Xavier Rixhon's PhD thesis - Answers to jury members

Exploration of uncertainty-aware energy transition pathways - Reinforcement learning and principal component analysis-based methods

I would like to thank the jury members for the comments, which significantly helped improving the manuscript and substantiating the novelty of my work. Based on the notes taken during the private defense, I hereby transcribed, as accurately as possible, the jury's comments.

I believe I have addressed all the issues raised in the following answers. Some of them required adaptations of the text. These adaptations are either directly in the thesis manuscript or left for further developments in subsequent papers. For each comment, I have first highlighted the issue, then provided an answer, and finally described how the manuscript was adjusted, if needed.

When a comment explicitly comes from specific members of the jury, they are listed at the beginning of the comment with the following color code: **Stefano** Moret, **Stefan** Pfenninger, **Sylvain** Quoilin and **Christophe** De Vleeschouwer. Here is how an answer to a comment is structured:

Text of the comment. When a page number is mentioned at the beginning of the comment, it refers to the page number of the manuscript submitted before the private defense, which might differ from the one in its final version.

The answer provided to the comment and, based on this, where the potential modification brought to the manuscript is located in the thesis manuscript using blue font.

New version of the text in the manuscript.

Contents

Stefano - Overall, many methods: PCE + RL + NN + PCA. At each stage, some assumption is made. Why not a simpler approach or a simpler model? Do you need all these steps? Explain the role of the different methods and why PCE instead of monthly version for uncertainty?

The purpose of each methods and the assumptions are discussed in the "Assumptions - Fine tuning" section of the present document. Regarding the choice of PCE instead of monthly version for uncertainty, as discussed during the private defense, monthly version of the model does not provide enough detail to provide sufficient confidence in the results given the need to massively integrate VRES for Belgium to succeed its transition. Given the hourly/daily intermittency, properly assessing the integration of wind and solar requires a fine time resolution that is not provided by the monthly model.

Given what is detailed further in this document and what has been discussed during the private defense, I have not brought modification to the manuscript in this regard.

Christophe - The variables and the uncertainties should be presented in a compact and mathematical way.

In my opinion, the main variables of EnergyScope Pathway are presented in Section 1.1 of the core of the manuscript. Further details are also given in Appendix B.2. Finally, these variables are even exhaustively detailed in [1] and [2] that are cited several times in the thesis manuscript. Regarding the uncertainties, the way the ranges are defined and the way they affect the value of some parameters in the model are explained in Section 1.2 of the core of the manuscript. Consequently, no modification has been brought to the manuscript regarding this topic.

ASSUMPTIONS - FINE TUNING

Stefano, **Sylvain** & **Stefan** - Many assumptions, e.g., alpha = 85% (p. 40) or reward = -300 (Chapter 4). How sensitive are the results to these assumptions? It looks like all these parameters have been tuned to obtain the desired results. How robust are they? Can the methodology be generalized to other models? Can we keep the same values for other applications? You need a model that runs pretty fast, right?
Stefan - Justification of the RL actions selected? why no other actions like the cost of some technologies?
Sylvain - p. 86 - A lot of heuristic and trial and error. Can the methodology be generalized to other models?

I have not carried out analysis to assess the sensitivity of the results to these assumptions. They result either from trial and error or observations made *a posteriori*. However, to discuss these assumptions and the methodological choices, I have added a specific section to each methodological parts of Chapter 1 to provide future users and developers of the methods proposed in this work with guidelines. These aim at helping other researchers in either using the same methodologies and assumptions on their own case study or keep on developing and improving these methodologies.

1.1.3 Discussion and guidelines for future researchers [EnergyScope Pathway]

Given the research questions targeted in this work, EnergyScope Pathway was the right model to choose for several reasons: its low computational burden, its hourly time-resolution, its operation and design optimisation of a whole-energy system and the openness of the code and availability of the documentation (see Appendix B.1).

However, depending on the research questions to address, other pathway energy system models might be more appropriate given their better spatial resolution or higher techno-economical details, for instance. Such models can be used and combined with the other methodological tools presented in this chapter. Although, the main (and only) requirement is to keep a low computational time as getting relevant results from the following approaches usually requires $10^3 \sim 10^4$ runs. In our case, we have implemented the model to keep the time to run a pathway composed of 7 representative years below 15 minutes on a personal laptop.

