thesis will be awesome



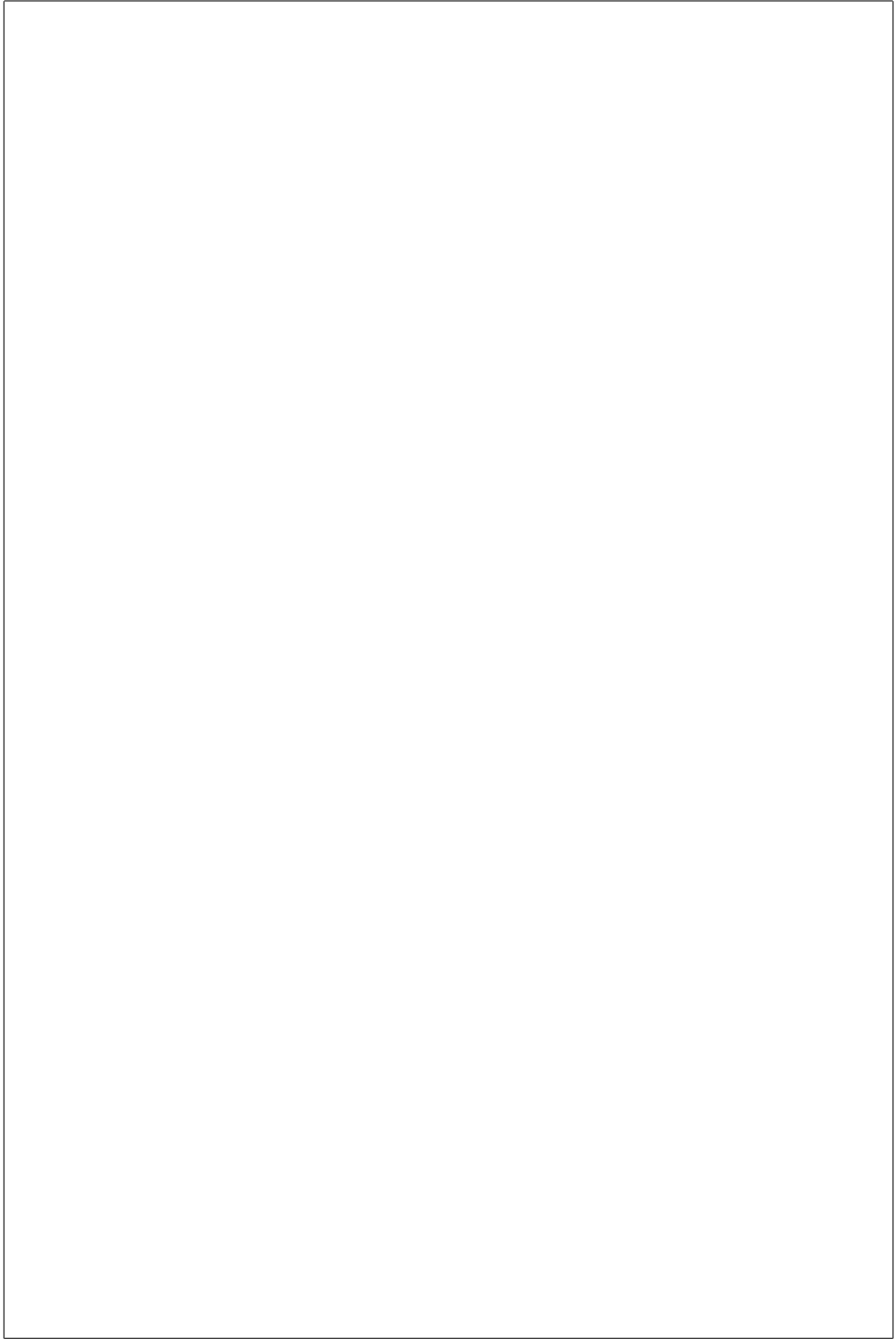
*“Pour ce qui est de l’avenir, il ne s’agit pas de le prévoir,
mais de le rendre possible”*

– Antoine de Saint Exupéry, Citadelle, 1948



Remerciements

Thank you, thank you, far too kind



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Symbols

Acronyms

API	application programming interface
BEV	battery electric vehicle
BTX	benzene, toluene and xylene
CAPEX	capital expenditure
CCGT	combined cycle gas turbine
CHP	combined heat and power
DHN	district heating network
ESOMs	energy system optimisation models
EnergyScope TD	EnergyScope Typical Days
EUD	end-use demand
FC	fuel cell
GHG	greenhouse gases
GSA	global sensitivity analysis
GWP	global warming potential
HP	heat pump
HVC	high value chemicals
IEA	International Energy Agency
IPCC	intergovernmental panel for climate change
LCA	life cycle assessment
LCOE	levelised cost of energy
LFO	light fuel oil
LOO	leave-one-out
LPG	liquefied petroleum gas
MMSA	Methanol Market Services Asia
MTBE	methyl tert-butyl ether

NED	non-energy demand
NG	natural gas
NN	neural network
NRE	non-renewable energy
NSC	naphtha steam cracker
OPEX	operational expenditure
PCE	Polynomial Chaos Expansion
PV	photovoltaic
RE	renewable energy
RL	reinforcement learning
SAC	Soft Actor Critic
SDGs	Sustainable Development Goals
SMR	small modular reactor
UQ	Uncertainty Quantification

List of publications

Limpens, G., **Rixhon, X.**, Contino, F., & Jeanmart, H. (2024). “*EnergyScope Pathway: An open-source model to optimise the energy transition pathways of a regional whole-energy system.*” In *Applied Energy*, (Vol. 358). URL: <https://doi.org/10.1016/j.apenergy.2023.122501>

Rixhon, X., Limpens, G., Coppitters, D., Jeanmart, H., & Contino, F.(2022). “*The role of electrofuels under uncertainties for the Belgian energy transition.*” In *Energies* (Vol. 14). URL: <https://doi.org/10.3390/en14134027>

Rixhon, X., Limpens, G., Contino, F., & Jeanmart, H. (2021). “*Taxonomy of the fuels in a whole-energy system.*” In *Frontiers in Energy Research*, Sec. Sustainable Energy Systems, (Vol. 9). URL: <https://doi.org/10.3389/fenrg.2021.660073>

Rixhon, X., Tonelli, D., Colla, M., Verleysen, K., Limpens, G., Jeanmart, H. ,& Contino, F.(2022). “*Integration of non-energy among the end-use demands of bottom-up whole-energy system models.*” In *Frontiers in Energy Research*, Sec. Process and Energy Systems Engineering, (Vol. 10). URL: <https://doi.org/10.3389/fenrg.2022.904777>

Rixhon, X., Colla, M., Tonelli, D., Verleysen, K., Limpens, G., Jeanmart, H., & Contino, F.(2021). “*Comprehensive integration of the non-energy demand within a whole-energy system: Towards a defossilisation of the chemical industry in Belgium.*” In *proceedings of ECOS 2021 conference* (Vol. 34, p. 154).

Limpens, G., Coppitters, D., **Rixhon, X.**, Contino, F., & Jeanmart, H. (2020). “*The impact of uncertainties on the Belgian energy system: application of the Polynomial Chaos Expansion to the EnergyScope model.*” In proceedings of ECOS 2020 conference (Vol. 33, p. 711).

Chapter 1

Methodology: Through a variety of complementary tools

Contributions

- Develop the myopic approach
- Apply Stefano's method on the pathway model with a similar approach as Guevara et al.
- Check that PCE was appropriate as a method for such a system (ECOS2020)
- Update the $C_{inv,etern}$ based on the initial investigation of Goffaux [1] and in line with Poncelet et al. [2].

Other authors' main contribution statement

On top of the main contributions of this thesis that are aforementioned, three main authors are to be mentioned for having brought a significant part of the methodological work. Based on Stefano Moret's monthly whole-energy system model (i.e. EnergyScope) [3], Gauthier Limpens has developed the hourly version of the snapshot model (i.e. EnergyScope TD) [4], as well as the perfect foresight pathway model [5], to which I personally contributed too. Diederik Coppitters has developed the RHEIA framework allowing to quantify the impact of uncertainties and carry out robust optimisation of energy systems [6]. The current work used this framework for the first of these functionalities. Finally, Stefano Moret extensively assessed the uncertainty char-

acterisation on the Swiss energy system [7]. This thesis follows the same methodology, updating the uncertainty ranges for the pathway model.

1.1 Whole-energy system transition model optimisation: EnergyScope Pathway

This work optimises the entire transition pathway from a known system in 2020 up to 2050 thanks to EnergyScope Pathway [5]. According to pathway models review (see Appendix A.1), EnergyScope Pathway can be categorised as an investment and operation optimisation model that assesses the whole-energy system, has a hourly time-resolution and is open-source documented model. Moreover, it maintains a low computational cost (i.e. around 15 minutes for a 30-year pathway with a hourly discretisation). From the perfect to the myopic foresight of the transition optimisation, this section presents only the main constraints of the former approach to further dig into more details about the latter. The reader is invited to refer to Appendix A.2 for more details about the formulation of the model and its extension from a snapshot approach, EnergyScope TD. More extensive information about the formulation choices, for instance, can be found in [5] and the documentation [8].

1.1.1 Perfect foresight: One global optimisation of the transition

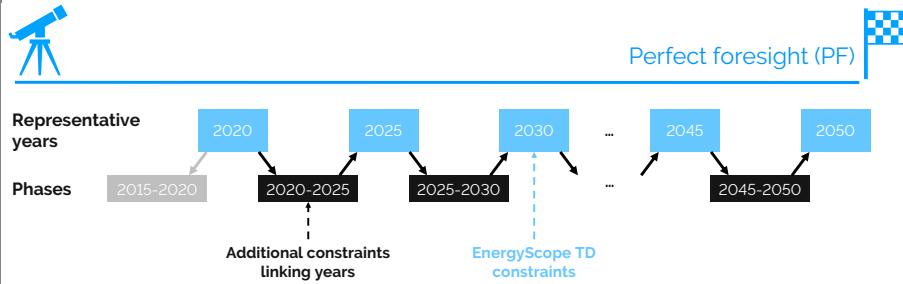


Figure 1.1. Illustration of the pathway methodology based on an existing energy system model. The methodology spans from 2020 to 2050, with one representative year every five years. The model EnergyScope Typical Days (EnergyScope TD) is applied in 7 representative years (light blue boxes). The formulation includes additional constraints (black boxes) that link the years together. The pathway’s initialisation assumes that all capacities installed in 2020 were built during the pseudo-phase of 2015-2020 (grey box). The overall problem is defined as the pathway model.

The whole-energy system model developed in this work originates from the perfect foresight (PF) formulation (Figure 1.1) of EnergyScope—the entire transition is computed in one optimisation, assuming a complete but uncertain knowledge of the different parameters until 2050 [5]. All the variables and constraints of the snapshot model, EnergyScope TD [4], and summarized in Appendix A.2.1, are kept as is with an extra-dimension to relate them to a specific representative year, y , of the pathway. For instance, the energy balance is guaranteed at every hour of each of these years.

The optimised objective of the pathway model, i.e. the total transition cost $C_{\text{tot,trans}}$, is computed as follows:

$$\min C_{\text{tot,trans}} = C_{\text{tot,capex}} + C_{\text{tot,opex}} \quad (1.1)$$

$$C_{\text{tot,capex}} = \sum_{p \in \text{PHASE} \cup \{2015_2020\}} C_{\text{inv,phase}}(p) - \sum_{j \in \text{TECH}} C_{\text{inv,return}}(j) \quad (1.2)$$

$$C_{\text{tot,opex}} = C_{\text{opex}}(2020) + t_{\text{phase}} \cdot \tau_{\text{phase}}(p) \cdot \sum_{p \in \text{PHASE} | y_{\text{start}} \in P_START(p), y_{\text{stop}} \in P_STOP(p)} (C_{\text{opex}}(y_{\text{start}}) + C_{\text{opex}}(y_{\text{stop}})) / 2 \quad (1.3)$$

$$\tau_{\text{phase}}(p) = 1 / (1 + i_{\text{rate}})^{\text{diff_2015_year}(p)} \quad (1.4)$$

$$C_{\text{inv,return}}(i) = \sum_{p \in \text{PHASE} \cup \{2015_2020\} | y_{\text{start}} \in Y_START(p), y_{\text{stop}} \in Y_STOP(p)} \tau_{\text{phase}}(p) \cdot (c_{\text{inv}}(y_{\text{start}}, i) + c_{\text{inv}}(y_{\text{stop}}, i)) / 2 \cdot \frac{\text{remaining_years}(i, p)}{\text{lifetime}(y_{\text{start}}, i)} \left(F_{\text{new}}(p, i) - \sum_{p2 \in \text{PHASE}} F_{\text{decom}}(p2, p, i) \right) \quad \forall i \in \text{TECH} \quad (1.5)$$

where $t_{\text{phase}} = 5$ years and $\text{diff_2015_year}(p)$ are respectively the duration of a phase between two representative years and the number of years between the middle of a phase and 2015 for a correct annualisation. $C_{\text{inv,return}}$ accounts for the residual value, also called *salvage value*, of the technologies installed during the transition and having not reached the end of their lifetime by 2050. This last variable is crucial to avoid penalising heavy (and potentially long-lifetime) investments at the end of the transition as these assets would still be operational beyond 2050. The interested reader will find more information about the formulation choices related to it in the work of Limpens et al. [5]. The other variables in Eq. (1.2-1.3) are detailed here below:

$$\mathbf{C}_{\text{opex}}(y) = \sum_{j \in \text{TECH}} \mathbf{C}_{\text{maint}}(y, j) + \sum_{i \in \text{RES}} \mathbf{C}_{\text{op}}(y, i) \quad \forall y \in \text{YEARS} \quad (1.6)$$

$$\mathbf{C}_{\text{inv,phase}}(p) = \sum_{j \in \text{TECH}} \mathbf{F}_{\text{new}}(p, j) \cdot \tau_{\text{phase}}(p) \cdot (c_{\text{inv}}(y_{\text{start}}, j) + c_{\text{inv}}(y_{\text{stop}}, j)) / 2$$

$$\forall p \in \text{PHASE} | y_{\text{start}} \in P_{\text{START}}(p), y_{\text{stop}} \in P_{\text{STOP}}(p) \quad (1.7)$$

where \mathbf{F}_{new} are the capacities newly installed. In Eq. (1.6-1.7), the costs related to each representative year are:

$$\mathbf{C}_{\text{inv}}(y, j) = c_{\text{inv}}(y, j) \mathbf{F}(y, j) \quad \forall y \in \text{YEARS}, \forall j \in \text{TECH} \quad (1.8)$$

$$\mathbf{C}_{\text{maint}}(y, j) = c_{\text{maint}}(y, j) \mathbf{F}(y, j) \quad \forall y \in \text{YEARS}, \forall j \in \text{TECH} \quad (1.9)$$

$$\mathbf{C}_{\text{op}}(y, i) = \sum_{t \in T} c_{\text{op}}(y, i) \mathbf{F}_t(y, i, t) t_{\text{op}}(t) \quad \forall y \in \text{YEARS}, \forall i \in \text{RES} \quad (1.10)$$

where the variable \mathbf{F} represents the size of the installed capacities (for all technologies j) and the variable \mathbf{F}_t is the hourly consumption of the resources; the parameters c_{inv} and c_{maint} are the CAPEX and the OPEX of the technologies, and the parameter c_{op} is the cost of purchasing resources. For the sake of simplicity, as done by Limpens et al. [5], the sum over the 8760 hours of the year is written as the sum over $t \in T$.

Then, as detailed in section 2.5, the CO₂-budget for the transition, $\mathbf{GWP}_{\text{tot,trans}}$, is computed and constrained as follows:

$$\mathbf{GWP}_{\text{tot,trans}} = \mathbf{GWP}_{\text{tot}}(2020) + t_{\text{phase}} \sum_{p \in \text{PHASE} | y_{\text{start}} \in Y_{\text{START}}(p), y_{\text{stop}} \in Y_{\text{STOP}}(p)} (\mathbf{GWP}_{\text{tot}}(y_{\text{start}}) + \mathbf{GWP}_{\text{tot}}(y_{\text{stop}})) / 2 \quad (1.11)$$

$$\mathbf{GWP}_{\text{tot,trans}} \leq gwp_{\text{lim,trans}} \quad (1.12)$$

where the computation of the yearly emissions are based on the global warming potential (GWP) of the resources:

$$\mathbf{GWP}_{\text{tot}}(y) = \sum_{i \in \text{RES}} \mathbf{GWP}_{\text{op}}(y, i) \quad \forall y \in \text{YEARS} \quad (1.13)$$

$$\mathbf{GWP}_{\text{op}}(y, i) = \sum_{t \in T} gwp_{\text{op}}(y, i) \mathbf{F}_t(y, i, t) t_{\text{op}}(t) \quad \forall y \in \text{YEARS}, \forall i \in \text{RES} \quad (1.14)$$

where gwp_{op} is the specific emissions (i.e. in kt_{CO₂,eq}/GWh) of each resource. Based on an approach developed by the Intergovernmental Panel on Climate Change (IPCC) [9], this work considers the indicator “GWP100a - IPCC2013” to compute the emissions related to the use of resources. This includes the emissions due to the extraction,

the transportation and the combustion of the energy carrier. EnergyScope proposes to account for the embodied emissions of the technologies based on a life cycle assessment (LCA). These stand for extraction of materials, refining, construction and end of life [10]. However, this work is still in progress and the database is not yet complete. Consequently, it is not included in this work and not accounted for.

Besides this constraint on the emissions, the main constraint to link years with each other is the one dictating the installed capacities at the end of each year:

$$\mathbf{F}(y_{\text{stop}}, j) = \mathbf{F}(y_{\text{start}}, j) + \mathbf{F}_{\text{new}}(p, j) - \mathbf{F}_{\text{old}}(p, j) - \sum_{p2 \in \text{PHASE} \cup \{2015_2020\}} \mathbf{F}_{\text{decom}}(p, p2, j)$$

$$\forall p \in \text{PHASE}, y_{\text{stop}} \in Y_{\text{STOP}}(p), y_{\text{start}} \in Y_{\text{START}}(p), j \in \text{TECH} \quad (1.15)$$

where the variables \mathbf{F}_{old} and $\mathbf{F}_{\text{decom}}$ are the capacities respectively having reached the end of their lifetime and prematurely decommissioned. Moreover, to account for the society inertia and to prevent unrealistically fast modal share change, constraints limit this change for the sectors of the low-temperature, the passenger mobility and freight mobility demands. The parameters $\Delta_{\text{change,LT_heat}}$, $\Delta_{\text{change,pass}}$ and $\Delta_{\text{change,freight}}$ respectively limit their respective modal share change up to 33%, 50% and 50% per phase of 5 years.

1.1.2 Myopic: Sequential optimisation of the transition with limited foresight

One of the main methodological contributions of this work regarding the development of the whole-energy system model consists in giving it the possibility to optimise the transition pathway in a myopic approach. After introducing the general concept of it, this section details more the additions brought to the model in terms of implementation.

General concept of the myopic optimisation

Compared to the perfect foresight, the myopic approach (Figure 1.2) has two main advantages: shorter computational time and more realistic representation of the short-sightedness of decision-makers. For this reason, several studies are based on this approach [2, 11–13]. Babrowski et al. [11] analysed the benefit of the myopic approach to reduce the computational time. Poncelet et al. [2] uses this approach to analyse the expansion planning of the power sector beyond 2050. Nerini et al. [12] analysed the impact of the horizon windows and overlapping time. Overall these studies decided to choose the myopic approach to analyse the speed of change compared to a perfect foresight approach. Moreover, the myopic approach allows a sequential optimisation

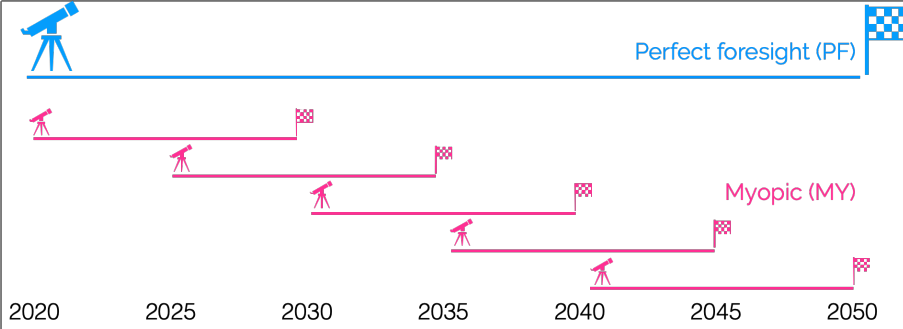


Figure 1.2. The myopic approach (in pink) uses several instances of the pathway model (illustrated in Figure A.3). In this example, the pathway instance has a time horizon of 10 years ($N_{\text{year, opti}} = 10$) with a 5 year-overlap ($N_{\text{year, overlap}} = 5$). As a comparison the Perfect foresight (in blue) has a time horizon of 30 years.

process that opens the doors to decision-making/policy-learning methodologies, like assessing shock events. This approach is used by Heuberger et al. [13] who assessed the speed of integration of technologies due to these events. In their analysis of the overcapacity in European power systems, Moret et al. [14] emphasised that such a “possibility of *recourse*” is very appropriate to address uncertainty gradually unfolding over time. Consequently, the development of the myopic approach represents the foundations of the further implementation of the agent-based reinforcement learning framework (see Section 1.3).