1.2.4 Discussion and guidelines for future researchers [Uncertainty quantification]

Carrying out a Global Sensitivity Analysis (GSA) requires two steps: uncertainty characterisation and uncertainty quantification. Characterising the distribution followed by uncertain parameters require a lot of data that are either seldom available or poorly documented in the literature. Consequently, once lower and upper bounds are computed following a method like the one developed by Moret et al. [3], a good practice is to consider uniform distribution. Preliminary analyses revealing key parameters impacting the most the feature of interest could direct further researches to refine the characterisation of these parameters.

About the method to quantify the uncertainty, PCE has the advantages to provide Sobol' indices as the impact indicators of the uncertain parameters and extract statistical moments of the output of interest. Based on our experience, considering a second-order PCE is the minimum to get a reasonably low LOO error (below 1%) and reliable results. However, as presented in Section 1.2.2, starting with a first-order PCE

is a good proxy to get a initial insight into the impact of the parameters and discard the negligible ones before moving to a higher order PCE to increase the accuracy of the results.

1.3.3 Discussion and guidelines for future researchers [Agent-based reinforcement learning to support myopic energy transitions]

Reinforcement Learning (RL) was found to be an appropriate approach to explore myopic transition pathways under uncertainties and assess the robustness of policies to support such pathways. As a novice user of a RL framework, we would recommend to opt for SAC as it is sample efficient, ensures a wide exploration and has a low sensitivity to hyper-parameters [4]. Using the SAC package developed by STABLE-BASELINES3 allows a handy introduction to apply RL.

Besides the choice of the algorithm, most of the work when using a RL framework consists in properly define the rules of the games following which the agent interacts with its environment: actions, states and reward. These are defined and discussed in Chapter 4.

1.4.3 Discussion and guidelines for future researchers [Robustness assessment via PCA]

Principal Component Analysis (PCA) was found to be an appropriate method to provide a metric that capture a major part of the system design variance through the transition while keeping the amount of information to a "graspable" level of details. Besides selecting the installed capacities of end-use-type categories (electricity, heat, mobility and non-energy), one could discuss the scaling of these data and the management of the outliers. Where scaling the data is fundamental before computing the PCs, future researchers could adapt the scaling factor. To avoid singularities in our PCs, we have decided *a posteriori* to put high and low outliers to the upper and lower fences, respectively. However,before managing the outliers, we would recommend to keep them and assess the provided results in terms of number of PCs and the key technologies that characterise them.

Finally, we have assumed thresholds to limit the number of principal components of each representative year, PC_y (90%), the similarity between two of these PC_y (90%) and to limit the number of $PC_{texttransition}$ (85%). These thresholds have been defined based on good practices discussed in the literature and *a posteriori* observations specific to our case study. We would recommend starting with these values and adapting them in a second time if needed to increase or decrease the level of details captured by the PCs.

Moreover, to discuss the rules of the RL games, presented in Section 4.2, I have added a Section 4.2.4 introduced at the end of the introductory paragraph of Section 4.2:

We end this section with justifications of actions, reward and states implemented in this work as well as guidelines for researchers that would like to apply the RL approach on their own case study with their own model.

4.2.4 Discussion and guidelines for future researchers

As introduced in Chapter 1, most of the work in applying RL is the definition of the interactions between the agent and its environment (i.e., actions, reward and states) that are very dependent on the case study and the research questions to answer. The elements presented in this work result from several trial and errors to end up with meaningful results according to our research questions.

Besides mimicking potential actual policies, the actions chosen in this work have a direct translation into constraints and we can therefore assess their effectiveness through the fact they are binding or not. In this work, we have investigated other actions like incentivising solar PV panels and wind turbines by "artificially" reducing their CAPEX. The result was not conclusive as these technologies need to take part to the Belgian energy transition and because it was harder to assess the impact of this action.

The reward function was designed to first aiming at respecting the CO_2-budget then minimising the total transition cost. The -300 penalty given in case of an infeasible optimisation problem was arbitrarily set. *A posteriori*, it seems to be a well-defined penalty given its significant relative difference with the values taken by the reward otherwise, between -120 and 44 (see Figure 4.4). Besides this penalty and given the observed results, we recommend to start with the same reward function if the objective is similar, first target cumulative emissions then cumulative costs. This requires to define the CO_2-budget according to a certain sharing principle (see Section 2.5) and to compute reference total transition cost. However, other researches focusing on reaching carbon-neutrality by 2050 could define a binary reward function as +1 for reaching the objective and -1 otherwise.