As illustrated in Figure 1.3, after optimising, in design and operation, one time window (e.g. from 2020 to 2030), the intermediate system design (i.e. the installed capacities) is set as initial conditions for the start of the next time window (e.g. from 2025 to 2035) as well as the historical investment decisions (i.e. \mathbf{F}_{new} , \mathbf{F}_{old} and $\mathbf{F}_{\text{decom}}$). Consequently, the solution obtained at the end of the first time window (e.g. 2030) as well as potential investment decisions between the start of the second time window and this end-year are discarded. In other words, they are not taken into account for the optimisation of the second time window. This process goes on until the stated end of the transition (i.e. 2050, in this case).

Additional sets, parameters and variables

The major add-on from the original EnergyScope Pathway model [15] to the myopic version developed in this thesis, is the possibility to carry out the optimisation on a limited time window, of which the duration is defined by $N_{\text{year, opti}}$. Moreover, to

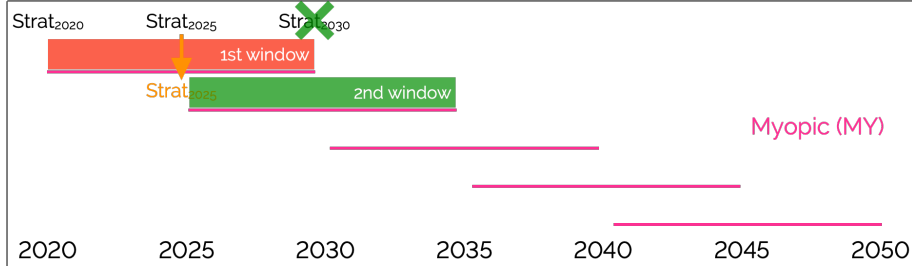


Figure 1.3. Sequential optimisation of the transition pathway in the myopic approach: (i) first time-window optimisation, (ii) set-up of the initial conditions of the second time-window, (iii) second time-window optimisation discarding intermediate results

ensure the “possibility of *recourse*”, there is also the possibility of having an overlap between two consecutive time windows. The timespan of this overlap is defined by the parameter $N_{\text{year,overlap}}$. The philosophy followed behind the development of the myopic approach was to add another layer on top of the perfect foresight model in order to make it more modular. For this reason, the already existing constraints are marginally adapted. This way, the newly developed model can easily be used to perform a perfect foresight optimisation by setting the time window to $N_{\text{year,opti}} = 30$ years (i.e. between 2020 and 2050) and the overlap between the time windows to $N_{\text{year,overlap}} = 0$. Consequently, as defining the actual time window on which the system is optimised as well as the history, i.e. what has already been optimised earlier in the transition, are fundamental, four new sets are implemented: $\text{YEARS}_{\text{WND}}$, $\text{YEARS}_{\text{UP TO}}$, $\text{PHASE}_{\text{WND}}$ and $\text{PHASE}_{\text{UP TO}}$ (see Table 1.1).

Table 1.1. New SETs for myopic pathway formulation.

Set	Index	Description
$\text{YEARS}_{\text{WND}}$	$y \in Y$	Representative years of the time window to optimize
$\text{YEARS}_{\text{UP TO}}$	$y \in Y$	Representative years including the years already optimised, i.e. the history
$\text{PHASE}_{\text{WND}}$	$p \in P$	Phases of the time window to optimize
$\text{PHASE}_{\text{UP TO}}$	$p \in P$	Phases including the phases already optimised, i.e. the history

$\text{YEARS}_{\text{WND}}$ and $\text{PHASE}_{\text{WND}}$ substitute YEARS and *textPHASE* in the constraints defined in the pathway model in Section 1.1.1. These two sets aim at setting the optimization to a more limited time window. Progressing through the transition, $\text{YEARS}_{\text{UP TO}}$ and $\text{PHASE}_{\text{UP TO}}$ allow keeping track of the history of the investments (e.g. technologies installation, decommissioning or retirement), the consumption of resources, the cumulative amount of emissions, etc.

On top of these four specific sets, some artefacts were also necessary to avoid computational rounding errors. Indeed, optimizing the first year of a time window that has already been optimized in the previous time window could lead to rounding errors preventing from the optimization to converge. For this reason, the set YEAR_{ONE} accounts for the first representative year of the time window to optimize that is excluded from $\text{YEARS}_{\text{WND}}$ to avoid these errors. This remark stays valid for any time window except the first one of the transition where the year 2020 is optimized even though its technological strategy is set according to the actual system presented in Appendix B.1. Finally, as the end of time windows changes for each of them, the parameter *remaining_years* has to be updated accordingly to keep a meaningful definition of $\text{C}_{\text{inv,return}}$ in Eq. 1.5.

Myopic pathway implementation

Starting this work in 2017, AMPL Optimization Inc. has developed a Python application programming interface (API) called *amplpy* [16]. In a nutshell, this API allows the pre/post-processing of an *ampl* optimisation problem by accessing its features (e.g. constraints, parameters, variables, objective function) from within Python. Using this API, this updated version of the model interacts with the AMPL problem representing the optimization of the whole-energy system transition pathway as represented in Figure 1.4.

1.2 Uncertainty quantification

In their systematic review, Yue et al. [17] highlighted that a wide majority of studies addressing the optimisation of energy systems (i.e. 75% out of the 134 reviewed studies) were not investigating the impact of uncertainties. However, disregarding these impacts can have drastic consequences on the system design. For instance, historical low natural gas (NG) prices have led to overcapacity of combined cycle gas turbine (CCGT) in Europe [14]. This is why accounting for uncertainty in energy system opti-

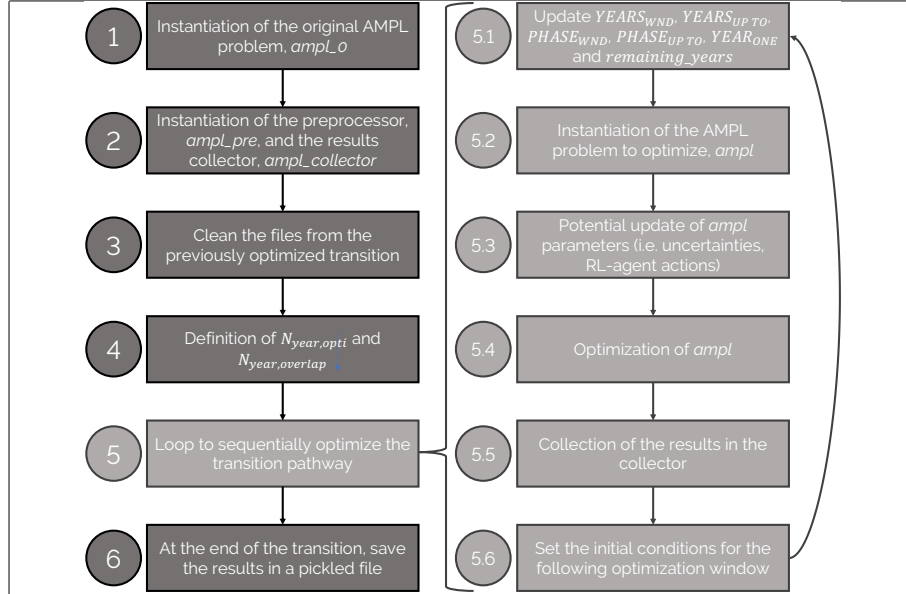


Figure 1.4. Schematic of the iterative optimization of the whole-energy system transition pathway.

minimisation models (ESOMs) is crucial [18], especially when it comes to optimise several decades in an inherently uncertain future [19].

This section aims at briefly presenting the methods followed to first characterise these uncertainties, then to quantify their impact on different outputs of interest of the model (e.g. amount of molecules imported from abroad, the installed capacity of SMR or the total transition cost) and finally, the screening and selection of the parameters to analyse.

1.2.1 Uncertainty characterisation

Characterising precisely the uncertainty—ideally with their respective probability density functions (PDFs)—of the thousands of parameters in the model is daunting if not impossible because of lack of data [20]. Therefore, we used a workaround developed by Moret et al. [7] that defines relative ranges of variation for different groups of parameters. These ranges have been adapted for the Belgian energy system and the pathway formulation. Moreover, some ranges have been added to account for new parameters coming from the pathway formulation described in Section 1.1 like the society inertia.

Like other works [21, 22], the uncertain parameters are assumed to be independent and uniformly distributed between their respective lower and upper bounds.

Following the methodology defined by Moret et al. [7], uncertainties of types I (investment-type) and II (operation-type, constant uncertainty over time) keep the same range for the whole transition. However, parameters with an uncertainty increasing over time, type III, (i.e. end-use demands, in this case) will have a wider and wider range over the transition. In this work, a +50% linear increase has been arbitrarily set between the width of the range of such parameters in 2025 and the same ranges in 2050. In Figure 1.5, this means that for type III uncertainties only, R_{2050}^+ is 50% bigger than R_{2025}^+ and R_{2050}^- is 50% smaller than R_{2025}^- . For uncertainties of types I and II, the relative variation versus the nominal value remain the same over the transition. Inspired by Guevara et al. [23], the values of the uncertain parameters are set at a fixed relative position from the nominal values for each sampled transition—the values do not zigzag from 2025 to 2050 within the bounds (Figure 1.5).

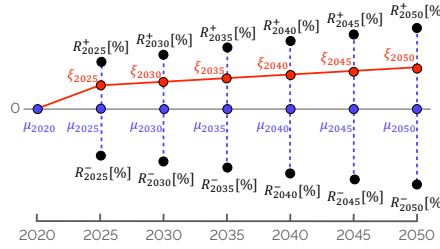


Figure 1.5. $\mu_{2020}, \mu_{2025}, \dots, \mu_{2050}$ are the nominal values equal to 0 as the uncertain parameters represent a relative increase/decrease of actual parameters of the model. R^+ and R^- are respectively the upper and lower bounds of the range and $\xi_{2025}, \xi_{2030}, \dots, \xi_{2050}$ are the values taken by one parameter for a specific sample of the global sensitivity analysis (GSA) for each of the representative years of the transition, always starting from the nominal value in 2020, μ_{2020} . The graph has been adapted from [23].

Finally, the model accounts for thousands of parameters. The computational burden to consider all of them separately would be completely overwhelming ($\sim 10^7$ model runs). Therefore, similarly to other works [7, 24], the model parameters that would follow the same uncertainty have been grouped to one single uncertain parameter. For instance, the uncertainty on the cost of purchasing renewable electrofuels, $c_{\text{op,electrofuels}}$, identically affects the cost of e-hydrogen, e-methane, e-ammonia and e-methanol. Indeed, besides their respective specificities, each of these fuels will be similarly affected by the variation of cost of electricity or the electrolyser, that drive

the majority of their cost of purchasing [25]. Similarly, the uncertainties impacting the industrial demand, *industry_EUD*, alters equally the industrial high- and low-temperature and electricity demands as well as the non-energy demand.

1.2.2 Polynomial Chaos Expansion

We used Polynomial Chaos Expansion (PCE), an approach for surrogate-assisted Uncertainty Quantification (UQ), to propagate uncertainties in input parameters through the system model. This allowed us to assess statistical moments on the quantity of interest and determine Sobol' indices [26]. To construct a PCE of the EnergyScope Pathway model, we employed the open-source Python framework RHEIA [27, 28]. Where the first part of this section is dedicated to the mathematical definition of this approach, the second details its choice and summarises the comparison made with another approach (i.e. Morris method) in a previous work [24].

Definition

The PCE model (\hat{M}) is a representation of the relationship between the input parameters and the output variable of interest (i.e. results) in the EnergyScope Pathway model (M). This representation is constructed as a truncated series of multivariate orthonormal polynomials Ψ , weighted by coefficients u :

$$\hat{M}(\xi) = \sum_{\alpha \in \mathcal{A}^{d,p}} u_{\alpha} \Psi_{\alpha}(\xi) \approx M(\xi), \quad (1.16)$$

where the vector $\xi = (\xi_1, \xi_2, \dots, \xi_d)$ comprises the independent random input parameters (section B.4), d corresponds to the number of input distributions and α is a multi-index, i.e. a vector of non-negative indices of length d , where each index corresponds to the degree of each univariate polynomial that forms the basis of the multivariate polynomial Ψ_{α} . As uniform distributions are considered, the Legendre polynomials are adopted, as they are the associated family of polynomials that are orthogonal with respect to standard uniform distributions [29].

A truncation scheme is implemented to restrict the number of multivariate polynomials in the series. This is done based on two factors: a specified limiting polynomial order (p) and the number of uncertain parameters (d) involved. The multivariate polynomial order $|\alpha|$ is the summation of the orders for each univariate polynomial in the multivariate polynomials space. Thus, only the multi-indices corresponding to an order that is less than or equal to the specified limiting order are retained and stored in the truncated series denoted as $\mathcal{A}^{d,p}$:

$$\mathcal{A}^{d,p} = \{\alpha \in \mathbb{N}^d : |\alpha| \leq p\}. \quad (1.17)$$

The number of multi-indices satisfying this condition is as the cardinality of \mathcal{A} , i.e. the number of its elements:

$$\text{card}(\mathcal{A}^{d,p}) = \binom{p+d}{p} = \frac{(d+p)!}{d!p!} = P+1. \quad (1.18)$$

The coefficients $(u_0, u_1, \dots, u_{P+1})$ are quantified using a regression method applied to orthonormal polynomials [29]. To ensure a well-posed least-square minimisation, it is recommended to have a number of training samples at least twice the number of coefficients [29]. Therefore, $2(P+1)$ samples are evaluated in the system model, and the model response for each quantity of interest is recorded. To generate the training samples, the quasi-random Sobol' sampling technique is employed [30]. As a low-discrepancy sequence, this technique exhibits the main advantage to investigate efficiently and (almost) uniformly the hypercube of uncertainties, unlike uniformly distributed random numbers.

The process of defining the polynomial degree includes incrementally increasing it until a desired level of accuracy is achieved [27]. Starting with $p = 1$, a PCE is constructed and the leave-one-out (LOO) error is evaluated. If the LOO error is below a specified threshold, the corresponding polynomial order is considered sufficient for generating an accurate PCE. However, if the error exceeds the threshold, the order is increased, and additional samples are generated following the rule of Eq. (1.18).

For the specific study of this work, a polynomial order of 2 is necessary (with 1260 training samples as per Eq. (1.18)) to achieve a LOO error below 1 % for the total transition cost.

Lastly, the statistical moments can be analytically derived from the PCE coefficients, eliminating the need for further model evaluations. The mean μ and standard deviation σ are obtained as follows:

$$\mu = u_0, \quad (1.19)$$

$$\sigma^2 = \sum_{i \neq 0} u_i^2. \quad (1.20)$$

Furthermore, the Sobol' indices can also be determined analytically. The total-order Sobol' indices (S_i^T) assess the overall influence of a stochastic input parameter on the performance indicator, encompassing all possible interactions:

$$S_i^T = \sum_{\alpha \in A_i^T} u_\alpha^2 / \sum_{i=1}^P u_i^2 \quad A_i^T = \{\alpha \in A | \alpha_i > 0\}. \quad (1.21)$$

Here, A denotes the collection of all PCE coefficients, and α_i corresponds to the coefficient associated with the uncertain parameter i .

Comparison with a proven method

Besides being an in-house used method, an early step of this thesis consisted in assessing PCE with similar approach used in the literature [24].

After characterising the uncertainty ranges, Moret et al. [7] quantified the impact of these uncertainties on the snapshot model of EnergyScope, i.e. ranking them, using the Morris method [31]. This method, as a statistical analysis, relies on individually randomized one-factor-at-a-time designs. Given the d model parameters $\vec{\xi} = (\xi_1, \xi_2, \dots, \xi_d)$, the first step of the method consists in generating independent random samples of $\vec{\xi}$ in a standardised and discretised p -level *region of experimentation*, ω . In this *region of experimentation*, each ξ_i , varying in the interval $[\xi_{i,min}, \xi_{i,max}]$, can take a random discrete value as follows :

$$\xi_i = \xi_{i,min} + j \cdot \frac{1}{p-1} (\xi_{i,max} - \xi_{i,min}) \quad \text{with } j \in \{0, 1, \dots, p-1\} \quad (1.22)$$

Then, given these random one-factor-at-a-time samples, Morris method defines, for a given set of $\vec{\xi}$, the elementary effect of the i th parameter (EE_i) as :

$$EE_i = \frac{M(\xi_1, \xi_2, \dots, \xi_i + \Delta, \dots, \xi_d) - M(\vec{\xi})}{\Delta} \quad (1.23)$$

where M is the objective function, $\vec{\xi} \in \omega$, except $\xi_i \leq 1 - \Delta$ and Δ is a set multiple of $1/(p-1) (\xi_{i,max} - \xi_{i,min})$. As in other studies [7, 32, 33], we consider p as even and $\Delta = p/[2(p-1)] (\xi_{i,max} - \xi_{i,min})$.

Finally, in order to evaluate the importance of the i th parameter over an output, Morris method relies on F_i , the distribution of r elementary effects. Computing the mean, $\mu_i = \mu(F_i)$, and the standard deviation, $\sigma_i = \sigma(F_i)$, of the F_i distribution, allows ranking the parameters based on their influence on the concerned output. Usually, in Morris method, p and r respectively get values as follows : $p \in \{4, 6, 8\}$ and $r \in [15; 100]$ depending on, d , the number of uncertain parameters. The higher this number is, the higher shall be, simultaneously, p and r . In the following comparative analysis, we set p and r to their maximum values, respectively 8 and 100 in order to get the most reliable parameters ranking.

Beyond the original Morris method, we used the standardized elementary effects, SEE_i , formulation [32], given by

$$SEE_i = EE_i \cdot \frac{\sigma(\xi_i)}{\sigma(M)}. \quad (1.24)$$

Among other things, the SEE allows comparing the influence of different inputs on the same output or compare the influence of a same parameter on different outputs, even if these parameters or outputs are significantly different in terms of variation range or average amplitude. Moreover, this standardized analysis does not require any additional model evaluations.

Therefore, in the following results, we rather use

$$\mu_i^* = \mu(|SF_i|) \quad (1.25)$$

to rank parameters among each other. In (1.25), SF_i is the distribution formed by the r standardized elementary effects, as done in Moret [33].

In [24], we have assessed the PCE approach, comparing the Top-14 most impacting parameters obtained from this approach with the one provided by the improved Morris method based on μ_i^* . Even if the output of each method does not have the same physical meaning, both methods can rank the parameters by their impact on the total annual cost of the energy system. Both rankings were very similar which validates the use of PCE in the rest of this work.

1.2.3 Preliminary screening and selection

After the initial phase of grouping (Section 1.2.1), a preliminary screening was necessary to identify the key parameters to account for in this GSA. Rixhon et al. [34] performed a similar sensitivity analysis on the 2050 Belgian whole-energy system under different CO₂-limits using the snapshot model, i.e. EnergyScope TD [4]. Screening the results of this work, we have discarded some parameters with negligible impact (e.g. CAPEX of electrolyzers or variation of the freight demand), selected a subset of parameters and added others that were intrinsic to the pathway formulation, e.g. modal share changes, or related to the integration of SMR, $f_{\max, \text{SMR}}$. The exhaustive list of these 34 parameters is presented in Appendix B.4.

1.3 Agent-based reinforcement learning for energy transition support

To navigate through the transition and investigate the efficiency of different policies, this work implements the reinforcement learning approach. This section aims first at presenting the general concepts of this approach as well as the policy optimisation algorithm. Then, the environment, actions, state and reward are detailed.

1.3.1 Reinforcement learning fundamentals and algorithm

At the initial state, i.e. the energy system in 2020, the agent gets an initial observation, o_0 . An observation represents a set of the characteristics of the environment accessible to the agent for it to take the next action. The state, though, is the exhaustive list of these characteristics. Even though an observation is a subset of the state, this work uses these two words interchangeably. Then, it takes an action, a_0 , impacting its environment, i.e. the energy system limited transition over the first decision window (2020-2030). Through this interaction with its environment, the agent is given a reward, $r_1 = r(a_0|o_0)$, and ends up in a new state, i.e. the energy system in 2025, characterised by a new observation, o_1 , and so on (Figure 1.6).

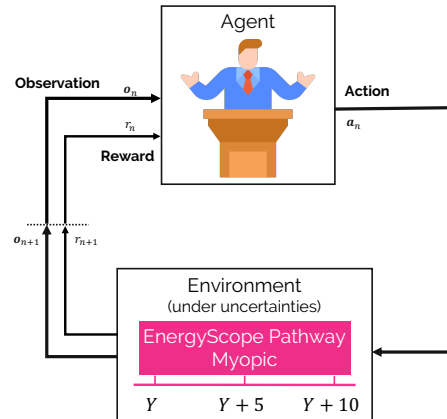


Figure 1.6. reinforcement learning (RL) framework made of the agent interacting with its environment, i.e. the energy-system model on a limited decision window of 10 years.

A learning episode is a succession of such learning steps. In the context of the transition pathway between 2020 and 2050, an episode can come to an end for different reasons. First, if the actions taken by the agent make the optimisation unfeasible, the

episode is prematurely stopped before reaching 2050. Similarly, cumulative emissions of the system over the predefined CO₂-budget (see Section 2.5) lead to an anticipated end of the episode. Finally, the “natural” end is the prescribed end of the transition, i.e. 2050. Consequently, the maximum value of steps for an episode is equal to $N_{ep,max} = 5$.