Finally, states aim at representing the information relevant to the agent to efficiently learn and progress through the transitions. For this reason, on top reward-related features (cumulative emissions and costs), we added other indicators that are actually monitored to help decision-makers assessing their policies to reach their targets (share of renewables in the mix and the system overall efficiency). For other studies, one might consider other information like the metrics considered by Pickering et al. [5] (e.g., heat electrification, average national import or level of curtailment).

In conclusion, future studies might start from the actions-reward-states defined in this work and adapt these rules depending on the research questions to answer, the case study and the energy system optimisation model.

Finally, I have added a sentence in the conclusion of the manuscript to remind that the methods and the assumptions presented in this work can serve as a good basis but will need to be adapted depending on the model and the case study:

Besides the formulated recommendations, the assumptions and the formulation choices made in this work can serve as a basis for further researches but will need to be adapted according to model that is used or the case study that is studied.

GRAPHS AND RESULTS

Stefano, **Stefan** & **Sylvain** - Many axes labels are missing, and the captions are often insufficient to read the figures.

I agree and have gone through all the figures of the manuscript to clarify them by adding axes labels or extending the caption where it was needed. Figures where y-axis (and its label) is missing are distribution (or density) plots (i.e., Figures 3.6, 4.4, 4.5, 4.6, 4.8 and E.1). Consequently, similarly to an histogram, the feature of interest and its span of values are represented on the x-axis. The y-axis has no real interest in terms of information. What matters is the shape of the curve to be able to point out for which values/ranges of values, the feature of interest occurred more or less often. For this reason, I have not added y-axis for the aforementioned figures but rather improved their respective caption, emphasising, among other things, that these figures represent distribution of occurrences. For instance, the caption of Figure 4.4 is now more explicit:

Exploration of the state space over the learning process: distribution of occurrence of cumulative emissions (left) and costs (right). Number of remaining attempts decrease with time since infeasible problem and solutions overshooting the CO_2-budget are discarded prematurely, i.e., before reaching 2050. Besides infeasible problems, distributions labelled as "Failure" represent the attempts that overshot the CO_2-budget by 2050 at the latest. The majority of successful transitions have cumulative emissions much lower than the CO_2-budget and are cheaper than the REF case.

Stefan - Some big topics are missing like storage. Why is storage not more discussed?

As discussed during the private defense, storage is not more discussed in the manuscript for two reasons. First, the storage technologies, for the case of Belgium assuming a copper-plate approach, consist in two main technologies: methane storage mostly (about 15 TWh) and, to a smaller extent, seasonal thermal storage (about 3 TWh), with limited variations through the transition (see Figure 1). Analyses under uncertainties have not shown major variations neither. Second, storage assets are intrinsically linked to the conversion technologies and, consequently, can be seen as by-products of the optimisation results. For these two reasons, I have rather focused my analyses on the use of resources and the installation and operation of conversion technologies. Given the discussion during the private defense and these further explanations, I have not brought modification to the manuscript in this regard.
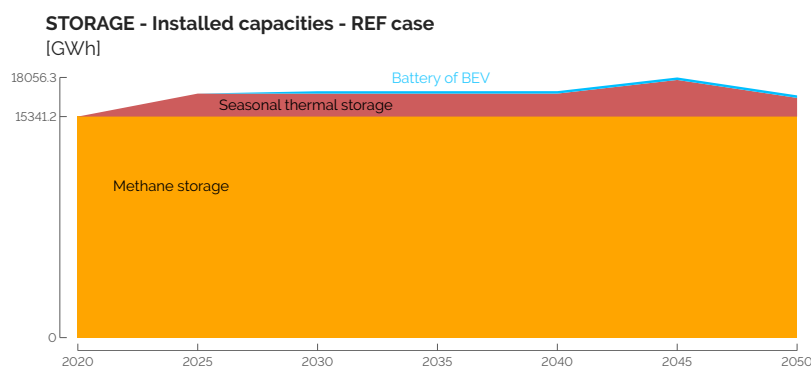

Figure 1: Storage installed capacities for the REF case

Stefan - Lot of the results hinge on the import of e-fuels with the assumption that they have GWP = 0; is it justified? Those fuels are directly available knowing they are no.

To succeed its energy transition, Belgium will need radical changes, "unicorn" solutions, and one of them would be the import of electrofuels. As presented in the introduction and reminded in the conclusion of the manuscript: "Chemically similar to their fossil-based equivalents, they [the electrofuels] can benefit from the current infrastructures and provide seasonal storage and flexibility against the intrinsic intermittency of solar and wind electricity." Besides these intrinsic advantages, considering these fuels as infinitely available (like their fossil equivalents) and with 0-GWP allow finding a solution for the Belgian case study, without considering a decrease of the demands. These are strong assumptions that can be challenged as suggested in the conclusion: "A future work would be to constrain the deployment of local renewables or the availability of electrofuels. This could provide different pathways where electrofuels would be produced more locally using carbon capture technologies. This

could also show the limits of the Belgian energy system to meet such an ambitious CO2-budget in its energy transition when solely relying on technological progress, highlighting the need for demand reduction. "

The assumption about 0-GWP molecules is similar to the one considered [6] which is the most recent study that addressed the case of the Belgian energy transition.

As discussed during the private defense, the first key-message of this work is the need for this (mix of) "unicorn" solution(s) given the ambitious objectives set to mitigate climate change. This need for this radical change and the fact that solutions rely a lot on assumed to be carbon-neutral and directly available electrofuels are explicitly mentioned in the conclusions of Chapter 3:

Given the ambitious CO_2-budget (i.e., 30-year budget representing 10 years of the current emissions), the global sensitivity analysis highlights the need for radical changes. Assumed to be carbon-neutral and directly available to a large amount, one of the "unicorn" solution for the case of Belgium is the import of renewable electrofuels, even at early stages of the transition. This is why the most impacting parameter on the variability of the total transition cost (around 45%) is the cost of purchasing these energy carriers.

and reminded in the conclusions of the manuscript:

Besides a wider electrification of the system and the integration of more efficient technologies, Belgium needs to go for radical changes, "unicorn" solutions. One robust policy would consist in massively investing in electrofuels.

STRUCTURE

Stefano & Stefan - The thesis structure makes it quite difficult to follow. Having all the methodology summarised in Chapter 1, makes it difficult to link it to the different chapters. As changing the structure may be now a major work, I would invite you to think how to better connect the different parts.

Initially, I wanted to group methodology and results per kind of analysis, i.e., UQ on Pathway (Chapter 3), RL (Chapter 4) and PCA (Chapter 5) but that would have made the RL, and even more PCA, methodology parts come too far in the manuscript. For this reason, I made the choice to group all the methodological approaches together in Chapter 1 and the results in their respective chapters. Given this explanation, I have added one sentence at the end of the introductory paragraph of the RL method in Chapter 1:

As Chapter 2 presents the input of the case study and Chapter 3 details the results of the GSA on the pathway model, the reader interested by the results of the RL method is invited to go to Chapter 4.

and at the end of the introductory paragraph of the PCA-based method in Chapter 1:

The reader interested by the results of the PCA-based method is invited to go to Chapter 5.

Finally, I have added a schematic at the end of the Introduction of the thesis to clarify the structure and highlight that Chapter 4 and 5 can be read after the methodological sections 1.3 and 1.4, respectively (see Figure 2).
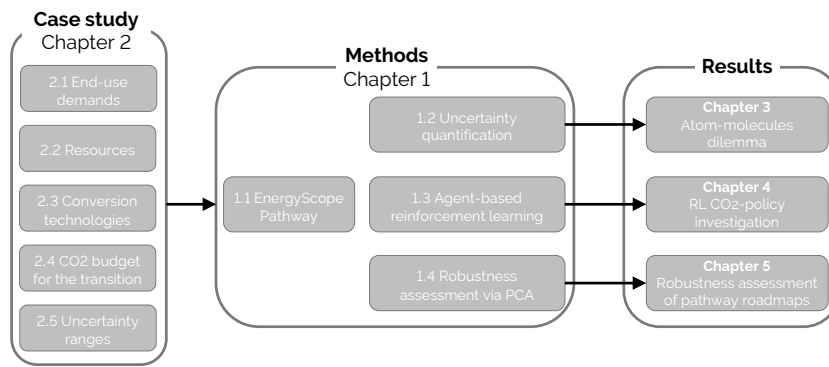

Figure 2: Structure of the thesis. Beyond Chapter 2 that describes the case study of Belgium, Chapters 3, 4 and 5 collect the analyses resulting from the application of the different methodologies developed in Chapter 1. Given the (quasi-)independence of the analyses presented in the last three chapters, they can be read separately.