The goal of a reinforcement learning (RL) approach is to optimise the mapping between inputs (i.e. the observations) and output (i.e. the actions), called the policy $\pi(\mathbf{a}_n|\mathbf{o}_n)$. To do so, an objective function, $J(\pi)$, built on the cumulative rewards collected during each episode. Finally, a back-propagation process updates the weights and biases of the neural network (NN) during the learning of the agent. Among the wide variety of RL algorithms applied in energy systems [35], this work opted for Soft Actor Critic (SAC) [36] to train and update the NN. This algorithm is model-free and off-policy. The former characteristic is necessary as the agent is assumed to have no knowledge about the dynamics of the environment, i.e. its transition or reward functions. The transition function is, given the current state of the environment and the action taken by the agent, a function that outputs a probability to end up to any of the next states. The reward function, on its turn, gives a reward given the current state and the taken action. In practice, in this model-free approach, the agent estimates the optimal policy directly from experience and without estimating the dynamics of the environment. However, model-free methods suffer from two major drawbacks: their sample inefficiency and their brittleness with respect to their hyper-parameters (e.g. learning rates, exploration constants) [36]. The former leads to a too expensive computational burden while the second requires meticulous settings to get good results. SAC overcomes these two challenges as an off-policy (i.e. efficiently re-using past episodes to update the target policy-network) actor-critic deep RL algorithm based on the entropy-augmented objective function:

$$J(\pi) = \mathbb{E}_{\pi} \left[\sum_{n=0}^{N_{ep}} \gamma^n r_n(\mathbf{o}_n, \mathbf{a}_n) - \zeta \log(\pi(\mathbf{a}_n|\mathbf{o}_n)) \right] \quad (1.26)$$

where γ is the discount factor and ζ the temperature parameter. The former determines how much importance we want to give to future rewards within an episode. The latter balances the trade-off between exploitation of proven actions via the return maximisation, i.e. $\sum_{n=0}^{N_{ep}} \gamma^n r_n(\mathbf{o}_n, \mathbf{a}_n)$, and exploration through the entropy¹ term, i.e. $\log(\pi(\mathbf{a}_n|\mathbf{o}_n))$. This way, SAC ensures sample efficiency and low sensitivity to

¹Where entropy represents the amount of energy in a system not available to produce work in thermodynamics, this term stands for the randomness or stochasticity of the policy in the current context.

hyper-parameters while improving exploration [37] and robustness [38]. These make SAC a state-of-the-art algorithm and one of the most efficient model-free deep RL method nowadays. In this work, the authors used the open-source SAC package developed by STABLE-BASELINES3 [39] where the policy NN is a fully connected multilayer perceptron (MLP) built with TENSORFLOW [40]. For further information on RL and the SAC algorithm, the interested reader is invited to refer to the works of Sutton and Barto [41] and Haarnoja et al. [36], respectively.

1.4 Principal Components Analysis

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Chapter 2

Case study: the Belgian energy system

As detailed by Limpens et al. [5], 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 B.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) [42]. 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 [8]. Then, the uncertainty ranges considered for some of the parameters are detailed. Finally, the CO₂-budget over the 2020-2050 transition is presented.

Contributions

First, as pointed out by Rixhon et al. [43], where most of the studies assessing whole-energy system integrate energy demands (i.e. electricity, heat 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*’ [44]. 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. [45], 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 [46].

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 [15]. 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 [47], and especially in Belgium, this thesis has integrated the potential to install SMR from 2040 onward.

Fourth, where previous works considered a prescribed CO₂ trajectory to reach carbon-neutrality by 2050 [5, 15], the case study analysed in this thesis is subject to a CO₂-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 [15]. 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 [46, 48], 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.

2.1 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 [15, 45]. 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 [46]).

2.1.1 Non-energy demand

Where previously published works of Rixhon et al. [43, 49] 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 [50]: (i) HVC (worldwide production of $\sim 365\text{Mt/year}$); (ii) ammonia ($\sim 185\text{Mt/year}$); (iii) methanol ($\sim 100\text{Mt/year}$) 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 ($\sim 80\%$ of global ammonia consumption). Its production is dominated by 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 [51].

The NED currently represents around 20% of the final energy consumption in Belgium [52]. 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, [53]: (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 [50, 51], 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 been 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 [54]. Besides this uncertainty, Belgium stays a major exporter as approximately 2/3 of plastic raw materials produced locally are exported abroad [55]. 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 [53]. 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 ($1.83t_{\text{naphtha}}/t_{\text{HVC}}$ and $1.67t_{\text{LPG}}/t_{\text{HVC}}$) [50], 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 [56] 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 [57]. 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. [58].

2.1.2 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, [58]. Looking at Figure 2.1, 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 2.1, 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 2.1 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 [45]. 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.

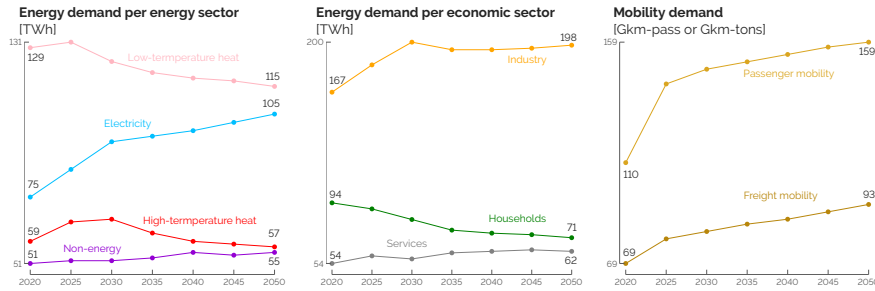


Figure 2.1. EnergyScope splits the whole-energy system end-use demands (EUD) into two sets: (non)-energy and transport-related. This figure presents the nominal values of each of these demands. In the center graph, the non-energy demand has been fully associated with the industrial demand. As detailed 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 [5].

2.2 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. [5]. Figure 2.2 depicts the evolution the respective costs of purchasing. Regarding “renewable electrofuels”, these are in line with the recent study of Genge et al. [59] who carried out an extensive review and “meta-analysis[60, 61] 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 [62]) 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 CO₂ in the atmosphere [63]. In practice, it means that their GWP is assumed to be zero in the model. Regarding specifically these electrofuels, the Hydrogen Import Coalition [25] 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 ($gwp_{op,coal} = 0.40 \text{ kt}_{\text{CO}_2,\text{eq}}/\text{GWh}$), natural gas ($gwp_{op,NG} = 0.27 \text{ kt}_{\text{CO}_2,\text{eq}}/\text{GWh}$) or the fossil-based molecules equivalent to the electrofuels (e.g. $gwp_{op,ammonia} = 0.46 \text{ kt}_{\text{CO}_2,\text{eq}}/\text{GWh}$ or $gwp_{op,methanol} = 0.41 \text{ kt}_{\text{CO}_2,\text{eq}}/\text{GWh}$).

2.3 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. 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

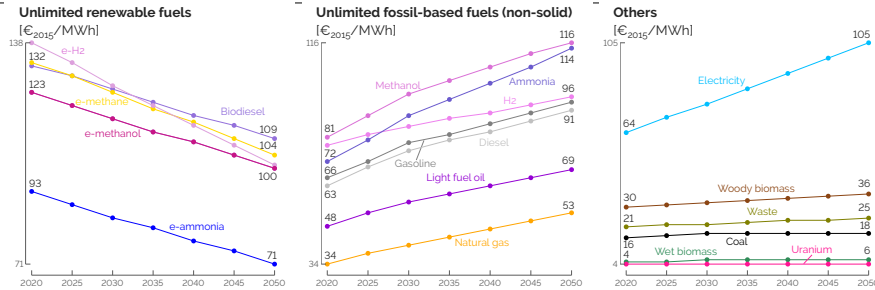


Figure 2.2. Cost of purchasing the different resources. Besides the free local renewables (i.e. sun, wind and hydro) limited by technical potentials, EnergyScope accounts for renewable energy carriers and their respective fossil counterparts (left and center graphs). These fuels can be imported from 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.

grid or the district heating network (DHN) that allow to account 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 [15].

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 [64], a Belgian consortium for energy research, and in line with the Belgian Nuclear Research Centre (SCK-CEN) [65], SMR are implemented with the features listed in Table 2.1. 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 2.3 gives the levelised cost of energy (LCOE) of the principal technologies to produce electricity, based on the computation used by Limpens [15]. Compared to the other flexible generation units, SMR is significantly

Table 2.1. 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.

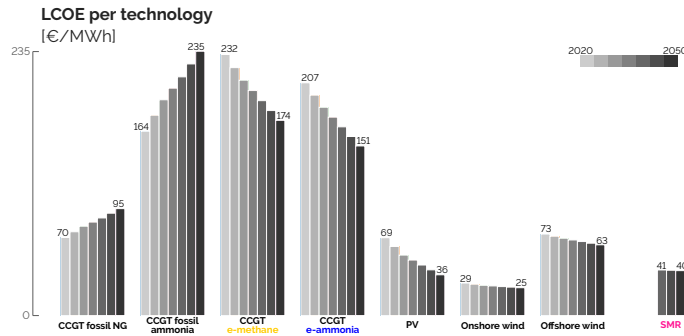


Figure 2.3. Levelised cost of energy (LCOE) for the main technologies in the power sector. Where SMR is cheaper than the other flexible options, CCGT running on e-ammonia is, a priori, cheaper than its e-methane alternative.

Figure 2.4 illustrates the different paths to produce the final molecules of the NED integrated within the model. Similarly to [66], 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 [67]. 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 [45]).

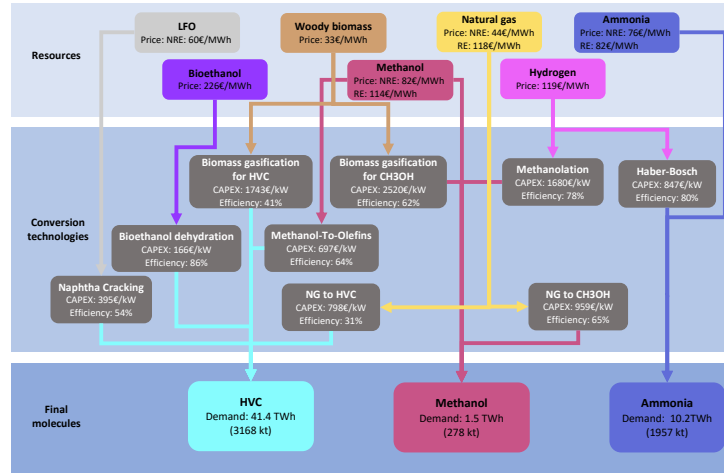


Figure 2.4. Schematic view of the different resources able to produce HVC, ammonia and methanol with their related conversion technologies (including energy efficiency and their CAPEX - in €/kW of final molecules). Values stand for 2035. Graph from [49]

2.4 Uncertainty ranges

Table 2.2 gives the uncertainty ranges of some key parameters. Like other works [21, 22], 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 2.2. As detailed before, the commercial availability of such a technology is uncertain but would not be before

2040. Consequently, for SMR, the parameter $f_{\max, \text{SMR}}$ 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 [64], 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 B.4.

Table 2.2. 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 [64].

Category	Parameter	Meaning	Type ^(a)	Relative variation ^(b)	
				min	max
Cost of purchasing	$c_{\text{op}, \text{fossil}}$	Purchase fossil fuels	II	-64.3%	179.8%
	$c_{\text{op}, \text{electrofuels}}$	Purchase electrofuels	II	-64.3%	179.8%
Investment cost	$c_{\text{inv}, \text{car}}$	CAPEX car	I	-21.6%	25.0%
	$c_{\text{inv}, \text{e_prop}}$	CAPEX electric motor	I	-39.6%	39.6%
	$c_{\text{inv}, \text{fc_prop}}$	CAPEX fuel cell engine	I	-39.6%	39.6%
	$c_{\text{inv}, \text{PV}}$	CAPEX PV	I	-39.6%	39.6%
	$c_{\text{inv}, \text{nuclear_SMR}}$	CAPEX SMR ^(c)	I	-40.0%	44.0%
Consumption	$\eta_{\text{e_prop}}$	Consumption electric vehicles	I	-28.7%	28.7%
Potential installed capacity	$f_{\max, \text{PV}}$	Max capacity PV	I	-24.1%	24.1%
	$f_{\max, \text{windon}}$	Max capacity onshore wind	I	-24.1%	24.1%
Hourly load factor	$c_{\text{p}, \text{t}, \text{PV}}$	Hourly load factor PV	II	-22.1%	22.1%
	$c_{\text{p}, \text{t}, \text{winds}}$	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%
	$\Delta_{\text{change}, \text{freight}}$	Modal share change freight mobility	-	-30%	30%
	$\Delta_{\text{change}, \text{pass}}$	Modal share change passenger mobility	-	-30%	30%
	$f_{\max, \text{SMR}}$	Potential capacity SMR	-	0	1

2.5 CO₂-budget for the transition

In most of the studies carried out on the pathway optimisation of a whole-energy system, a CO₂-trajectory is *a priori* set to reach carbon-neutrality by 2050. Nerini et al. [12] 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. [68] analysed different CO₂-trajectories considering more or less severe water scarcity for the US. Poncelet et al. [2] with LUSYM (Leuven University SYstem Model) and EnergyVille [64] 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. [13] 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 CO₂-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"[69]. This budget (1.2 Gt_{CO₂,eq}) corresponds to the proportion of Belgium's emissions in the world emissions in 2020 (34.8 Gt_{CO₂,eq} [70]) applied to the global budget to have a 66% chance of limiting warming to 1.5°C of 420 Gt_{CO₂,eq} [71]. Therefore, in this work, a limit has been put on $gwp_{lim,trans} = 1.2 \text{ Gt}_{CO_2,eq}$ in Eq. (1.12). 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. [5], this budget represents a 60% reduction of the cumulative emissions over the transition. Appendix B.3 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.

Chapter 3

The atom-molecules dilemma: deterministic and uncertain analyses

Contributions

- Pathway UQ
- Contrast analysis between atom and molecules and local renewables
- Influence of the parameters on the import of molecules and the installation of SMR

Add here references and analyses of nuclear and/or molecules as THE solution
[72]

The model and the frameworks have been introduced in ?? and the case study presented in ?. This section focuses on the results in two ways. First, Section ?? targets the impact of integrating SMR from 2040 onward on the whole-energy system, in a deterministic way (i.e. considering only nominal values of the parameters). Second, accounting for uncertainties as presented in section ??, section ?? will identify the key factors driving higher or lower imports of electrofuels as well as the installation of SMR.

3.1 Deterministic impact of integrating SMR in 2040

In this section, like in the rest of the paper, the **REF** case is without any deployment of SMR anytime during the transition and whereas in the **SMR** case this technology

is available, up to 6 GW, from 2040 onward. After investigating the deployment of SMR through the power sector, the first part of this section focuses on this impact on macro/system-level considerations (i.e. overall transition costs, primary energy mix and yearly emissions per sector). The second part will address the impact of SMR on each of the other sectors of the system.

3.1.1 Power sector

Figure 3.1 shows that SMR is deployed as soon as available, i.e. 2040, to their maximum capacity, i.e. 6 GW, substituting other flexible power generation units: no ammonia-CCGT at the end of the transition and the anticipatory reduction of methane CCGT (i.e. 2.1 GW in 2040 versus 3.7 GW for the REF case). To a lesser extent, the last 2% deployment of solar-PV is slightly delayed as the capacity in 2025 is 1.3 GW smaller than in the REF case. Overall, given the smaller efficiency of SMR, i.e. 40% versus 51% for ammonia-CCGT, the restriction on yearly availability and the slightly higher electrification (Figure 3.2), the total power capacity installed by 2050 is 3.5% higher for the SMR case.

When assessing the electricity production-versus-consumption-balance (Figure 3.2), SMR, as a cheaper, flexible and low-emitting power generation system, produces to its full capacity, given the 15% maintenance off-time assumed in this work: 44.6 TWh. By 2050, it represents 24.6% of the total electricity production which is less than the current share of conventional nuclear in Belgium, 38.5%. This resurgence of nuclear electricity occurs at the expense of other, although more efficient technologies: CCGT and industrial combined heat and power (CHP). Besides the unchanged end-use-demand, we observe a slight increase of the electrification of the rest of the system: +9.4% which corresponds to +5.8 TWh, mostly consumed by electric heaters in industry (+48%) to produce industrial high-temperature heat.

3.1.2 System-level impacts

First of all, as far as the objective function (i.e. the total transition cost) is concerned, Figure 3.3 shows that the 6 GW SMR installed from 2040 allow reaching a 3.3% (-36.9 b€, ~6% of the Belgian GDP) cheaper overall transition. Interestingly, as the model can freely spend the constrained CO₂-budget over the transition, knowing ahead (i.e. perfect foresight) that cheaper and low-emitting SMR will be available in the future, cost-savings, that are more important after 2040, also occur before 2040. This is mostly due to the extended use of cheaper LFO at the beginning of the transition to produce HVC, that is then compensated by the deployment of SMR (Figure 3.3). Then,

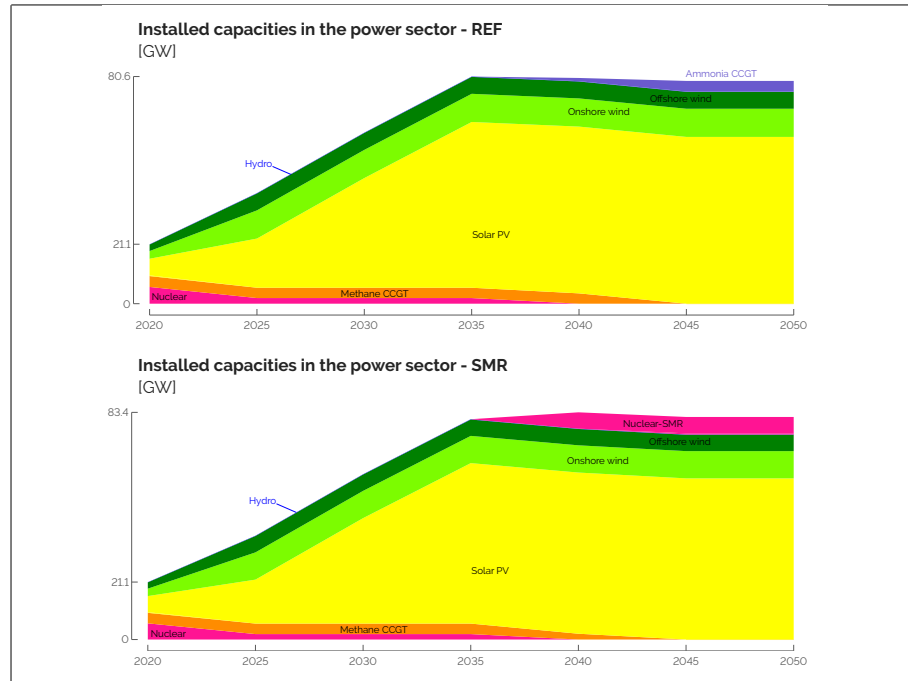


Figure 3.1. As soon as available (i.e. 2040), small modular reactor (SMR) is deployed to their maximum potential (i.e. 6 GW) to substitute more expensive flexible generation units (i.e. gas and ammonia CCGT).

the capital-intensive investments in SMR, mostly recovered by the end of the transition as salvage value, are widely compensated by the smaller resource-related OPEX. This leads, at the end, aggregating the OPEX and the annualised CAPEX, to a system that is yearly 8.8% less expensive by 2050.

Then, considering the primary energy mix shown in Figure 3.4, three phases in the transition can be identified. Before 2040, thanks to the perfect foresight approach, the model finds it more economical in 2025 to keep on using 33.2 TWh of LFO to produce HVC through naphtha/LPG-cracking. In 2040, uranium-driven SMR substitutes the electricity originally produced from industrial CHP and CCGT running respectively on fossil gas and renewable ammonia. Finally, from 2045 onward, the significant drop in the consumption of electrofuels comes from the same industrial CHP. This is the illustration of the atom-molecules dilemma where the consumption of local renewables is, on its side, not much affected. In other words, SMR competes with importing electrofuels while both support the integration of local solar and wind energies. Then, like

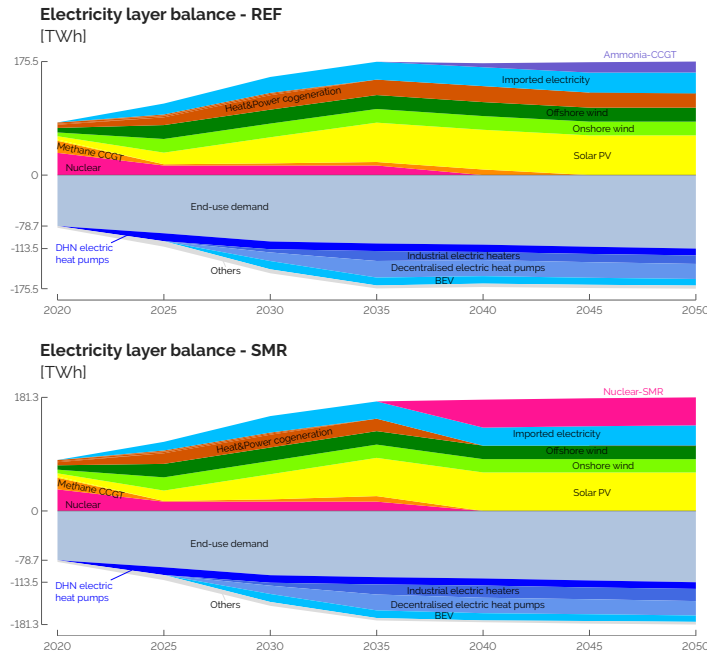


Figure 3.2. The production of electricity from SMR substitutes more efficient technologies (i.e. CCGT and CHP) and boosts the electrification of the rest of the system, mostly the industrial high-temperature heat sector.

the power sector, the SMR case ends up in a less efficient whole-energy system by 2050 at it consumes 47 TWh (+12.7%) primary energy more to supply an unchanged EUD. Interestingly, in both cases, given the assumptions made on the GWP of the resources (i.e. $gwp_{op,electrofuels} = 0 \text{ kt}_{CO_2,eq}/GWh$ and $gwp_{op,uranium} = 0.004 \text{ kt}_{CO_2,eq}/GWh$), the constraint on the CO_2 -budget leads to “carbon-neutrality” by 2050¹.