Christophe - Formal description of the problem is missing even in described in the text to make the link between the ideas and the implementation. Add some flow charts to introduce key elements

This point is addressed with the structure chart presented in the previous comment as well as the improvement of Figure 1.4 presenting the implementation of the myopic approach as well as the way uncertainties and RL change the values of some parameters (see Figure 3 of the present document).

REFERENCES

Stefano & **Sylvain** - I found it unusual to see many references to own work (Rixhon et al.) throughout the thesis. Unless the articles are unrelated to the thesis, these references should be removed and the associated content should be included in the manuscript. As an example, at p. 25, results are mentioned which are not reported in the thesis. The reader currently must refer to [48] to see these results, which should instead be included in the thesis.

This choice to sometimes refer to own works was made to focus only on the main contributions of the thesis. However, I agree that some content should be included in the thesis to enhance its reading. I hereby list the references to works I have been involved in (with the reference number of the manuscript version submitted before the private defense) and detail the potential modifications brought to the manuscript for each of them.

- *[2] Limpens et al., Energyscope pathway: an open-source model to optimise the energy transition pathways of a regional whole-energy system*: Mostly cited to give credits to Gauthier Limpens' work in developing the Pathway version of EnergyScope, I have decided to refer to the paper about the formulation choices rather than including them in the thesis manuscript. Consequently, no further modification regarding this reference.

- *[7] Limpens et al., The impact of uncertainties on the Belgian energy system: Application of the Polynomial Chaos Expansion to the EnergyScope model*: The table gathering the results of the comparison between Morris' and PCE methods has been included at the end of Section 1.2.2:

In [7], we have assessed the PCE approach on the cost-optimum Belgian energy system in 2035, using EnergyScope TD. To do so, we compared 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 validated the use of PCE in the rest of this work (see Table 1).

- *[9] Rixhon et al., The role of electrofuels under uncertainties for the Belgian energy transition*: This paper is cited to highlight the GSA performed on the snapshot model with different GWP limits. The main contribution of this work in the context of the thesis was to provide a preliminary screening and selection of parameters to carry out the GSA on the pathway model. The result of this selection is given in Section 2.4 where the uncertain parameters and their respective ranges are listed. Consequently, no further modification regarding this reference.

Table 1: Comparison of the Top-14 rankings for the improved Morris method (left) and total-order PCE method (right). We used the DTU's implementation of Morris method [8] (with $p = 8$, $r = 100$).

Parameter	Morris Ranking (μ_i^*)	PCE Ranking (S_i^T)
Prices of hydrocarbons	1 (0.7141)	1 (0.6434)
Cost of increased efficiency	2 (0.3046)	2 (0.1014)
Cost of maintenance	3 (0.2371)	4 (0.0534)
Discount rate	4 (0.2019)	5 (0.0467)
Price of imported electricity	5 (0.1974)	3 (0.0809)
CAPEX of the grid	6 (0.1498)	6 (0.0252)
CAPEX of PV	7 (0.1270)	7 (0.0187)
Increase of electricity demand	8 (0.1168)	8 (0.0154)
CAPEX of nuclear power plant	9 (0.0963)	9 (0.0119)
Increase of space heating demand	10 (0.0856)	11 (0.0088)
Price of coal	11 (0.0856)	12 (0.0087)
Price of renewable fuels	12 (0.0794)	10 (0.0104)
Price of uranium	13 (0.0607)	13 (0.0047)
Onshore wind load factor	14 (0.0600)	14 (0.0046)

- *[10] Rixhon et al., Integration of non-energy among the end-use demands of bottom-up whole-energy system models*: Reference used to highlight the fact that whole-energy systems usually do not account for the non-energy demand. Consequently, no further modification regarding this reference.

- *[11] Rixhon et al., Comprehensive integration of the non-energy demand within a whole-energy system: towards a defossilisation of the chemical industry in Belgium*: Reference to graphs that have either been adapted from the paper or directly taken from it. Consequently, no further modification regarding this reference.