3.1.3 Non-power sectors

High-temperature heat As aforementioned, the main impact of including SMR from 2040 onward on the high-temperature heat sector is (i) its higher direct electrification and (ii) the reduction of overall more efficient heat-and-power co-generation in the benefit of single-output industrial boilers. On the one hand, in the REF case, industrial electric heaters are mainly used to absorb, instead of curtailing, the “over-production”

¹The model being constrained to keep on using all the waste that would keep on being locally produced, the system in 2050 reaches a $\sim 3.5 \text{ Mt}_{CO_2,eq}/\text{year}$.

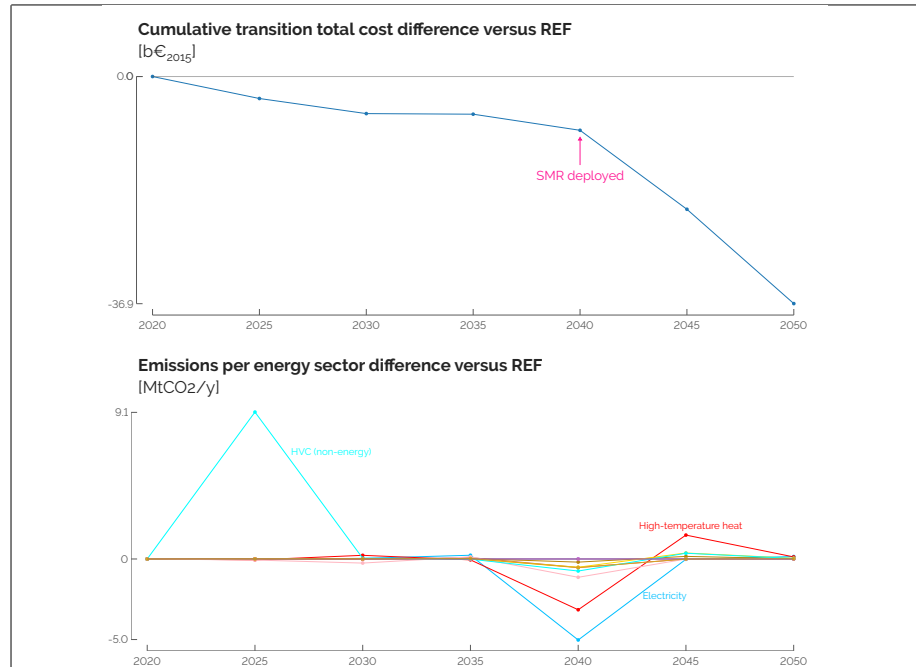


Figure 3.3. (Left) Cumulative transition cost difference between the SMR and the REF cases. Including SMR ends up in a cheaper overall transition (i.e. -3.3%, -36.9 b€). (Right) Emissions per energy sector difference between the SMR and the REF cases. The deployment of SMR from 2040 onward allows maintaining longer the use of light fuel oil (LFO) for the production of high value chemicals (HVC).

of the 59 GW solar-PV when fully deployed, in the sunny days. With SMR, by 2050, an additional 1.7 GW (+13%) of these heaters can rely on a more constant supply of defossilised electricity, consequently increasing their load factor and yearly production respectively by 31% and 48%. On the other hand, given the 44.6 TWh of electricity produced by SMR, cogeneration units are less relevant and, by 2050, 2.6 GW industrial gas boilers completely substitute CHP to produce 16.6 TWh (i.e. 23%) of the total production of high-temperature heat.

Low-temperature heat This sector is marginally impacted. In both cases, the major shift of supply from decentralised to centralised productions operates early in the transition, to hit the constraint that DHN cannot supply more than 37% of the ??-heat production. Then, from a mix between oil (53%), gas (43%) and wood (4%) boilers for the decentralised production of ??-heat in 2020, the system progressively shifts to

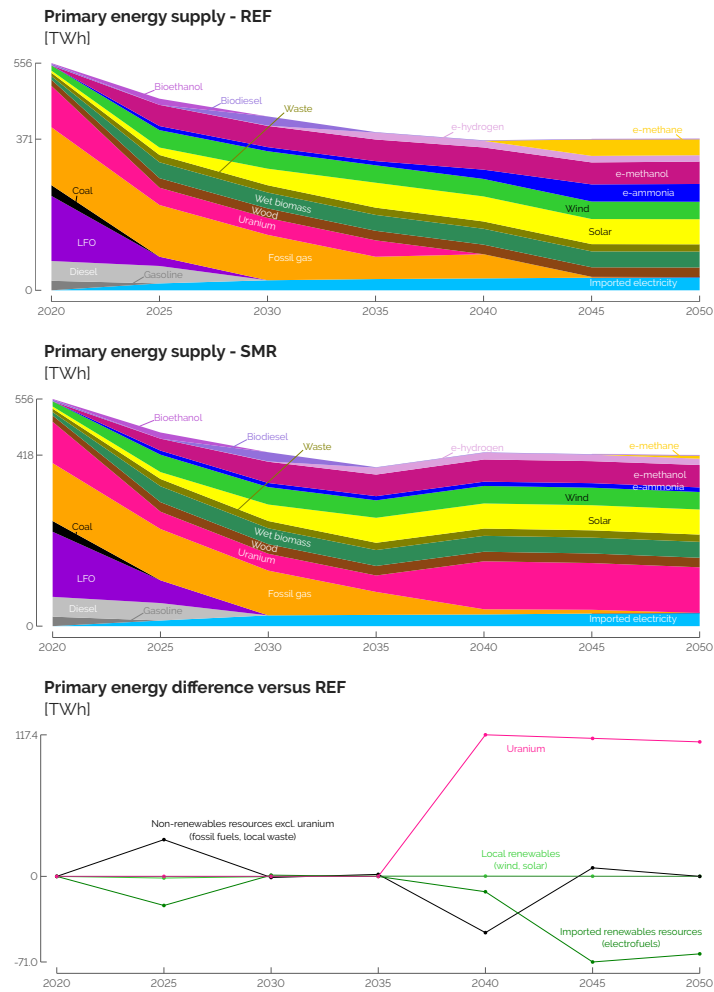


Figure 3.4. (Up) Primary energy mix over the transition for the REF and SMR cases. (Bottom) Difference of the mix between the two cases after aggregation per category. In Uranium, considered as a non-renewable resource in line with Rixhon et al. [63], is nevertheless dissociated from other non-renewable resources for the sake of clarity.

The imported electricity is split between imported non-renewable and renewable resources assuming a linear decrease between the current share of renewables, i.e. 37.41% [?], and an assumed 100%-renewable European electricity mix by 2050.

wards electric heat pump (HP) only. Similarly for the centralised production of ??-heat, electric HP remains the most efficient and economic option.

Mobility The passenger mobility is not affected either as the electrification of the system is preferentially done in this sector with BEV progressively substituting ?? cars for the private sector. About the public mobility, trains and tramways supply their *a priori* set maximum share, respectively, 50% and 30% complemented by ?? buses substituting diesel-driven buses. Similarly, considering the freight transport, technology shifts (i.e. from diesel to fuel cell (FC) trucks) or modal shares (i.e. 53%-47% split between NG and (bio)-diesel boats) are identical between the two cases.

Non-energy demand The supply of ammonia (i.e. from Haber-Bosch to direct import of renewable ammonia) and methanol (i.e. import of renewable methanol) are unchanged between the two cases. However, as introduced previously, to produce HVC, the full substitution of naphtha/LPG-cracking by ?? is delayed as the emissions of the former are compensated by the later integration of SMR.

3.2 Uncertainty quantification on the cost, the atom and the molecules

"It is difficult to make predictions, especially about the future." (Niels Bohr, foundational contributor to the understanding of atomic structure and quantum theory). Besides the deep understanding of the deterministic results, it is important to challenge these conclusions out-of-sample, accounting for the uncertainty of the parameters. To mitigate the computational burden, we have used the PCE approach (??) on the monthly version of EnergyScope Pathway. As detailed by ?], this simplified model does not implement daily storage technologies and integrates much more easily intermittent renewables (PVs and wind turbines) in the system as the daily supply-demand intermittency and mismatch are not at stake. Consequently, it requires less flexibility options (i.e. electrification of the heating sector or import of electricity from the neighbouring countries) and ends up with a cheaper transition (-3%). Although, it allows to quantify the full set of 34 uncertain parameters (i.e. 1260 samples for an order-2 PCE), and avoid the computational burden of the hourly pathway. Nevertheless, comparing the UQ on the hourly pathway with a limited set of uncertain parameters and on the monthly model, Appendix ?? shows that the most impacting parameters are correctly captured by the latter.

After briefly assessing the GSA on the objective function of the model, the total transition cost, this section investigates more deeply the atom-molecules dilemma. This time, the Sobol' indices are computed for import of renewable molecules and installed capacities of SMR.

3.2.1 Total transition cost

Exhaustively listed in Appendix ??, Table 3.1 gathers the most impacting parameters² on the total transition cost, highlighting the cost of purchasing electrofuels as well as the potentiality to install SMR and its CAPEX. The former is the most impacting parameter whereas the two others have much lower influence on the variation of the total transition cost. Given the uncertainty characterisation presented in Section ??, there are 60% chance that no SMR could be installed. In other words, the variation of the parameter $f_{\max, \text{SMR}}$ has zero impact on the variation of the total transition cost in 60% of the samples. Then, in perspective with the local sensitivity analysis of Section ??, the 3.3% reduction has been observed when SMR is installed from 2040 onward. This represents only 10% of the samples. Moreover, given its characteristics detailed in Table 2.1, mostly its cheap and low-emitting fuel (i.e. uranium) and the long lifetime leading to lower annualised CAPEX and higher salvage value, this explains why SMR has this lower impact. On the contrary, more expensive renewable electrofuels are always imported, to a smaller or larger extent depending on the sample. For instance, in the REF case (Section ??), the imported electrofuels represent, by 2050, 152.9 TWh (i.e. 41% of the primary energy mix) with an average 93€/MWh cost of purchasing and, over the entire transition, a 273 b€ cumulative OPEX (i.e. 25% of the total transition cost).

Given the relatively wide uncertainty range (i.e. up to [-30.8%; +24.0%] by 2050) and, above all, the major share among the total demand, between 53% and 60%, the industrial EUD is the second most impacting parameter. Then, as the driving factor for the annualisation and the salvage value of the assets, the interest rate has a 11% Sobol' index³. Finally, similarly to electrofuels, the cost of purchasing fossil fuels is also to consider in the perspective to reduce the uncertainty over the total transition

²Per [?], parameters are considered as "impacting" if their Sobol' index is above the threshold $= 1/d$, d being the total number of uncertain parameters after the pre-selection phase. In this case, $d = 34$, and, consequently, the threshold is equal to 2.9%.

³It is important to note here that the model considers an overall interest rate for the entire system (i.e. 1.5% as a nominal value). In practice, the interest rate would vary depending on the technology investment risk. This variation would have, for instance, a major impact on the LCOE of technologies like nuclear power plants [?], given the important capital needs and long time horizons [?].

Table 3.1. Total Sobol' indices of the uncertain parameters over the total transition cost. Where the cost of purchasing electrofuels is the top-1 parameter, SMR-related parameters have a negligible impact on this cost.

Parameter	Ranking	Sobol' index
Purchase electrofuels	1	47.4%
Industry EUD	2	23.5%
Interest rate	3	11.0%
Purchase fossil fuels	4	6.9%
⋮	⋮	⋮
Potential capacity SMR	11	0.9%
⋮	⋮	⋮
CAPEX SMR	32	<0.1%

cost. However, due to the ambitious CO₂-budget, phasing out of fossil fuels is urgent and makes their uncertain impact smaller than their renewable alternatives.

3.2.2 Atom and molecules

The samples used to carry out the GSA on the total transition cost, also provide the distribution of other outputs of the model. Among them, Figure 3.5 shows the evolution of the import of renewable electrofuels over the transition.

As the general trends are increasing, discrepancies exist between the different energy carriers. E-methane, as the renewable alternative to fossil natural gas, substitutes it, sometimes at a very early stage of the transition, 2025, and to a somehow unrealistically large extent, 173 TWh, which is more than 13% more than the total import of electrofuels in the REF case. The necessity to import this molecule is progressive through the transition to supply mostly industrial CHP and boilers.

E-hydrogen becomes rapidly the main stream of hydrogen in the system, on top of steam-methane-reforming or electrolysis, to reach a median and a maximum values of, respectively 13.6 TWh and 40.7 TWh in 2050. Hydrogen is more frequently used in the mobility sector. Like in the REF case, fuel cell trucks are often the first option but, in some outlying cases, fuel cell cars and buses appear to completely substitute respectively BEV cars and ?? buses by 2050. Moreover, some samples lead to local production of methanol via the methanolation process, to produce up to 16.3 TWh of methanol (i.e. 30% of the total supply of methanol of the nominal REF and SMR cases).

Then, the imported e-ammonia, becoming rapidly cost-competitive against its fossil alternative (Figure 2.2), quickly substitutes it and the Haber-Bosch process. Where

the initial purpose of ammonia is to satisfy a relatively limited non-energy demand (NED) (i.e. 10 ± 3 TWh by 2050), the variation of its import is mostly due to the higher or lower need for ammonia-CCGT as a flexible option to produce electricity. From 2035, out of the four considered electrofuels, the imported e-ammonia is the one exhibiting the largest uncertainty with, for instance, an interquartile range (IQR)⁴ of about 50 TWh. In some extreme cases, e-ammonia is the most imported molecules, i.e. up to 233 TWh or 63% of the total primary mix in the REF case in 2050.

Likewise, e-methanol early becomes the selected option to supply methanol even though alternatives like biomass-to-methanol or synthetic methanolation exist in some outlying cases. Given its lower NED (i.e. 1.5 ± 0.5 TWh_{NED,methanol} by 2050), the variation of imported e-methanol is almost exclusively due to its role in the industrial production of HVC, i.e. 78% of the total NED, through the ?? (??) process. In some rare samples, methanol is also used to supply the freight transport sector via boats or trucks.

Appendix ?? gives a more detailed information. On the one hand, it compares the statistics (i.e. quartiles and median) with the quantity of imported electrofuels in the REF and SMR cases. On the other hand, this appendix shows the distributions of the different sources of supply and consumption of gas, hydrogen, ammonia and methanol.

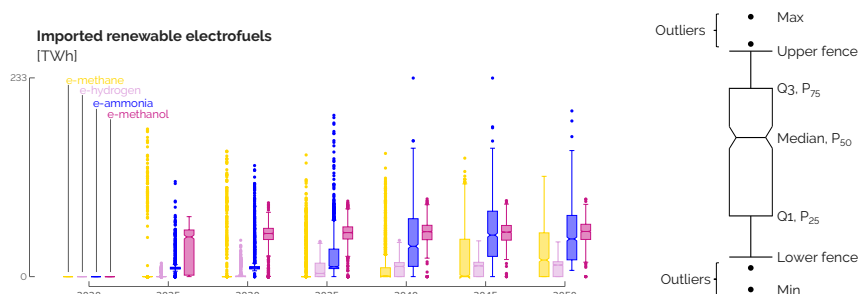


Figure 3.5. Distribution of the imported renewable electrofuels over the transition. Starting from no electrofuel in 2020, their respective import rises progressively along the transition (i.e. increasing median) at different growth rates and with different ranges of values. Observations being either 1.5 times the interquartile range (IQR) less than the first quartile (Q1) or 1.5 times the interquartile range greater than the third quartile (Q3) are defined as outliers.

After investigating the distribution of imports of electrofuels over the transition, this part assesses the space of uncertainties, like ?] who investigated the space of feasibility to reach carbon neutrality in Europe. Figures 3.6 and 3.7 give the trend

⁴The interquartile range is the difference between the third quartile ($Q3$ or P_{75}) and the first ($Q1$ or P_{25}). It is an indicator of statistical dispersion around the median, $Q2$ or P_{50} .

lines of the key parameters for these imports in 2050⁵, as well the installed capacities of SMR. Next to the name of a parameter, one can read its Sobol' index versus the output of interest⁶. Box plots also point out the distribution of this output for the extreme low or high values of some parameters.

As aforementioned, the industrial EUD impacts the most the import of e-methane. This parameter directly dictates the demand of industrial high-temperature heat for which industrial gas CHP, and industrial gas boilers to a lower extent, represent, on average over all the samples, respectively 25.6% and 6.1% of the total production. Then, considering the smaller-impact parameters, we notice that SMR plays a non-negligible role. Indeed, if deployed, SMR produces abundant low-emitting electricity for industrial electric heaters that substitute, even completely in some cases, gas alternatives. This confirms the observation made in Section ?? . Highly available local biomass also leads to smaller import of e-methane to supply bio-hydrolysis and produce methane-equivalent gas. Finally, and surprisingly, costs of purchasing electrofuels and fossil fuels have a positive and negative correlation with the amount of e-methane, respectively. In other words, by 2050, more expensive electrofuels induce to more e-methane import and *vice versa* for the fossil fuels. Given the techno-economic optimum sought by EnergyScope, if electrofuels are more expensive, the system will, overall, import less of them, especially e-ammonia, mainly used by CCGT. Subject to the CO₂-budget for the transition, the system goes towards more efficient technologies, like industrial methane-CHP to substitute e-ammonia-CCGT in the production of electricity. First running on fossil natural gas, these CHP consume more e-methane by 2050. In the contrary, if electrofuels are cheaper, there is more import of them, and especially of e-ammonia. This leaves room for more emitting and cheaper resources to be used while respecting the CO₂-budget, i.e. coal in industrial boilers that produce, in these cases, on average 24% of the high-temperature (HT) heat in 2050. Consequently, there is smaller investment in methane CHP, and consequently import of e-methane as more abundant renewable electricity is produced via e-ammonia-CCGT and more HT-heat is supplied by industrial coal boilers. Even though we might expect that no more coal will be consumed in Belgium by 2050, the model still has the opportunity to use it if the CO₂-budget allows it. About the cost of purchasing fossil fuels, the parameter has mainly an impact on the import of fossil NG as the most versatile energy carrier in the whole-energy system. If NG is more expensive, the system will import less of

⁵The authors picked this specific year as it is the one where electrofuels, if imported, are imported in the largest amount, in general, compared to the other years of the transition.

⁶For these outputs of interest, different from the total transition cost, the LOO error is generally higher than the threshold of 1 % defined in Section ?? . Consequently, the Sobol' indices are less accurate but already allow a fair relative comparison between the different parameters.

it. Subsequently, the investments in methane-CHP and boilers are more limited. This ends up in smaller need for e-methane by 2050.

In relation to e-hydrogen, the sensitivity analysis highlights its dependence on various driving parameters, particularly those linked to the transport sector. As depicted in ?? in Appendix ??, the utilisation of e-hydrogen is most prevalent in FC trucks, followed by FC cars and buses to a lesser extent. The adoption of fuel cell engines in trucks contributes, on average, to 63.5% of the total road freight transport, thereby affecting the level of e-hydrogen imports. Consequently, the smaller is the CAPEX of fuel cell engines, the more the system imports e-hydrogen. Similarly, the cost of purchasing electrofuels influences e-hydrogen imports. Subsequently, the cost of purchasing biofuels emerges as the third most influential parameter. Indeed, biodiesel trucks are the mostly picked alternative to FC trucks to provide, on average, 27.6% of the total. Additionally, ?? buses are preferred in public road transport (34.9%), followed by FC buses (11.2%) competing with biodiesel and hybrid biodiesel buses, accounting for 27.8% and 26.1%, respectively. Finally, the last noticeable parameter at stake is the CAPEX of electric vehicles. In competition with BEV that stand for 83.4% on average of the private mobility sector, the cheaper these cars are, the more cost-competitive are these vehicles, and vice versa, versus FC cars (i.e. 13.7% of the total passenger mobility, on average).

As already pointed out in Section ??, the installation of SMR drastically reduces the import of e-ammonia. As ammonia CCGT is the biggest consumer of ammonia by the end of the transition, low-emitting and cheap electricity flexibly produced by SMR substitutes the CCGT. With a higher cost of purchasing electrofuels, this import of e-ammonia drops down to 7.3 TWh, 83.4% less than in the REF case. Then, with a 9%-Sobol' index, industrial EUD also influences the need for this molecule, due to its NED.