- *[12] Rixhon et al., Taxonomy of the fuels in a whole-energy system*: Where the content of this paper is the Appendix A of the thesis, some references to this paper aimed at clarifying the meaning of "renewable fuels" (Section 2.2) or the fact that uranium is considered neither fossil nor renewable (Sections 3.1.2 and 4.2.2). Consequently, no further modification regarding this reference.

Christophe - State of the art mainly European. Why not reference to other regions of the world.

It is an interesting topic for further investigations, especially how they address the subject in other parts of the world like Australia/Asia. This could be linked with

the political perception of energy system optimisation models and the subsequent analyses. However, no modification has been brought to the manuscript regarding this topic.

Writing style

Stefano - While a more "friendly" writing style can be pleasant, there are many colloquial expressions that not do not fit well in the thesis, e.g., "carrot and stick", "apples with apples", etc. I recommend reducing them to the bare minimum, or completely getting rid of them.

The listed colloquial expressions have been transformed and, overall, I have reviewed the manuscript to reduce them.

There are various typos in the thesis, e.g. "storagR" (page 3), "therefore, therefore" (p. 11), "The" (p.14), "Moleclues" (p. 61), etc.. Also, the use English language can be improved, e.g. "calls FOR a variety" (p. 9), "cumulative emissions ARE" (p. 14), "than to" (p. 34), etc. The document will benefit from a spelling/grammar check.

The listed typos have been corrected and, overall, the manuscript has gone through Grammarly to improve the spelling and the grammar.

Documentation

Sylvain - Where is the repository for the code? Don't forget the documentation?

As discussed during the private defense, this is a task that is already planned for the year to come, after the public defense. A better reference towards these repository and documentation will be given in the subsequent paper on RL. Consequently, there has not been further work done in this regard in the manuscript by the public defense.

Introduction

Stefano & **Stefan** - At page 1, it is mentioned that you focus on the technical levers of the transition, "renewables" and "efficiency". From this I understand that you are not focusing on "sufficiency". This seems to contradict a statement at p. 2, where it is mentioned that one objective of the thesis is to "support interdisciplinary projects in the assessment of sufficiency policy". I suggest clarifying this potential misunderstanding.

I totally agree with this remark, especially because I do not want to overlook the necessary third pillar of the transition which is "sufficiency", even though my thesis does not address directly this aspect. Consequently, I have adapted page 2 of the introduction:

> Among all the lenses through which it is necessary to assess sufficiency policies, one of the objectives of this work is to support these interdisciplinary projects by providing informed techno-economic guidelines.

This technical contribution to the interdisciplinary debate of sufficiency is reminded in the last sentence of the conclusion.

> In this sense, this work provided insight about possible transition pathways for Belgium to bring the technical dimension into the intrinsically political and interdisciplinary discussions and decisions that must be made in the coming years.

CHAPTER 1 - METHODOLOGY

ENERGYSCOPE PATHWAY

Stefano - p.11 : The stated computational time seems low for a pathway model with hourly resolution. Were there approximations (e.g., disabling crossover) added and what was their impact?

To decrease the computational time by one order of magnitude, besides opting for Gurobi to solve the LP, I disabled crossover. Besides this significant reduction of computational time, I observed no other impact regarding the values of the objective function or the design variables at the optimum. As disabling crossover is a very LP-specific aspect, I added this information in a footnote in the first paragraph of Section 1.1:

> To keep this low computational time, crossover was disabled to solve the optimisation problem. This had no observed impact regarding the values of the objective function or the design variables at the optimum.

3.1.1 End-of-time-horizon, myopic pathway and salvage value

Stefano - Often, multi-stage models are affected by the end-of-time-horizon effects. Did you observe those and how did you deal with them? See, e.g. Figure 3.3 p. 66.

To cope with these "end-of-time-horizon effects", we have implemented the salvage value, $C_{inv,return}$. This represents the residual investment that would remain after

2050. As detailed in Section 1.1.1: "the salvage value avoids penalising the capital intensive technologies towards the end of the transition" [13]. The sensitivity analysis on the formulation of the salvage value has been added in Appendix B.2.2 (see further comments on the salvage value).

As discussed during the private defense, instead of implementing a salvage value another alternative would be to implement artificial representative years after 2050 that are then excluded from the total transition cost and emissions in while post-processing the results of the optimisation. Even though the choice of the formulation of the salvage value accounts for assumptions (discussed in Appendix B.2.2), we opted for this rather than "artificial future years" for several reasons. First of all, it allows mitigating the computational burden of the pathway problem. Indeed, the more there are representative years, the bigger are the matrices and the longer it takes to solve the problem. Second, the salvage value-approach is also used in other works [13, 14]. Finally, implementing "artificial future years" would require to either collect more data, which is quite time-consuming, or make other kind of assumptions on the evolution of costs, GWP and other features beyond 2050.

Since the implementation of the salvage value and the formulation choices are the work developed by Limpens et al. [2] (partly integrated in Appendix B) and given the above explanations, I have not brought further modification to the manuscript in this regard.

Stefano - p.17-19: is the myopic version modeled as a single LP or as a sequence of LPs? This should be better clarified. The diagram at p. 19 focuses on the code, it would be better replaced by a code showcasing the logic of the approach.

Even though this sequence of LPs was already mentioned in the caption of Figure 1.3, I have complemented the text in the paragraph "Myopic pathway implementation" of Section 1.1.2,

[...] The myopic optimisation of the pathway consists of a sequence of smaller LP problems limited to their respective 10-year time-window, until eventually reaching 2050.

reminded it in the caption of Figure 1.2

The myopic approach (in pink) uses several instances of the pathway model, illustrated in Figure 1.1, as a sequence of different and linked LP problems.

and extended the caption of Figure 1.4. However, besides highlighting the key step 3.3 where there is an update of parameters value, I have decided to keep the figure as is since, on the one hand, the extension of the caption provides now a better understanding and, on the other hand, the code itself is exactly what is schematically represented on the diagram.
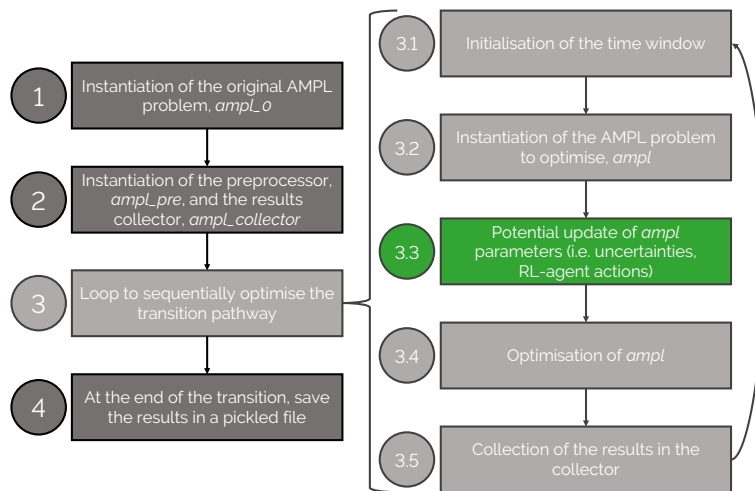
Figure 3: Diagram of the iterative optimisation of the whole-energy system transition pathway. Myopic optimisation of the pathway consists of a sequence of smaller LP problems limited to their respective 10-year time-window. If the optimisation is not deterministic, step 3.3 is the one where the value of some parameters is changed due to uncertainties (see Section 1.2) or the actions taken by the Reinforcement Learning-agent (see Chapter 4)

Stefan - With the myopic approach, are you predicting what will come or drawing a path that is the best? Is that a desirable feature to mimic the way we proceed now. Why artificially limit the model as we know we have to go to zero in 2050?

As written in the manuscript and discussed during the private defense, the purpose of the myopic approach is to challenge the assumption of the complete knowledge about the uncertain future and mimic the short-sightedness of the decision-making process. This sequential optimisation allows showcasing robust policies to support myopic transitions (see Chapter 4) and the robustness of roadmaps (see Chapter 5). The myopic approach is also the methodological basement to support the implementation of the RL and PCA-based methods.

Given these explanations and what is already in the manuscript, I have not brought modification in this regard.

Stefan - p.18 : Surprising that myopic leads to a sooner investment to the transition? Is it an effect of the salvage value? was there a sensitivity analysis on this salvage value? Perhaps include more details on this. The salvage value plays a large role in the decision of the model. Give more details to give more confidence in the choice.