The conclusions are more straightforward for the import of e-methanol and the installed capacity of SMR. For the former, industrial EUD is, by far (i.e. 81% Sobol' index), the key factor. Due to its own NED but, above all, since it is the low-emitting alternative picked by the model to supply the significant NED of HVC, the lower this demand, the lower the need to import e-methanol, and vice versa. For the latter, it is the availability of the technology that drives its installation. Not shown here but all the samples of the GSA highlight that SMR is installed to its maximum capacity, i.e. 6 GW, as soon as possible. In other words, the only parameter "Potential capacity

SMR” dictates the installation of this technology⁷. Surprisingly, the [-40%; +44%] variation of its CAPEX has a negligible impact, with a Sobol’ index of 0.9%.

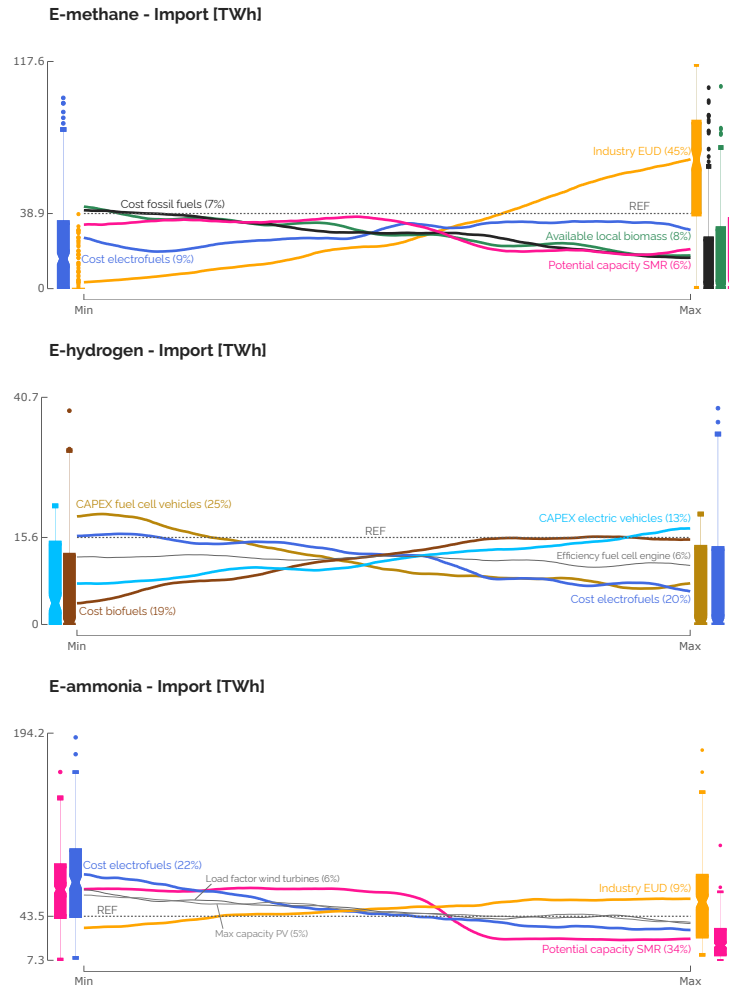


Figure 3.6. Trend lines of the key parameters on the import of e-methane, e-hydrogen and e-ammonia. Around these lines, box plots point out the distribution of the output of interest for the extreme values (either bottom-15% or top-15%) of some parameters. The grey dashed line gives the value of the output of interest in the REF case. Part A

⁷In practice, we observe that as soon as this parameter is equal or higher than 0.9, 0.8 and 0.6, 6 GW SMR is installed from, respectively, 2040, 2045 and 2050.

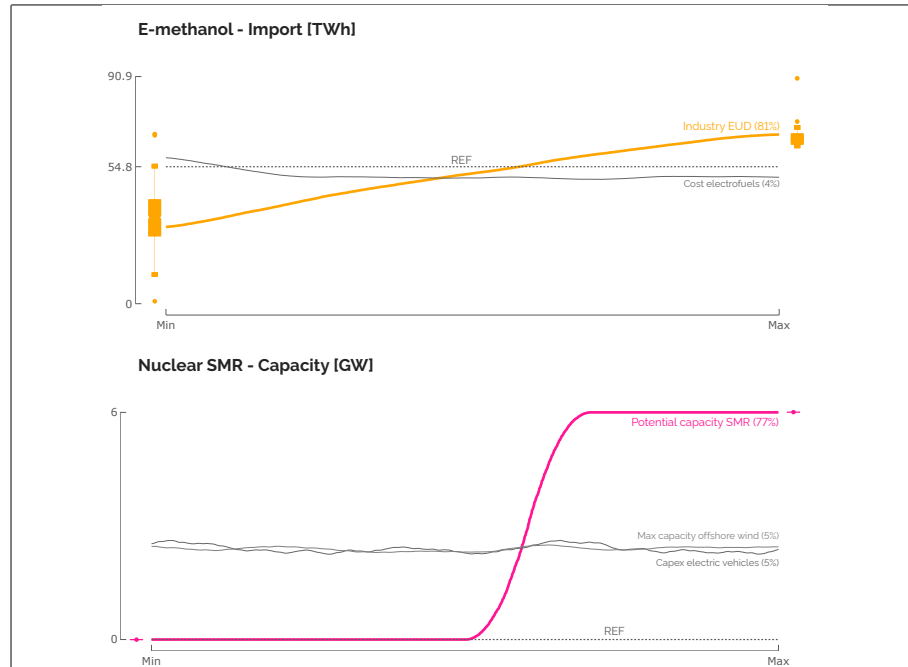


Figure 3.7. Trend lines of the key parameters on the import of e-methanol and the installed capacity of SMR, in 2050. Around these lines, box plots point out the distribution of the output of interest for the extreme values (either bottom-15% or top-15%) of some parameters. The grey dashed line gives the value of the output of interest in the REF case. Part B

3.2.3 Local renewables

In line with results given in Section ??, the GSA shows that SMR has negligible impact on the deployment of local ?? (i.e. PV, onshore and offshore wind turbines). Figure 3.8 gives the evolution of Sobol' indices for the most impacting parameters on the deployment of PV and offshore wind⁸. The key factor that drives the installed capacities of these two technologies is mostly their respective maximum potential, especially at the end of the transition, much more than their CAPEX. Given its higher LCOE (Figure 2.3), PV is more impacted in the short-term by the variation on the cost of purchasing electrofuels supplying e-methane (and e-ammonia to a lesser extent) CCGT. However, this impact gets negligible by 2050.

⁸As the installed capacities of onshore wind is totally driven by the uncertainty on its maximum potential, $f_{\max, \text{windon}}$, it is not represented in the figure.

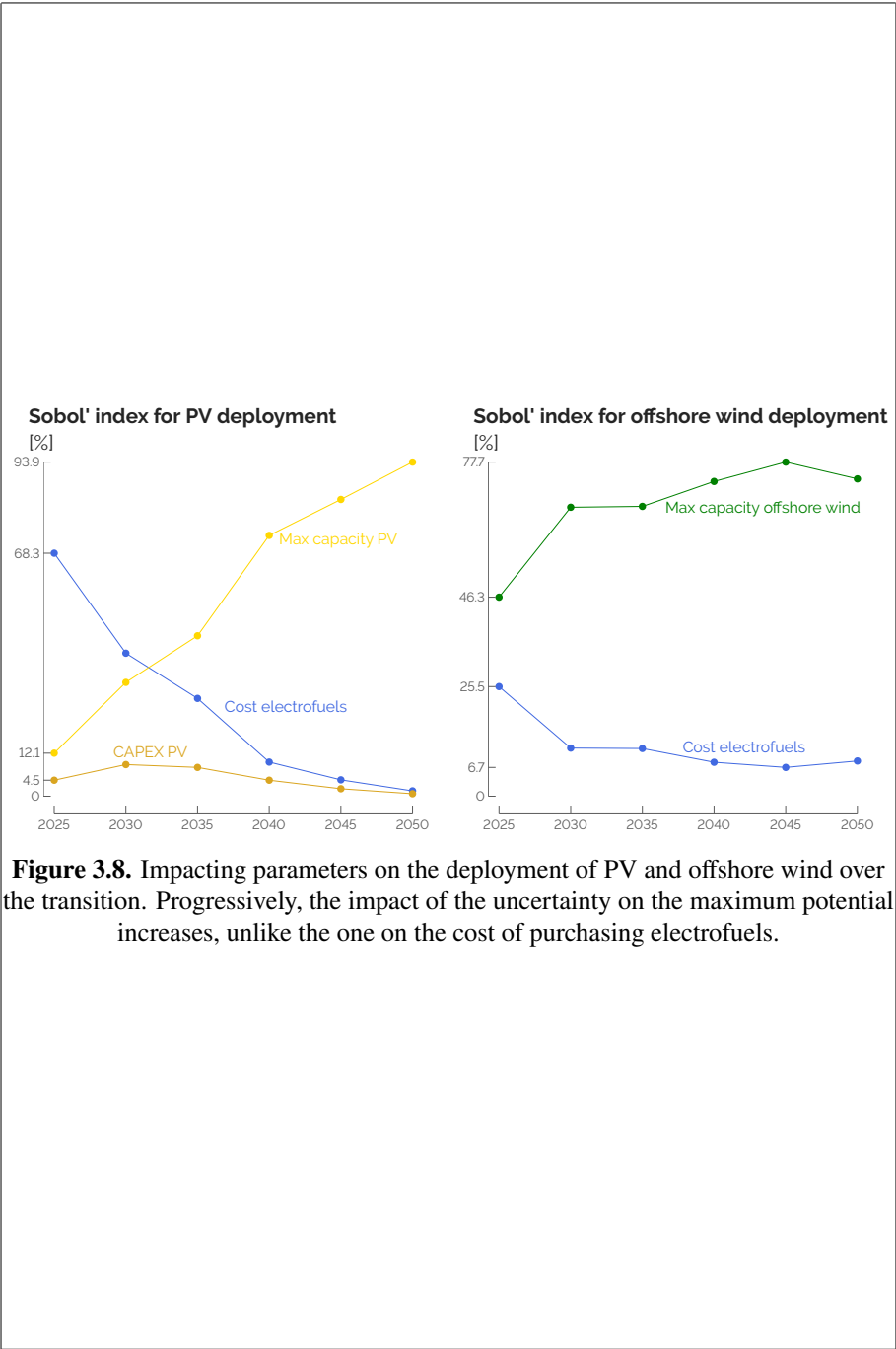
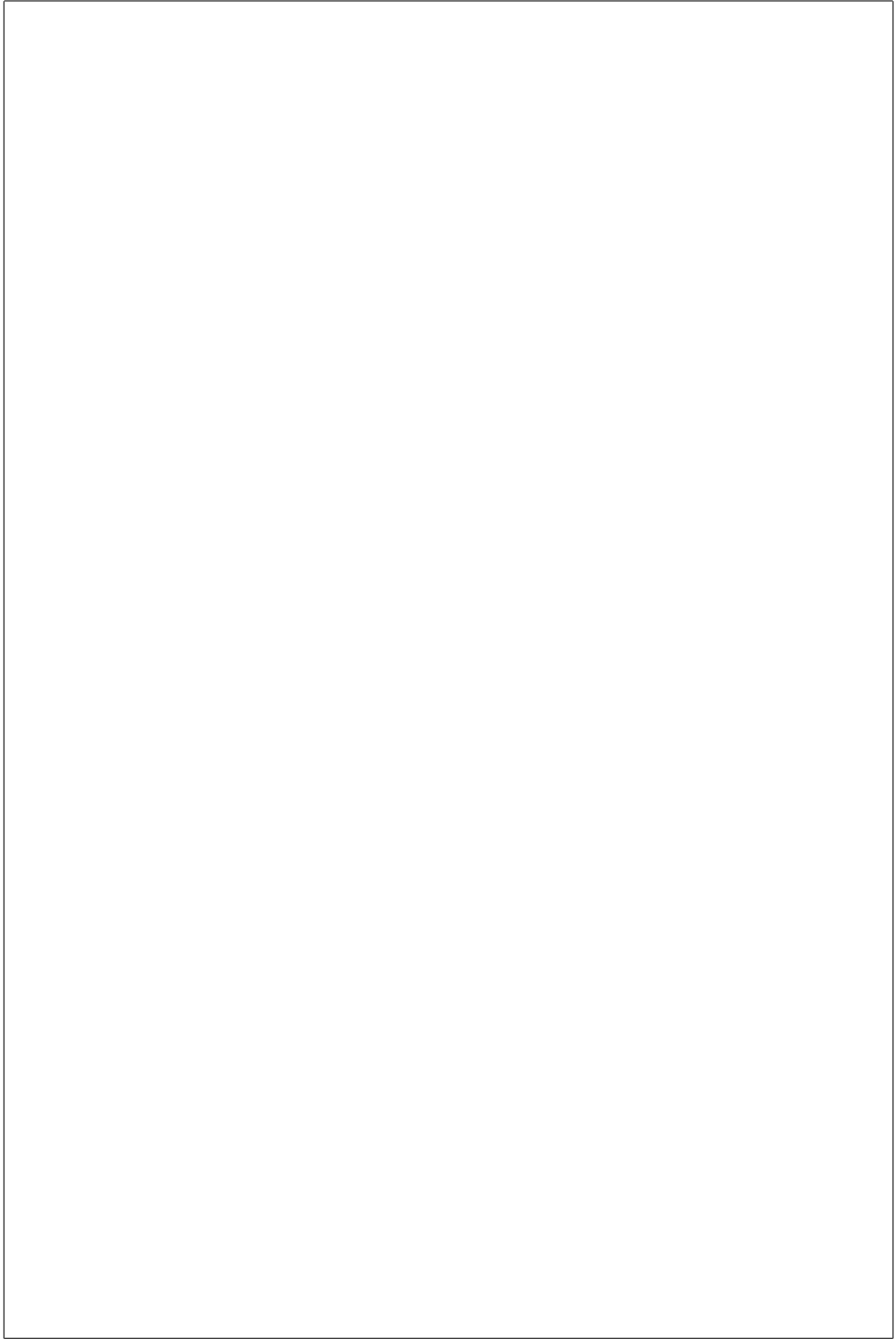


Figure 3.8. Impacting parameters on the deployment of PV and offshore wind over the transition. Progressively, the impact of the uncertainty on the maximum potential increases, unlike the one on the cost of purchasing electrofuels.



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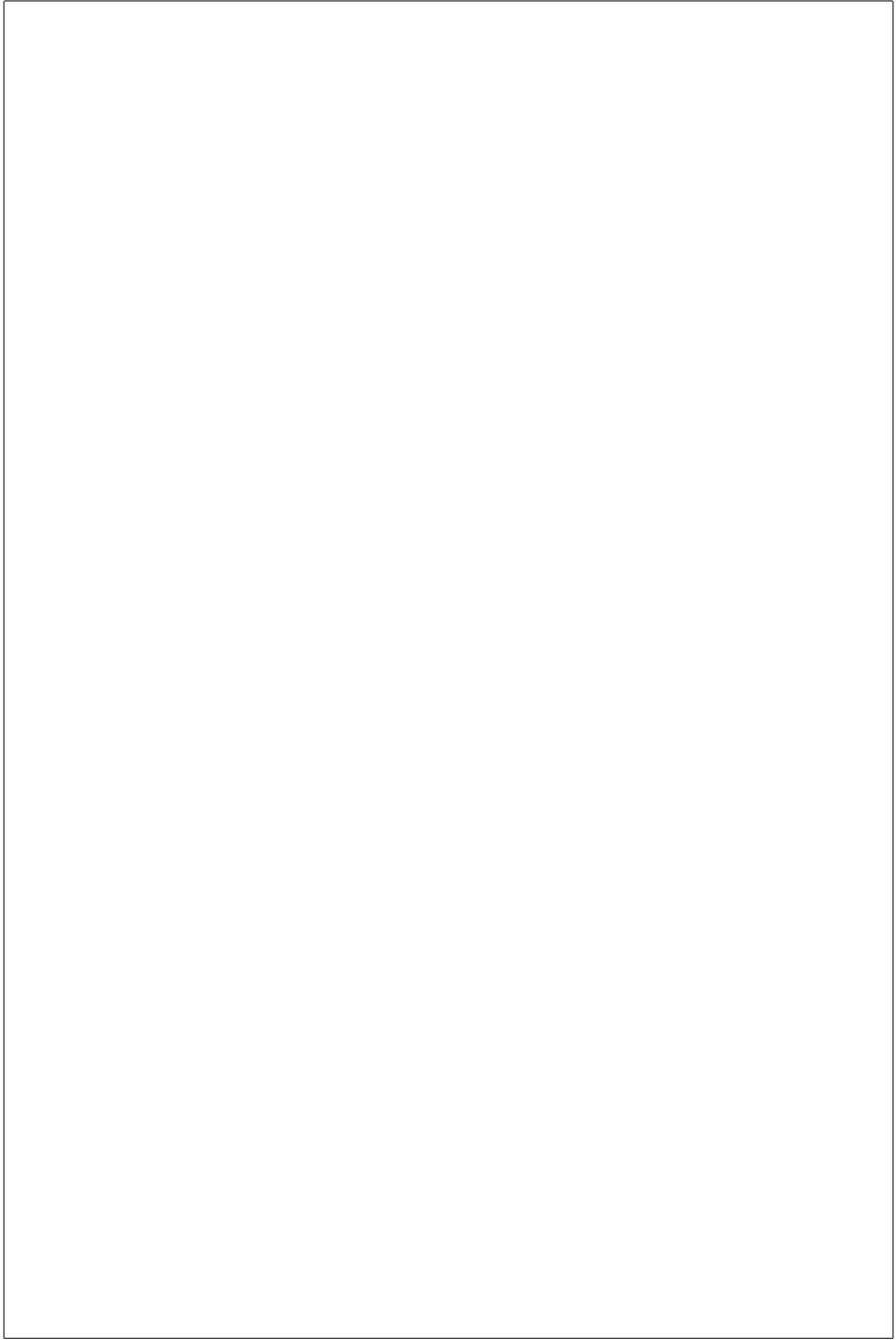
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Appendix A

EnergyScope Pathway: Its choice and its formulation

A.1 EnergyScope Pathway: The right model to choose

Energy system models of varying complexity are valuable tools for guiding policy-makers and projecting future trends. These models enable the exploration of different energy scenarios and the assessment of their consequences based on the underlying assumptions. Specifically, techno-economic models play a crucial role in identifying technically feasible pathways for the energy transition while considering the associated economic costs. These models can be classified based on two key factors: technical resolution and simulation horizon, as illustrated in Figure A.1.

Increasing the technical resolution of energy system models often comes at the expense of a shorter simulation horizon, and vice versa. For instance, day-ahead grid operation models prioritise accurate grid resolution and capacity reserves for uncertainties, but they may not incorporate long-term market trends. Different model classes cater to various needs, with decreasing technical resolution. These include machine-level control, network dispatch, unit commitment, maintenance, power plant expansion, planning for new infrastructure, and scenario analysis. Each class serves a specific purpose, from fine-grained control within a machine to the exploration of multiple assumptions across different scenarios.

In accordance with the previous classification, models aimed at aiding decision-makers in the energy transition primarily fall under the categories of planning and scenario analysis, with a relatively lower technical resolution. Nonetheless, ensuring technical accuracy is of paramount importance to ensure the effective functionality of

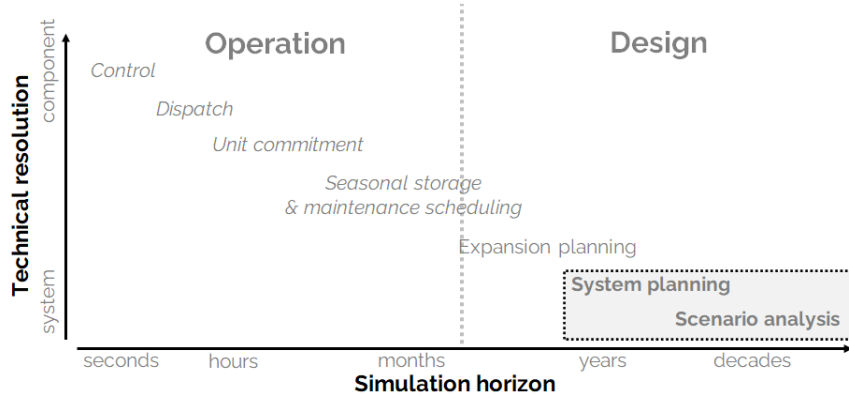


Figure A.1. Model can be classified by their core focus: **Operation** or **Design**.

These categories can be broken down into subcategories. This paper focuses on the system planning and scenario analysis models. Inspired from [73].

future energy systems. Hence, these models should meet the following requirements as a minimum: (i) assessment of intermittent renewable energy integration; (ii) accounting for all energy flows in different sectors, including the measurement of greenhouse gas emissions in the energy sector; (iii) exploration of all available options; (iv) consideration of investments throughout the transition process; and (v) ensuring a reasonable computation time for analysing different trajectories. Additionally, to enhance result reproducibility and user understanding, it is advantageous for such models to: (vi) maintain transparency and preferably be open-source, accompanied by collaborative documentation.

These requirements can be transposed into criteria that a model should match: (i) it should have an hourly resolution spanning a one-year time horizon; (ii) it should encompass the entire energy system, including all types of demands (such as heat, electricity, mobility, and non-energy), as well as all resources, conversion processes, and storage technologies; (iii) it should optimise the system design, accounting for all the options; (iv) it should have a long-term investment horizon, spanning several decades; (v) its computational time should be reasonable, typically less than one hour on a personal laptop; (vi) it should be open-source, with accessible data and comprehensive documentation. These requirements are commonly found in reviews of energy system models. In 2010, Connolly et al. [74] reviewed 68 tools, considering similar criteria: (i-iv) and (vi), along with others such as the number of users and market equilibrium. In 2019, Prina et al. [75] reviewed 12 “most established” models, focusing on criteria

(i-ii) and (iv). This review was followed by a classification where criteria (i-iv) were taken into account [76]. In 2021, Chang et al. [77] conducted a survey-based review of 42 models for energy transition modelling, covering all criteria except computational time. Based on these reviews, Tables A.1 and A.2 compare models based on all the previous criteria except the computational time (v). Indeed, the latter is hard to compare as models are not apply to the same case study and the information is rarely given. The table includes only the models that achieved partially at least four out of the five criteria. We endeavored to refresh the model's information by consulting the model's website and repository, yet there is a possibility that some information might have been overlooked or omitted inadvertently.

Table A.1. Comparison of existing models that partially satisfy at least four of the six criteria (in alphabetical order). Legend: ✓ criterion satisfied; ✓ criterion partially satisfied; ✗ criterion not satisfied. Data from [74–77] (part A)

Model	Ref.	Hourly	Whole-energy	Optimis. invest. & operation	Pathway	Open-source
Calliope	[78, 79]	✓	✓	✓	✗ ^a	✓
COMPOSE	[80]	✓	✓	✓	✓	✓ ^b
DER-CAM	[81, 82]	✓	✓ ^{c,d}	✓	✗ ^e	✓ ^f
DIETER	[83]	✓	✓ ^{d,g}	✓	✗ ^e	✓
E2M2	[84]	✓	✓ ^{c,d,h}	✓	✓	✗ ⁱ
EMPIRE	[85]	✓	✗ ^{c,d,g,h}	✓	✓	✓ ^b
Ener. Trans. Model	[86]	✓	✓	✗ ^j	✓	✓
EnergyPLAN	[87]	✓	✓	✗ ^k	✗ ^l	✓ ^f
energyRt	[88]	✓	✓	✓ ^m	✓	✓
EnergyScope TD	[4]	✓	✓	✓	✗ ^l	✓
Enertile	[89]	✓	✓ ^d	✓	✓	✗ ⁿ

^aTopic is being discussed in the chat of their repository but not yet included in their documentation.

^b'Free under some special conditions'.

^c Transport not accounted.

^d Industry not accounted

^e Not specified but time horizon is 1 year.

^f Freeware.

^g DHN not accounted.

^h individual heating not accounted.

ⁱ Commercially (paid) licensed.

^jThe ETM is a simulation model with a simple merit order 'optimisation' for electricity, flex and heat.

^k Simulation model.

^l Yearly horizon without pathway.

^m EnergyRT optimises investments only.

ⁿ Only for internal use.

From Tables A.1 and A.2, four models almost check all the boxes (partially the pathway one): Calliope, GENeSYS-MOD, PyPSA and TIMES. The TIMES model,

Table A.2. Comparison of existing models that partially satisfy at least four of the six criteria (in alphabetical order). Legend: ✓ criterion satisfied; ✓ criterion partially satisfied; ✗ criterion not satisfied. Data from [74–77] (part B)

Model	Ref.	Hourly	Whole-energy	Optimis. invest. & operation	Pathway	Open-source
ESO-XEL	[90]	✓	✗ ^{a,b,c,d}	✓	✓	✓
GENeSYS-MOD	[91]	✓	✓	✓	✓ ^e	✓
H2RES	[93]	✓	✗ ^f	✓ ^f	✓	✓
iHOGA	[95]	✓	✗ ^{a,b,c,d}	✓ ^g	✓	✓ ^h
IMAKUS	[96]	✓	✓ ^{a,b}	✓	✓	✗ ⁱ
OpenDSS	[97]	✓	✓	✗ ^j	✓	✓
Plexos	[98]	✓	✓ ^k	✓	✓	✗ ⁱ
PyPSA	[100, 101]	✓	✓	✓	✓ ^l	✓
RamsesR	[103]	✓	✓ ^{a,b,d}	✓	✓	✓
ReEDS	[104]	✗ ^m	✓ ^{b,c,d}	✓	✓	✓ ^h
TIMES	[105]	✓	✓	✓	✓	✓ ⁿ

^a Transport not accounted.

^b Industry not accounted

^c DHN not accounted.

^d individual heating not accounted.

^eLöffler et al. [91] applied a pathway transition, but the time resolution was increased to 12h and it uses 3 typical days over a year. Bartholdsen et al. [92] performed a multi-regional pathway (16 nodes) for the case of Germany from 2020 to 2050 with a time step of 5 years. However, the time resolution is 16 time slices representing 4 hours per day and one day per season.

^fIn their review in 2021, Prina et al. [94] classified H2RES as a simulation model on power sector only. In their work, Herc et al. [93] presented a new version of H2RES claiming to optimise the power system and partially represent other sectors. Their study applied the model to a transition pathway for Croatia. In the conclusion, it is claimed ‘H2RES offers practically unlimited potential for functionality expansion since it is an open-source program’ which open the doors for future developments to encompass new features.

^g iHOGA conducts optimisation and simulation without specifying timing or scope.

^h‘Free under some special conditions’.

ⁱ Commercially (paid) licensed.

^j Simulation model.

^kDoes not account for all sectors but allow to implement them according to Waucquez [99].

^lPedersen et al. [102] applied PyPSA to a whole energy system split in 37 nodes. Using a myopic approach, the model optimises the energy transition with a 3-hours resolution).

^mSeasonal time slice.

ⁿModel is now open-source with limited access to data [106].

short for The Integrated MARKAL-EFOM System, is a well-established framework renowned for its capacity to generate comprehensive energy models. It encompasses a rich array of features, including support for multi-cell modeling, pathway analysis, full-scale representation of energy systems, and the consideration of market equilibrium dynamics, all of which facilitate thorough scenario exploration. This model has a widespread adoption and has been utilized by worldwide institutions such as the International Energy Agency (IEA) or technical ones such as VITO (Vlaamse Instelling voor Technologisch Onderzoek) research institute in their research endeavors. Notably, TIMES was reported commercial in 2010 [74]. A more recent survey conducted in 2020-2021 confirmed that the model was using a commercial interface [77]. Recent developments by the IEA-ETSAP have resulted in a version that is compatible with open-source solver CBC. In various studies conducted in different regions, including Canada, Sweden, the EU, and Denmark, TIMES has been shown to utilize 12 to 32 time-slices annually [76]. It is noteworthy that Haydt et al. [107] conducted a study focusing on the electrical sector, using 288 time slices, equivalent to a 12-day time resolution, highlighting the sensitivity of results to time resolution. Regarding data accessibility, while some publications partially present the used dataset, the overall accessibility of TIMES data remains an area of ongoing inquiry [106]. Calliope is a *‘tool that makes it easy to build energy system models’* at different geographical scale. Even if the framework offers the possibility of modelling multi-year systems, we did not find a relevant publication on this topic. In fact, the model is typically employed for scenario analysis with a specific focus on the electricity system. Previous studies have used the model to investigate the phasing out of fossil and nuclear energies in a multi-regional UK power system [108]. More recently, the model has been applied to analyse a scenario of a multi-energy district in Switzerland [109]. Moreover, the model has been used with decades of weather data. However, its application has been limited to assessing the impact of inter-year variability in wind and PV on the results, rather than evaluating a transition pathway [110]. Similarly GENeSYS-MOD presents some limitations. This model is an application of the open-source energy modelling system (OSeMOSYS), itself represented as a model with a poor time discretisation and a heavy computational burden according to [75]. Löffler et al. [91] applied the model to the world by splitting it into 10 regions and most of the energy demand sectors, the time disaggregation being chosen by the user. For their application they used representative years with three days and two time slice per day. Among the open-source models with an active community, PyPSA is one of the best-performing, with a large and active community, development at the state of the art, worldwide applications, and usage not only limited to academia. A study conducted by Bartholdsen et al. [92]

centered on Germany employed a representation comprising 16 time slices for representative years. This choice was substantiated by the work of Welsch et al. [111], which demonstrated that this level of temporal granularity yields consistent results in comparison to hourly time resolution over a year. However, it is noteworthy that the utilization of a limited number of time slices may simplify the optimization of storage technologies, especially those designed for inter-month energy storage. This simplification can be viewed as a pragmatic approach to reduce the computational burden while over-simplifying the challenge of accurately integrating intermittent renewable energy sources. Furthermore, PyPSA, a modeling framework recognized for its robustness and active user community, has also been employed to investigate scenarios related to myopic transitions [102]. Hence, it is worth noting that while Calliope, OS-eMOSYS, PyPSA and TIMES frameworks have the potential to be used for evaluating a transition pathway, we have not come across any publication that explicitly demonstrates their application to such cases with an hourly time resolution over significant time slices.

Hence, it appears that none of the models of Tables A.1 and A.2 fully meet all five criteria outlined in the table, topped with the additional consideration of acceptable computational time. This observation is consistent with the findings presented by Prina et al. [75] who identified two approaches for optimising the energy transition pathway based on the six criteria. The first approach involves running a snapshot model multiple times using an algorithm that optimises the transition path and validates the operability of the system. The second approach aims to extend a snapshot model to represent the entire transition pathway. However, they excluded this option due to the lack of models that met the requirements of being fast enough and easily adaptable. Therefore, they developed a new model based on the first methodology, named EPLANoptTP. It uses a multi-objective evolutionary algorithm to optimise the EnergyPLAN model [87]. To manage computational time, the number of decision variables is limited to three: PV, wind turbine and battery capacities. Thus, the model does not investigate all the options (i.e. criteria (iii)).

For the aforementioned reasons, the current work opted for EnergyScope Pathway, an extension of the open-source and documented EnergyScope TD model [4] listed in Tables A.1 and A.2. The latter has an horizon time of one year and does not account for the pathway from an existing energy system to a long-term target. The pathway version extends the time horizon to decades and accounts for the pathway transition from an existing energy system to a long term target. The computational time is kept low (i.e. around a 15 minutes on a personal laptop), mostly due to keeping the linear formulation after extending the snapshot model. Limpens et al. [5] provides more detailed insights

into the modeling choices made during methodological development. In the spirit of the EnergyScope project, the code is fully open-source (under the License Apache 2.0, see repo [112]) with a collaborative documentation [8]. Compared to existing models, EnergyScope Pathway introduces a rapid computational optimisation tool for exploring diverse transition pathways within an entire energy system while maintaining high temporal precision to accurately capture the integration of intermittent renewables. To the best of our knowledge, there are potentially frameworks that could be extended to similar capabilities, but their computational time for similar case study have not been found.

A.2 EnergyScope Pathway and its linear formulation

EnergyScope Pathway is the extension of EnergyScope TD [4] that follows the snapshot approach [113], consisting in optimising the system in a target future year. The objective of this section is to present the fundamental variables and constraints of the latter based on which the former was developed. There have been formulation choices to be made but they are not discussed in the current manuscript. However, the interested reader is invited to refer to the Appendix B of [5] for further information in this regard.

A.2.1 The starting point: a scenario analysis model

Overview of the snapshot model

EnergyScope TD [4] is a model that optimises both the investment and operating strategy of a 'whole'-energy system, encompassing electricity, heating, mobility, and non-energy sectors. According to Contino et al. [114], a model qualifies as a 'whole-energy' system when it considers all energy sectors, including the non-energy demand such as the production of plastics and other materials using feedstocks that are also considered as energy carriers, with the same level of detail.

The model's hourly resolution over a year makes it well-suited for integrating intermittent renewables. Its formulation incorporates typical days and a reconstruction method that captures different time scales from the hour to the season while accounting for the inter-weeks patterns of wind. This approach minimally affects the design while significantly reducing computational time [115]. The model investigates all the possibilities by optimising the investment decisions and hourly operations over a year, with a computational time of less than a minute on a personal laptop. This charac-

teristic was intentionally incorporated into the model design to facilitate uncertainty quantification and other studies that require numerous iterations [34].

EnergyScope TD has been successfully applied to various national energy systems, including Switzerland [4, 116], Belgium [45], Italy [117], and other European countries [42]. Furthermore, it has been extended to a multi-region energy system model [115], coupled with other energy models [118], or employed to focus on specific sectors such as the power networks of electricity, gas, and hydrogen [119].

Formulation of the snapshot model

The conceptual structure of the model is illustrated in Figure A.2: given the end-use energy demand, the efficiency and cost of energy conversion technologies, the availability and cost of energy resources, the model identifies the optimal investment and hourly operation strategies to meet the demand and minimise the total annual cost or greenhouse gas emissions of the energy system. Typically, the two objectives are integrated by placing a limit on emissions while simultaneously striving to minimize costs.

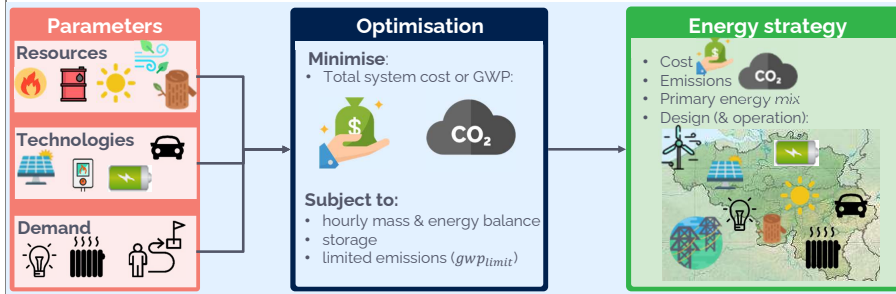


Figure A.2. EnergyScope TD model is a flow model with inputs (Parameters), an optimizing model (Optimisation) and results (Energy strategy). The image illustrates what is included (non-exhaustively).

Linear formulation

The following section illustrates, non-exhaustively, the original EnergyScope TD model. The objective function, cost and GHG formulation will be detailed. The rest of the formulation is detailed and available in previous works [15]. This work uses the following nomenclature: SETs are in capital letters, **Variables** are in bold and with first letter capital, and *parameters* are in italic.

$$\min \mathbf{C}_{\text{tot}} = \sum_{j \in \text{TECH}} \left(\tau(j) \mathbf{C}_{\text{inv}}(j) + \mathbf{C}_{\text{maint}}(j) \right) + \sum_{i \in \text{RES}} \mathbf{C}_{\text{op}}(i) \quad (\text{A.1})$$

$$\text{s.t. } \tau(j) = \frac{i_{\text{rate}}(i_{\text{rate}} + 1)^{\text{lifetime}(j)}}{(i_{\text{rate}} + 1)^{\text{lifetime}(j)} - 1} \quad \forall j \in \text{TECH} \quad (\text{A.2})$$

$$\mathbf{C}_{\text{inv}}(j) = c_{\text{inv}}(j) \mathbf{F}(j) \quad \forall j \in \text{TECH} \quad (\text{A.3})$$

$$\mathbf{C}_{\text{maint}}(j) = c_{\text{maint}}(j) \mathbf{F}(j) \quad \forall j \in \text{TECH} \quad (\text{A.4})$$

$$\mathbf{C}_{\text{op}}(i) = \sum_{t \in T} c_{\text{op}}(i) \mathbf{F}_t(i, t) t_{\text{op}}(t) \quad \forall i \in \text{RES} \quad (\text{A.5})$$

The objective, Eq. (A.1), is the minimisation of the total annual cost of the energy system (\mathbf{C}_{tot}), defined as the sum of the annualised investment cost of the technologies ($\tau \cdot \mathbf{C}_{\text{inv}}$), the operating and maintenance costs of the technologies ($\mathbf{C}_{\text{maint}}$) and the operating cost of the resources (\mathbf{C}_{op}). The annualised factor τ is computed *a priori* based on the interest rate (i_{rate}) and the technology lifetime, (*lifetime*), Eq. (A.2). The total investment cost (\mathbf{C}_{inv}) of each technology results from the multiplication of its specific investment cost (c_{inv}) and its installed capacity (\mathbf{F}), see Eq. (A.3). The installed capacity is defined with respect to the main end-uses output type, such as electricity for PV or heat for a boiler. The total operation and maintenance costs are calculated in the same way, Eq. (A.4). The total cost of the resources is calculated as the sum of the end-use over different periods multiplied by the period duration (t_{op}) and the specific cost of the resources (c_{op}), Eq. (A.5). To simplify the reading, we write the sum over typical days as $t \in T$ such as in Eq. (A.5) and following equations. The period T represents the sequence of hours and typical days over a year (8760h)¹. The full formulation is detailed in [4] or in the documentation [120].

$$\mathbf{GWP}_{\text{tot}} = \sum_{i \in \text{RES}} \mathbf{GWP}_{\text{op}}(i) \quad (\text{A.6})$$

$$\mathbf{GWP}_{\text{op}}(i) = \sum_{t \in T} gwp_{\text{op}}(i) \mathbf{F}_t(i, t) t_{\text{op}}(t) \quad \forall i \in \text{RES} \quad (\text{A.7})$$

The global annual GHG emissions are calculated using a LCA approach, i.e. taking into account emissions of the resources ‘*from cradle to use*’. It is based on the indicator ‘*GWP100a-IPCC2013*’ developed by the intergovernmental panel for climate change (IPCC) [121]. For climate change, the natural choice as indicator is the global warming potential, expressed in ktCO₂-eq./year. In Eq. (A.6), the total yearly emissions of the system ($\mathbf{GWP}_{\text{tot}}$) are defined as the emissions related to resources (\mathbf{GWP}_{op}). The total emissions of the resources are the emissions associated to fuels (from cradle

¹The exception is storage level which is optimised over the 365 days of the year instead of typical days.

to combustion) and imports of electricity (gwp_{op}) multiplied by the period duration (t_{op}), Eq. (A.7). Thus, this version accounts only for operation without accounting for the GWP emitted during the construction of the technologies. This makes the results comparable with metrics used in the reports by the European Commission and the International Energy Agency (IEA).

The above equations (Eqs. (A.1) - (A.7)) represent only a part of the formulation and illustrate the syntax that is used. Those representing the energy balance, network implementation, sectors representation, etc. are not presented in this work but are detailed in the latest version of the model, see [15] and on the documentation [120].

Finally, energy storage has two dimensions to be optimised: the stored energy quantity (also referred to as 'storage level') and the hourly power flow, encompassing both charging and discharging. EnergyScope TD optimises the hourly charge and discharge operations based on the hourly resolution of the typical days. In contrast, the optimisation of stored energy is conducted over the entire span of 8760 hours in a year. This formulation allows for the effective integration of a wide range of energy storage technologies, spanning short-term solutions like small thermal storage units and daily-use batteries, to longer-term options such as hydro-dam storage for seasonal storage, and even large-scale thermal storage for intra-week patterns. A previous study delved into the roles of various storage technologies, considering their sectoral applications and temporal aspects, within the context of the Swiss energy system [116].

A.2.2 Extending the model for pathway optimisation

In this section, we delve into the extension of EnergyScope TD from a static yearly snapshot model to a comprehensive pathway model. While snapshot models provide insights into the energy system for individual years, they lack the capacity to capture the dynamics inherent in investment strategies throughout a transition period. The proposed approach involves segmenting the transition into five-year intervals, during which the energy system is optimized for one specific year. This approach results in seven instances of EnergyScope TD – called representative years – spanning the 30-year transition period, covering the years from 2020 to 2050. To bridge these representative years, we introduce additional constraints that capture the investments changes between consecutive periods, accounting for societal inertia and evaluating both the cost implications and emissions of the transition. Overall, these constraints are integrated into a linear framework, ensuring computational efficiency, with an approximate computational time of 14 minutes on a personal laptop (2.4 GHz Intel Core i5 quad-core).

Figure A.3 illustrates the pathway concept. Simplification and choices were necessary to implement linearly the problem while keeping a tractable computational time. In this section, we present the formulation retained.

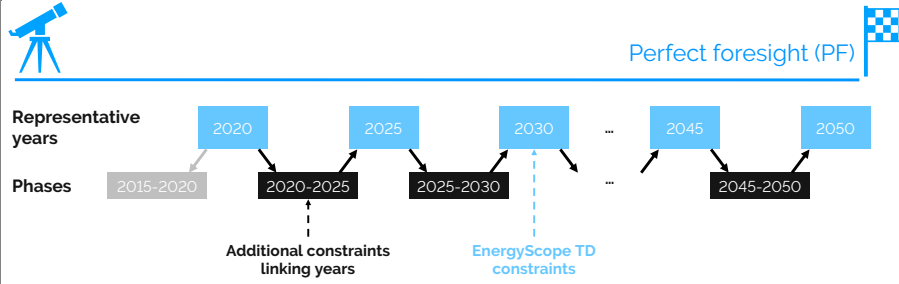


Figure A.3. The pathway methodology relies on 7 representative years (blue boxes) where the model EnergyScope TD is applied. Moreover, the formulation accounts for linking constraints (black boxes) and an initial condition (grey box). The overall problem is the pathway model.

The proposed formulation relies on representative years, selected every 5 years from 2020 to 2050. The period between two of them is called ‘*PHASE*’. For each of these 7 representative years, the EnergyScope TD model is run using the relevant data (such as energy demand, technology costs or GHG emissions constraints).

As a consequence, a new dimension ‘*year*’ is added to all **Variables** and parameters, except the interest rate (i_{rate}) assumed constant during the transition. This new dimension is necessary to represent the changes of technology and resource characteristics over the representative years. As an example, the investment cost (c_{inv}) of a solar photovoltaic panels could drastically vary in the next decades (e.g. data used ranges between 1220 to 870 [$\text{€}_{2015}/\text{kW}$] between 2020 and 2035).

Linking years

At this stage, all years are independent. In the following, we introduce new constraints to link representative years. The formulation allows to install new capacity (\mathbf{F}_{new}), remove a capacity that has reached its lifespan (\mathbf{F}_{old}) or decommission a technology prematurely (\mathbf{F}_{decom}). These capacity changes occur during a phase, this implies that there is no capacity change during a representative year. Figure A.4 illustrates the concept.

$$\mathbf{F}(y_{stop}, i) = \mathbf{F}(y_{start}, i) + \mathbf{F}_{new}(p, i) - \mathbf{F}_{old}(p, i) - \sum_{p \in PHASE \cup \{2015_2020\}} \mathbf{F}_{decom}(p, p2, i)$$

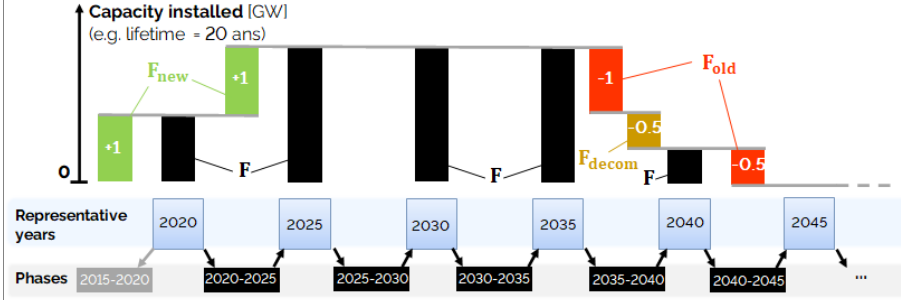


Figure A.4. Example of how the technologies capacity and associated variables are evolving. The example uses a technology with a 20 years lifetime. Initially 1 GW of capacity exists (F_{new} during phase 2015_2020). Then another 1 GW is deployed (F_{new} during phase 2020_2025). 15 years later, a part of the capacity reaches its lifetime limit and is removed (F_{old} phase 2035_2040). Moreover, during the latter phase, additional capacity is decommissioned prematurely (F_{decom}). Finally, the technology reaches its expected lifetime and is fully withdrawn (F_{old}).

$$\forall p \in PHASE, y_{stop} \in Y_{STOP}(p), y_{start} \in Y_{START}(p), i \in TECH \quad (A.8)$$

Similarly to a mass balance, Eq. (A.8) is the technology capacity balance. The constraint forces the installation or withdrawing of capacities between two representative years: at the end of the phase (y_{stop}), the available capacity is the one used in the next representative year ($F(y_{stop})$). This capacity is equal to the one available in the previous representative year ($F(y_{start})$) plus the new installed capacity (F_{new}) minus the capacity that has reached its lifetime (F_{old}) minus the early decommissioned capacity (F_{decom}). One notices that the capacity available for each representative year depends on a year (y_{start} or y_{stop}), while the other capacity changes depend on a phase (p or $p2$). Moreover, the decommissioning term depends on another phase, which is the one when the technology decommissioned has been built. As an illustration, Figure A.4 gives an example where 0.5 GW of a capacity built in 2015_2020 is decommissioned in 2030_2035 ($F_{decom}(2030_2035, 2015_2020, i)$).

$$F_{decom}(p, p2, i) = 0$$

$$\forall i \in TECH, p \in PHASE, p2 \in PHASE \cup \{2015_2020\} | decom_{allowed}(p, p2) = 0 \quad (A.9)$$

$$\begin{aligned}
\mathbf{F}_{\text{old}}(p, i) = & \text{if}(age = \text{ } \text{STILL_IN_USE}') \text{ then } 0 \\
& \text{else } \left(\mathbf{F}_{\text{new}}(age, i) - \sum_{p2 \in PHASE} \mathbf{F}_{\text{decom}}(p2, age, i) \right) \\
& \forall p \in PHASE, \forall j \in TECH | age \in AGE(p, j) \quad (\text{A.10})
\end{aligned}$$

In linear programming, a solution might be mathematically correct, while not making sense in practice. As an example, a technology could be decommissioned before being built ($p < p_{\text{built}}$). Eqs. (A.9-A.10) allow preventing these non-sense while keeping the formulation linear. Eq. (A.9) forces the decommissioned capacity to zero when technology will be built after. To do so, a parameter ($decom_{\text{allowed}}$) is defined *a priori* and is equal to 0 or 1 when decommissioning is not possible or possible, respectively. Eq. (A.10) defines the capacity reaching its lifetime limit at a certain phase, the concept is illustrated in Figure A.4. For each phase, a set (AGE) is calculated *a priori*. It relates, for a given phase and technology, when the technology should have been built. In the case the technology has already reached its lifetime limit, the set (AGE) returns the phase when the technology has been built. The first part of Eq. (A.10) indicates that the technology is still available, and thus no capacity needs to be removed. The second part of the equation represents the capacity that reached its expected lifetime minus a part of the capacity that would have been decommissioned. As an example, Figure A.4 shows a 20 years lifetime technology with 1 GW of capacity installed before 2020. One will highlight the use of a ‘if’ in Eq. (A.10), this formulation is linear as the if is applied to a parameter and not a variable.

$$\mathbf{F}_{\text{new}}(2015_2020, i) = \mathbf{F}(\text{YEAR_2020}, i) \quad \forall i \in TECH \quad (\text{A.11})$$

To initialise the problem in 2020 with the existing design, an additional phase ‘2015_2020’ is created. Eq. (A.11) requires that the capacity used in 2020 is installed in the previous phase.

Society inertia

To avoid unrealistically fast changes in the system, additional constraints are needed during the phases for the mobility and low temperature heat sectors. Without the following constraints, the model would eliminate certain technologies in one phase, such as oil and gas decentralised boilers. Even if this result is mathematically and physically correct, (i.e. fuels are expensive and investing in more efficient technology is economically and environmentally more profitable), this swap of technology cannot occur in one phase (i.e. 5 years). Indeed, society inertia to change, available manpower, supply chains and manufacturers limit the change.

$$\Delta_{\text{change}}(p, i) \geq \sum_{t \in T} (F_t(y_{\text{start}}, i, t)) - \sum_{t \in T} (F_t(y_{\text{stop}}, i, t))$$

$$\forall j \in \text{TECH}, p \in \text{PHASE}, y_{\text{start}} \in Y_{\text{START}}(p), y_{\text{stop}} \in Y_{\text{STOP}}(p) \quad (\text{A.12})$$

$$\sum_{i \in \text{TECH}(\text{HeatLowT})} \Delta_{\text{change}}(p, i) \leq \lim_{LT, \text{ren}} \cdot (eui(y_{\text{start}}, \text{HotWater}) + eui(y_{\text{start}}, \text{SpaceHeat}))$$

$$\forall p \in \text{PHASE}, y_{\text{start}} \in Y_{\text{START}}(p) \quad (\text{A.13})$$

$$\sum_{i \in \text{TECH}(\text{MobPass})} \Delta_{\text{change}}(p, i) \leq \lim_{\text{MobPass}} \cdot eui(y_{\text{start}}, \text{MobPass})$$

$$\forall p \in \text{PHASE}, y_{\text{start}} \in Y_{\text{START}}(p) \quad (\text{A.14})$$

$$\sum_{i \in \text{TECH}(\text{MobFreight})} \Delta_{\text{change}}(p, i) \leq \lim_{\text{MobFreight}} \cdot eui(y_{\text{start}}, \text{MobFreight})$$

$$\forall p \in \text{PHASE}, y_{\text{start}} \in Y_{\text{START}}(p) \quad (\text{A.15})$$

Eq. (A.12) calculates the upper limit of change (Δ_{change}) in terms of supplied demand instead of installed capacity. Based on this quantification, the amount of change per phase is limited for low temperature heat ($\lim_{LT, \text{ren}}$), Eq. (A.13), passenger mobility (\lim_{MobPass}), Eq. (A.14) and freight mobility ($\lim_{\text{MobFreight}}$), Eq. (A.15). For instance, if the maximum allowable variation in supplied low temperature heat is set at 25%, it would restrict the technology-related changes in low temperature heat to 25% within a given phase. Consequently, if a technology supplies more than 25% of the low temperature heat, it would require multiple phases to replace it with a different technology.

Cost and emissions of the transition

To optimise the energy system, two key metrics must be adapted: the transition cost and the total global warming potential (GWP). Concerning the first one, all costs are expressed in €_{2015} and an annualisation factor is used to distinguish investments over the transition. For the GWP, the metric used is based on the contributions of the gases over 100 years. It is assumed that the impact of emitting at the beginning or the end of transition are equivalent and thus no annualisation is used.

$$\min C_{\text{tot,trans}} = C_{\text{tot,capex}} + C_{\text{tot,opex}} \quad (\text{A.16})$$

$$C_{\text{tot,capex}} = \sum_{p \in \text{PHASE} \cup \{2015_2020\}} C_{\text{inv,phase}}(p) - \sum_{i \in \text{TECH}} C_{\text{inv,return}}(i) \quad (\text{A.17})$$

$$C_{\text{tot,opex}} = C_{\text{opex}}(2020) + t_{\text{phase}} \cdot \tau_{\text{phase}}(p) \cdot \sum_{p \in \text{PHASE} | y_{\text{start}} \in P_START(p), y_{\text{stop}} \in P_STOP(p)} (C_{\text{opex}}(y_{\text{start}}) + C_{\text{opex}}(y_{\text{stop}})) / 2 \quad (\text{A.18})$$

$$\tau_{\text{phase}}(p) = 1 / (1 + i_{\text{rate}})^{\text{diff_2015_year}(p)} \quad (\text{A.19})$$

The objective function to be minimised is the total transition cost of the energy system ($C_{\text{tot,trans}}$), defined as the sum of the total capital expenditure (CAPEX) ($C_{\text{tot,capex}}$) and the operational expenditure (OPEX) ($C_{\text{tot,opex}}$), according to Eq. (A.16). The total CAPEX ($C_{\text{tot,capex}}$) is the sum of the investment during each phase ($C_{\text{inv,phase}}$), Eq. (A.17), to which the residual asset investment cost in 2050 is withdrawn ($C_{\text{inv,return}}$). Thus, the investments account for the installation and dismantlement costs of the technologies. The total OPEX ($C_{\text{tot,opex}}$) is the sum of the OPEX in 2020 and the annualised sum of the OPEX during each phase (C_{opex}), Eq. (A.18). During a phase, the system OPEX is the product of the annualised phase factor, defined in Eq. (A.19), and the arithmetic average of OPEX cost for the representative years before and after the phase. The annualised phase factor is defined based on an average interest rate during the transition.

$$C_{\text{opex}}(y) = \sum_{i \in \text{TECH}} C_{\text{maint}}(y, i) + \sum_{j \in \text{RES}} C_{\text{op}}(y, j) \quad \forall y \in \text{YEARS} \quad (\text{A.20})$$

For each year, the yearly OPEX (C_{opex}) is the sum of the operating and maintenance costs of technologies (C_{maint}) and the operating cost of the resources (C_{op}), Eq. (A.20).

$$C_{\text{inv,phase}}(p) = \sum_{j \in \text{TECH}} F_{\text{new}}(p, j) \cdot \tau_{\text{phase}}(p) \cdot (c_{\text{inv}}(y_{\text{start}}, j) + c_{\text{inv}}(y_{\text{stop}}, j)) / 2 \quad \forall p \in \text{PHASE} | y_{\text{start}} \in P_START(p), y_{\text{stop}} \in P_STOP(p) \quad (\text{A.21})$$

The investment during a phase ($C_{\text{inv,phase}}$) results from the multiplication of the newly built technologies (F_{new}) with their annualised arithmetic averaged specific cost, Eq. (A.21). The annualised phase factor (defined by Eq. (A.19)) is used. The specific cost during the phase is defined as the average between the investment cost for the first and last year of the period.

$$\begin{aligned}
C_{\text{inv,return}}(i) = & \sum_{p \in \text{PHASE} \cup \{2015_2020\} | y_{\text{start}} \in Y_START(p), y_{\text{stop}} \in Y_STOP(p)} \tau_{\text{phase}}(p) \cdot (c_{\text{inv}}(y_{\text{start}}, i) + c_{\text{inv}}(y_{\text{stop}}, i)) / 2 \cdot \\
& \frac{\text{remaining_years}(i, p)}{\text{lifetime}(y_{\text{start}}, i)} \left(F_{\text{new}}(p, i) - \sum_{p2 \in \text{PHASE}} F_{\text{decom}}(p2, p, i) \right) \quad \forall i \in \text{TECH}
\end{aligned} \tag{A.22}$$

A part of the investment will remain after 2050. This residual investment, also called salvage value, can be calculated for each technology. A parameter, calculated *a priori*, gives for each technology and construction phase, the remaining amount of years (*remaining_years*). As an example, if a PV panel has been built in 2045 and has a 20 years lifetime, the parameter will equal to 15 years. Thus, the salvage value is a fraction of the investment cost of this technology when it has been built. This fraction is the ratio between the number of remaining years and the lifetime of the technology. In the previous example, the residual investment of the PV built is 75%. Eq. (A.22) computes, for each technology, the residual value that must be deducted from the total cost. The residual value reflects the fact that the technology can still be used after the horizon of the model and is not fully amortised. The residual value is not applied to technologies that are removed prematurely. This differs from other models, such as Plexos where a technology removed prematurely will benefit from its salvage value (see analysis of [99]).

$$\text{GWP}_{\text{tot,trans}} = \text{GWP}_{\text{tot}}(2020) + t_{\text{phase}} \sum_{p \in \text{PHASE} | y_{\text{start}} \in Y_START(p), y_{\text{stop}} \in Y_STOP(p)} / 2 (\text{GWP}_{\text{tot}}(y_{\text{start}}) + \text{GWP}_{\text{tot}}(y_{\text{stop}})) \tag{A.23}$$

$$\text{GWP}_{\text{tot,trans}} \leq \text{gwp}_{\text{lim,trans}} \tag{A.24}$$

The total global warming potential (GWP) emissions during the transition ($\text{GWP}_{\text{tot,trans}}$) are equal to the sum of the total emissions per period (GWP_{tot}), Eq. (A.23). The emissions during a phase is estimated as the arithmetic average of the representative years before and after the phase. Eq. (A.24) limits the total GWP emissions during the transition by a maximum ($\text{gwp}_{\text{lim,trans}}$).

Appendix B

Case study: the Belgian energy system

B.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 [122]. Given the data available in the literature (mostly for the power sector) and, when not available, following the assumptions made by Limpens et al. [45], Table B.1 gives the major technologies used in 2020 to supply the different demands of Figure 2.1.

B.2 Belgian energy transition pathway towards carbon-neutrality in 2050

This section presents the results of the deterministic (i.e. all parameters at their respective nominal value) perfect foresight optimisation of the Belgian energy transition pathway constrained to a linear decrease of the GHG emissions from 2020 (121 MtCO_{2,eq}) to carbon-neutrality in 2050. After performing a technical investigation of the pathway by checking the greenhouse gas breakdown by energy sectors, the primary energy mix is analysed. To illustrate the sector coupling, a focus is made on the electrification of other sectors. Then, the cost implications in terms of investments and operations are discussed.

Table B.1. Major technologies used to supply the 2020-demands of Figure 2.1 in terms of share of production and installed capacity.

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%	-

^aThe decentralised heating units provide 98% of the low-temperature heat demand.

^bThe private mobility accounts for 80% of the passengers mobility.

B.2.1 Greenhouse gases and primary energy

Figure B.1 shows the greenhouse gases (GHG) per sector. The system reaches its upper bound (i.e. maximum emissions) every year.

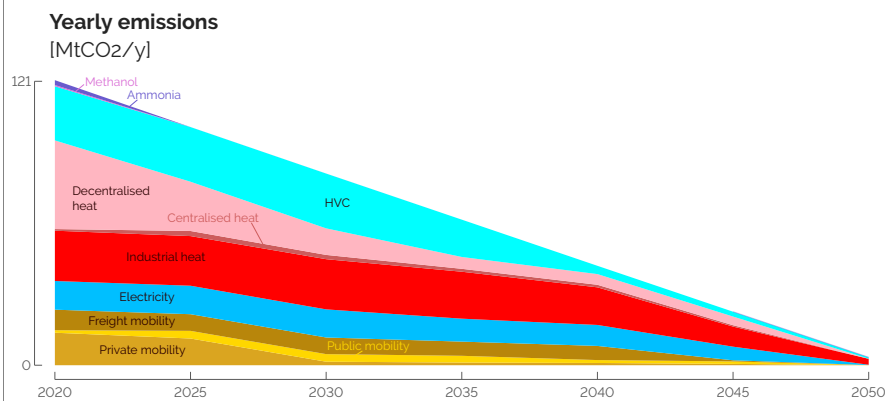


Figure B.1. Energy sectors have different speed to reduce GHG emissions over the transition. The system uses all the allowed GHG prescribed by the linear decrease from the emissions in 2020 until carbon-neutrality in 2050.

The defossilisation¹ of the different sectors are not performed at the same rate. The non-energy demand of methanol and ammonia are substituted by electrofuels. These are the first use of electrofuels as e-ammonia is the cheapest electrofuel thanks to the high maturity of the Haber-Bosch process. The decentralised heat and mobility sectors are also dropping first. This is a combination of efficiency and substitution of fossil fuels with electricity. Efficiency comes mainly from district heating networks and electrical heat pumps for the heat sector, and public mobility and electric cars for the mobility sector. From 2040 onward, the decreases are mainly due to the substitution of the remaining fossil fuels by electrofuels as illustrated in Figure B.2.

Figure B.2 shows the primary energy mix for the different representative years. The pathway verifies five trends: (i) reduction of primary energy thanks to energy efficiency; (ii) massive integration of endogenous renewable energies; (iii) importance of electrification; (iv) the usage of gas as the last fossil resource; and (v) the obligation to rely on renewable fuels to achieve carbon neutrality.

¹In a more sustainable future, some of the energy carriers, currently produced mostly from fossil resources, will still consist of hydrocarbons (e.g. e-methane or e-methanol). This is why this paper rather uses “defossilisation” rather than “decarbonisation” as carbon will still play a key role in a carbon-neutral energy transition [123].

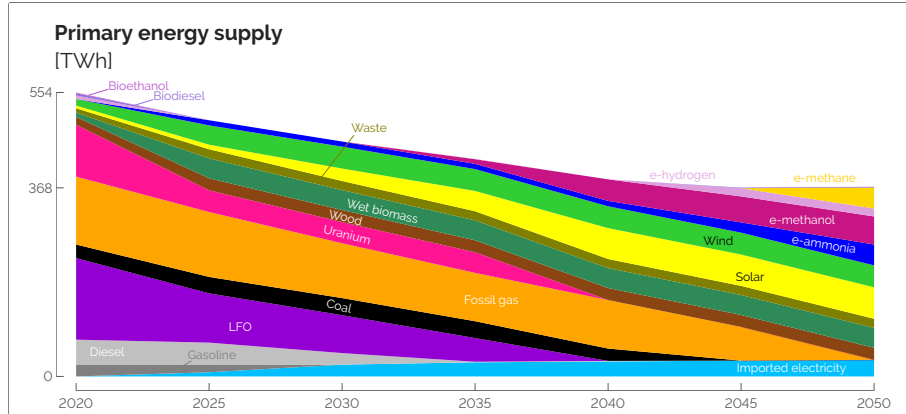


Figure B.2. Primary energy emitting GHG (below Uranium) are reducing linearly with fossil gas remaining until 2045. A part of this energy is replaced by renewable ones and starting from 2040, a significant share of electrofuels. As end-use demands slightly increase (see Figure 2.1), the drop represents energy efficiency (i.e. providing the same services with less primary energy).

The energy supply decreases from 554 TWh/y in 2020 down to 368 TWh/y in 2050 (i.e. -34%) whereas, in the meantime, the demands have increased by 19%, on average. This drop of primary energy consumption reflects the penetration of efficient measures and technologies, such as the previously mentioned public mobility, DHN or heat pumps. The results in 2050 are aligned with other studies, such as Devogelaer et al. [124]² and My2050³ [126] which estimates respectively a range of 305-417 TWh/y and 307-364 TWh/y for their central scenarios.

The first fossil energy to phase out is gasoline, which is exclusively used for private cars. Indeed, private mobility is partially replaced by public one⁴; and the cars are switching from gasoline and diesel to electricity. Then, diesel and LFO are decreasing. As diesel is used for trucks and buses mobility, it is harder to phase out compared to gasoline exclusively burned in cars. The first drop of LFO reflects the switch from oil boilers to other technologies: heat pumps and gas cogeneration mainly. Then, it is

²This study was ordered by the National Planning Bureau in 2013. Five scenarios are proposed.

³The Climate Change Service of the Federal Public Service Health launched an initiative in 2012 entitled 'Low Carbon Belgium by 2050'. This initiative resulted in a report and a calculator in 2013 [125]. The Belgian calculator has been improved since then into a recent expert version called **My2050** [126]. From this study, the results of two scenarios will be used: one based on an optimistic evolution of technologies (Technology), and one focusing on an increased dependence on neighbouring countries (EU integration).

⁴Given the major role played by private cars in the Belgian passenger mobility nowadays (i.e. around 80% [127]), public transport (e.g. tramways, buses and trains) is assumed to be able to supply only half of it.

mainly used for the production of HVC, this reflects that HVC is a feedstock hard to defossilise. Finally, coal is kept mainly for industrial usage because it is a cheap fossil fuel (mainly for industrial usage). To phase it out beforehand, a penalty mechanism, such as a carbon tax, would be required, or its strict ban should be put in place. The last fossil energy present in the system is fossil gas, used for the production of electricity and heat, through cogeneration mainly. Indeed, gas plays a key role to balance the intermittency of solar and wind.

The consumption of uranium declines in 2025, dropping to 2 GW, primarily due to the political framework aimed at phasing out nuclear energy [128]. In the initial stages, significant deployment of endogenous energies takes place. This includes the utilization of wood, wet biomass, and wind energy, followed by the introduction of solar energy. However, solar energy is not fully deployed during this period due to higher integration costs. Starting from 2025, the importation of electrofuels begins, although their significant utilisation is observed from 2035 onwards. Initially, these fuels are predominantly employed as feedstocks in non-energy sectors. From 2040, e-methanol is additionally utilised for the production of High-Value Chemicals (HVCs), e-hydrogen is employed for mobility purposes, and both e-methane and e-ammonia are used for electricity generation through gas CHP and ammonia-based CCGT plants (see Figure B.3).

In 2020, Belgium has been a net-exporter of electricity, however with the shut-down of nuclear power plants and the increase of electricity consumption, Belgium will become a net importer of electricity. These imports reach their maximal allowed capacity by 2035 (i.e. 30% of electricity end use). This strong dependence on imported electricity illustrates the need for balancing intermittent renewables without relying on fossil fuels.

B.2.2 Electricity sector: Capacities and yearly balance

To better understand the electricity sector, the installed production capacities are given in Figure B.3, while the supply-demand yearly balance is illustrated in Figure B.4.

As introduced in the primary energy analysis (see Figure B.2), renewable capacities soar. By 2050, wind and solar technologies deployments are 60 GW of PV, 10 GW of onshore wind turbines and 6 GW of offshore wind turbines. To compensate the intermittency, the system relies on imported electricity, gas CCGT, sector coupling and storage. As an illustration, in 2050, 176.8 TWh of electricity transit on the grid which includes 32.4 TWh of electricity imported and 15.4 TWh of electricity from CCGT. This result is aligned with other studies that estimates different ranges: 180-310 TWh/y

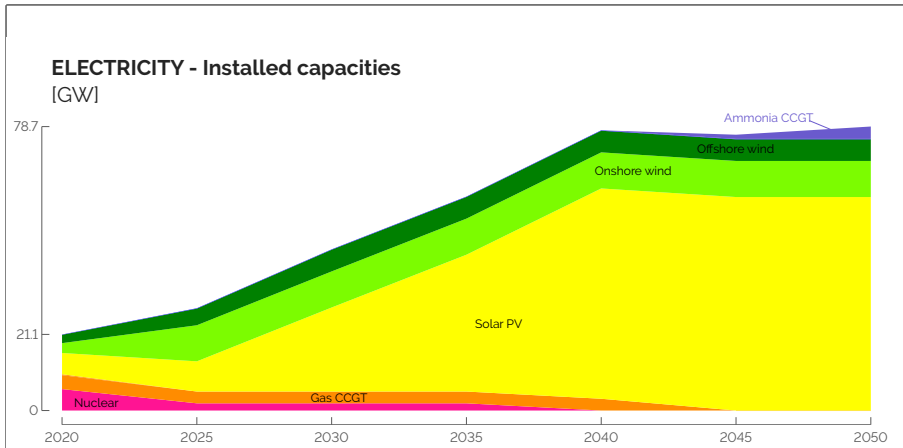


Figure B.3. The electrical production capacity will experience massive expansion of wind turbines (onshore and then offshore) and a soaring installed capacity of PV. Ammonia CCGT are installed at the end of the transition to provide a flexible capacity as gas CCGT are phased out.

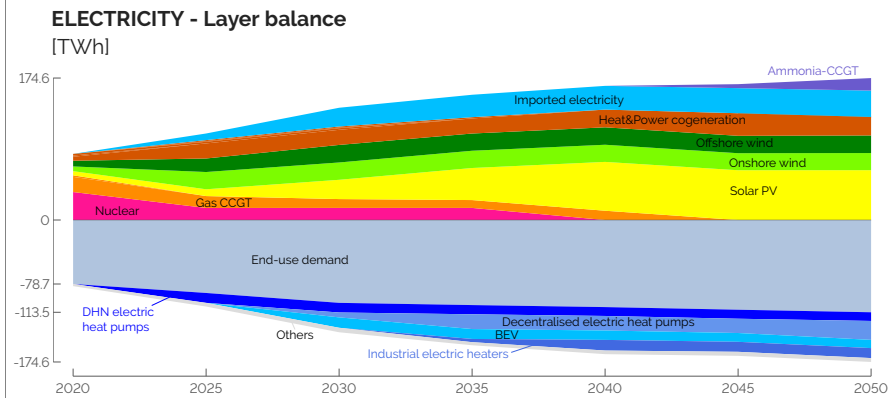


Figure B.4. The electricity supply (positive values) will remain a mix of different technologies where backup is first mainly provided by gas-CCGT and then imported electricity, heat and power cogeneration and later ammonia-CCGT. The electricity demand (negative values) is led by the electricity end-use demand, but the share used to electrify heat (heat pumps), vehicles (cars, trains, trams, ...) and industrial heaters drastically increase. This enables a flexible demand that can facilitate the integration of intermittent renewables.

[124], 126-140 TWh/y [126] and in a more recent study using the TIMES-BE model, 185-196 TWh/y [64]. Higher values from Devogelaer et al. [124] illustrate an almost exclusively electrified energy system. The differences between the study ranges reflect the different assumptions in terms of renewable potentials and availability of nuclear energy. A general trend is that Belgium should maximise its use of endogenous renewable resources, which Dubois et al. [129] identified as a cheaper option than importing additional renewable energies from abroad. Demand management reflects the flexible use of electricity, mainly through heat pumps that uncouple the heat demand and the electricity consumption when combined with thermal storage. Gas CCGT is also a useful asset to compensate intermittent renewables. However, its capacity remains the same as the one installed in 2020. These results are verifying an hourly adequacy of the power demand. Moreover, in a previous study by Pavičević et al. [118], the snapshot version of the model has been coupled with Dispa-SET, a dispatch optimisation model. Results showed that the backup capacity was underestimated by less than 20% to respect reserve capacity, mainly due the lack of reserve capacity for grid stability.

From 2025, the electricity mix has a strong renewable share that rises up to 60% in 2050. The remaining 40% are mainly gas (or ammonia) in CCGT and cogeneration and imported electricity. From a demand perspective, the electrification first starts with DHN heat pumps, then electric cars, then decentralised heat pumps and finally industrial heaters. The latter reflects the usage of cheap PV production peaks.

B.2.3 Costs: Investments and operation

In the following paragraphs, the results are analysed from an economic perspective to decipher the choices made by the model, as the overall cost of the transition is 1 004 b€₂₀₁₅ split unequally among the sectors.

Figure B.5 illustrates the cumulative investments made throughout the transition, amounting to a total of 377.8 b€₂₀₁₅. Initially, the infrastructure, transport, and electricity sectors each account for approximately one-third of the investments. The investments in infrastructure are primarily driven by the electricity grid and the district heating network (DHN), representing a combined investment of 73 b€₂₀₁₅. The electricity sector's investment is led by power plants, totalling 31.5 b€. Notably, the investment costs in the mobility sector are primarily attributed to private cars, constituting 71% of the total. A rough estimation confirms the significant investment in cars, with an average of 500,000 vehicles registered annually in Belgium over the last decade [130] and assuming an average cost of 20 k€ per car, the funds allocated to private cars amount to 10 b€ per year. This trend in private cars explains why the private mobility sector

accounts for half of the investments required to achieve the transition by 2050. This finding aligns with other studies, such as Devogelaer et al. [124], which estimates cumulative investment expenditures of approximately 600 b€₂₀₀₅ for the transport sector between 2013 and 2050, which confirms our conservative approach in the estimation.

As a comparison, the investments required to fully deploy the PV and wind potentials from 2020 to 2050 amount to 74.4 b€₂₀₁₅, with an additional 22.2 b€₂₀₁₅ allocated to reinforce the grid. The electrification of the heating sectors necessitates investments of 29.2 b€₂₀₁₅, including 6.5 b€₂₀₁₅ for the deployment of the DHN infrastructure. Storage investments, primarily focused on DHN seasonal storage, amount to 3.6 b€₂₀₁₅. Apart from the investment required to replace all private vehicles (accounting for 44% of the overall investments), the remaining sectors represent a total of 212 b€₂₀₁₅. To mitigate the cost of the transition, My2050 suggests deploying a fleet of no more than one million vehicles and implementing a car sharing system, distinct from car-pooling, as an inevitable measure [126].

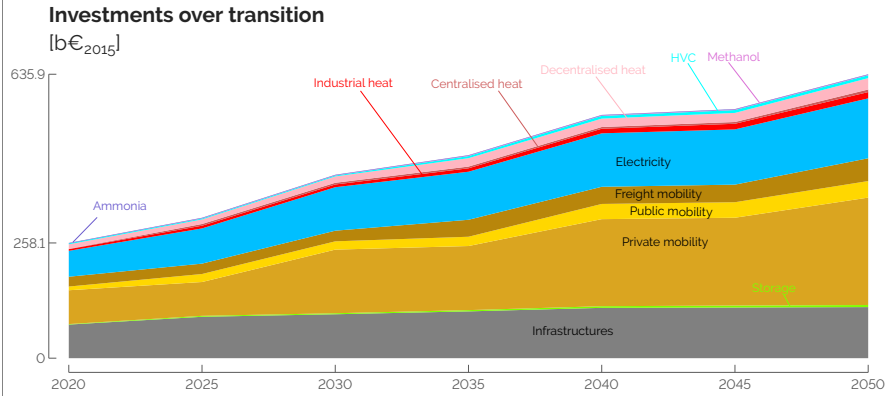


Figure B.5. The cumulative investments over the transition is unequally spread between the sectors. The energy system in 2020 is imposed to the existing energy system and its expenses are split in three main categories: mobility (mainly vehicles), infrastructure (mainly grids) and electricity (mainly thermal power plants). The investments required during the transition represents 150% the initial investment and mainly in the same three sectors.

A part of the investment will be recovered at the end of the transition based on the remaining lifespan of the technology after 2050. Figure B.6 illustrates the salvage value by sectors, calculated according to Eq. (1.5). Out of the 114.4 b€₂₀₁₅ of investments in the infrastructure (i.e. mostly power grid and gas network), 55.9% remain available after 2050, due to their long lifetime. On the contrary, private mobility has a lower

salvage value due to a major drop within the first four years and an average lifetime below 10 years [130].

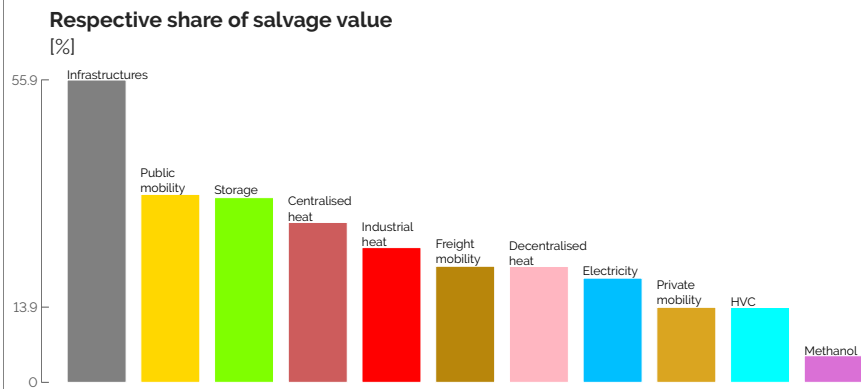


Figure B.6. By the end of the transition (i.e. in 2050), the ratio between the salvage value and its cumulative investment, per sector, is unequal. Investments in infrastructures, public mobility, storage and other long-lifetime technologies experience an important salvage value, at the contrary, investments in private mobility will not be recovered as vehicles have a short lifetime. All together, these salvage values represent 160.1 b€₂₀₁₅, 25% of the cumulative investment costs in 2050.

In addition to investment decisions, the operational expenditure (OPEX), which accounts for resource utilisation and technology maintenance, are significant. Figure B.7 shows the yearly system cost for each sector except the OPEX related to resources that are grouped together. The latter dominates the OPEX, with a significant share of non-renewable resources (i.e. 63.6% in 2020) until 2040, followed by a steep increase in the share of renewable resources (i.e. 66.2% in 2050). The substantial reliance on non-renewable resources reflects the prevalent use of fossil fuels in our current energy system. The high cost-share of non-renewable fuels underscores the economic challenges of simply substituting fossil fuels with renewables, particularly evident when emphasizing that electrofuels are 2-3 times more expensive. Maintenance expenses in the private mobility sector rank second in terms of expenditure. On the other hand, maintenance expenses in other sectors are relatively small compared to the aforementioned sectors.

The annualised cost of the energy system in 2020 is estimated to 44.3 b€/y and increases by 5.5 b€/y to reach 49.8 b€/y by 2050. **My2050** estimates the annualised cost in 2050 between 63 and 82 b€/y [126], while the other studies just indicate the cost increase compared to 2015 (+11.7 to +21) [64, 124]. The differences come from the

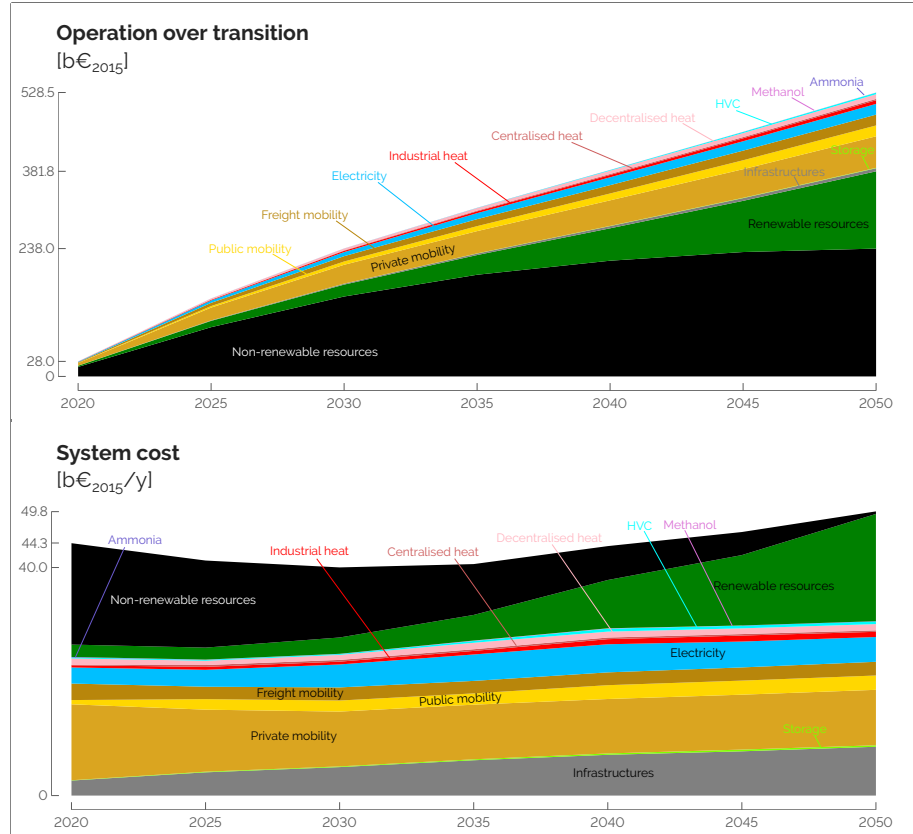


Figure B.7. The yearly system cost shows the shift from non-renewable to renewable resources (mainly electrofuels). Operation cost and maintenance represents almost 50% of the expenses.

scope of the energy system, as an example **My2050** also accounts for the agriculture sector. These differences highlight the difficulty to compare different studies due to difference of scope and partial availability of used data. Overall, comparing with existing studies shows the consistency of the results provided by EnergyScope Pathway.

B.3 CO₂-budget versus linear decrease of emissions

Figure B.8 shows the yearly emissions attributed for each sector in the REF case (i.e. imposed CO₂-budget) and a case where the CO₂-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.

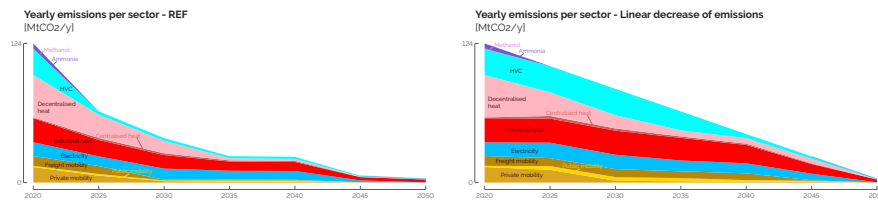


Figure B.8. Respecting the CO₂-budget imposed in the REF case drastically cuts the emissions of the system, especially in the production of high value chemicals (HVC) and the high-temperature heating sector.

B.4 Uncertainty characterisation for the 5-year steps transition

Table B.2 summarises the uncertainty ranges for the different groups of technologies and resources, for the year 2025. Refer to [7, 33] 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. [34] 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 B.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 main-

tenance 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 $f_{\max, \text{SMR}}$ 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 B.2. Application of the uncertainty characterization method to the EnergyScope Pathway model for the year 2025.

Category	Parameter	Meaning	Type ^a	Relative variation ^b	
				min	max
Cost of purchasing	$c_{op,fossil}$	Purchase fossil fuels	II	-64.3%	179.8%
	$c_{op,elec}$	Purchase electricity	II	-64.3%	179.8%
	$c_{op,electrofuels}$	Purchase electrofuels	II	-64.3%	179.8%
	$c_{op,biofuels}$	Purchase biofuels	II	-64.3%	179.8%
Investment cost	$c_{inv,car}$	CAPEX car	I	-21.6%	25.0%
	$c_{inv,bus}$	CAPEX bus	I	-21.6%	25.0%
	c_{inv,ic_prop}	CAPEX ICE	I	-21.6%	25.0%
	c_{inv,e_prop}	CAPEX electric motor	I	-39.6%	39.6%
	c_{inv,fc_prop}	CAPEX fuel cell engine	I	-39.6%	39.6%
	$c_{inv,efficiency}$	CAPEX efficiency measures	I	-39.3%	39.3%
	$c_{inv,PV}$	CAPEX PV	I	-39.6%	39.6%
	$c_{inv,grid}$	CAPEX power grid	I	-39.3%	39.3%
	$c_{inv,grid_enforce}$	CAPEX grid reinforcement	I	-39.3%	39.3%
	$c_{inv,nuclear_SMR}$	CAPEX SMR ^c	I	-40.0%	44.0%
Maintenance cost	$c_{maint,var}$	Variable OPEX of technologies	I	-48.2%	35.7%
Consumption	η_{e_prop}	Consumption electric vehicles	I	-28.7%	28.7%
	η_{fc_prop}	Consumption fuel cell vehicles	I	-28.7%	28.7%
Potential installed capacity	$f_{max,PV}$	Max capacity PV	I	-24.1%	24.1%
	$f_{max,windon}$	Max capacity onshore wind	I	-24.1%	24.1%
	$f_{max,windoff}$	Max capacity offshore wind	I	-24.1%	24.1%
Hourly load factor	$c_{p,t,PV}$	Hourly load factor PV	II	-22.1%	22.1%
	$c_{p,t,winds}$	Hourly load factor wind turbines	II	-22.1%	22.1%
Resource availability	$avail_{elec}$	Available electricity import	I	-32.1%	32.1%
	$avail_{biomass}$	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%
	$\%_{pub,max}$	Max share of public transport	I	-10%	10%
	$\Delta_{change, freight}$	Modal share change freight mobility	-	-30%	30%
	$\Delta_{change, pass}$	Modal share change passenger mobility	-	-30%	30%
	Δ_{change, LT_heat}	Modal share change LT-heat	-	-30%	30%
	$f_{max,SMR}$	Potential capacity SMR	-	0	1

^aPer [33], "I: investment-type, II: operation-type (constant uncertainty over time), III: operation-type (uncertainty increasing over time)".

^bThe nominal values of each of the parameters is 0, meaning no variation compared to the nominal values of the impacted parameter in the model.

^cThis range has been inferred from the local sensitivity analysis performed by EnergyVille [64].