Indeed, it is an effect of the salvage value as already written in the last paragraph "Impact of myopic formulation on the system" of Section 1.1: "The main difference

lies in the myopic transition itself and especially in the earlier deployment of PVs and offshore wind turbines. These induce the reinforcement of the grid that is a capital-intensive and long-lifetime asset. This is mostly due to impact of the salvage value, Equation (1.4), in the objective function.".

Sensitivity analysis has been performed on the formulation of the salvage value by Goffaux [15]. The overall conclusion of this sensitivity analysis was that the salvage value expression has little influence on the energy system at the end of the time horizon. The methodology and results of this analysis is now summed up in Appendix B.2

In the work of Goffaux [15], we carried out a sensitivity analysis on the formulation of the salvage value. First and foremost, this analysis confirmed the need to account for the salvage value to avoid penalising the capital intensive technologies towards the end of the transition [13]. Then, the sensitivity analysis focused on two elements in the expression of the salvage value: $\tau_{phase}(p)$ and $\mathbf{F_{decom}}(p2, p, i)$.

In Equation (B.22), τ_{phase} is the annualisation factor corresponding to the phase where the technology was built. With this expression, if a technology is still operational for half its lifetime after 2050, then half its initial investment is subtracted to the total transition cost. However, one could wonder if a technology that is still operational for half of its lifetime is not worth less than half of its initial investment cost, given the depreciation of the asset. In that case, the annualisation factor should account for the last phase of the optimisation (i.e., 2045_2050) when the residual value of the technologies are calculated and subtracted from the total transition cost.

On top of this, we also investigated the impact of accounting for the decommissioned technologies or not in the expression of the salvage value. In Equation (B.22), if a technology is decommissioned before 2050, then the salvage value of this technology will be 0. This is relevant since a technology decommissioned before 2050 would not be available after 2050. The issue is that the model could keep unnecessary technologies to subtract their salvage value from the total transition cost in order to decrease it. This would be done if the fixed OPEX of an unused technology is lower than its salvage value. Therefore, one could wonder if it would not be better to take into account the decommissioned technologies in the salvage value. In that case, a technology that would have been operational after 2050 but that had been prematurely decommissioned before 2050, would have a salvage value.

The overall conclusion of this sensitivity analysis was that the salvage value expression has little influence on the energy system at the end of the time horizon.

and a reference to this appendix is present in Section 1.1 where Equation (1.4) is detailed:

After assessing the sensitivity of the formulation of the salvage value (see Appendix B.2), we have kept the one given by Equation (1.4), being also similar to the expression used by Prina et al. [14].

3.1.2 Discount rate and annualisation

Sylvain - Wouldn't it be more appropriate to talk about "discount rate" rather than "interest rate"?

Indeed, as we want to capture the time preference associated with obtaining finance for the project, effectively quantifying the trade-off between present and future financial value, it is more appropriate to refer to "discount rate" when considering the parameter i_{rate}. We have changed every occurrence of "interest rate" into "discount rate" in the entire manuscript.

Sylvain - Value of the discount rate is generally above 6% in other works. You should have a better justification of selecting 1.5%.

Indeed, the discount rate is usually between 7.5% and 12% in other studies. The main justification for this choice was to be in line with G. Limpens' work [16]. However, assessing the impact of i_{rate} on τ_{phase}, we see that a lower value of i_{rate} will favour less late expenses compared to a high value. In other words, considering $i_{rate} = 1.5\%$ rather than 10% will less postpone investments (see Figure 4). I have added some explanations in this regard in Section 1.1.1:

τ_phase	Phase of expenses						
	2015_2020	2020_2025	2025_2030	2030_2035	2035_2040	2040_2045	2045_2050
1.5%	96%	89%	83%	77%	72%	66%	62%
2.0%	95%	86%	78%	71%	64%	58%	53%
2.5%	94%	83%	73%	65%	57%	51%	45%
3.0%	93%	80%	69%	60%	51%	44%	38%
3.5%	92%	77%	65%	55%	46%	39%	33%
4.0%	91%	75%	61%	50%	41%	34%	28%
4.5%	90%	72%	58%	46%	37%	30%	24%
5.0%	89%	69%	54%	43%	33%	26%	20%
5.5%	87%	67%	51%	39%	30%	23%	18%
6.0%	86%	65%	48%	36%	27%	20%	15%
6.5%	85%	62%	46%	33%	24%	18%	13%
7.0%	84%	60%	43%	31%	22%	16%	11%
7.5%	83%	58%	40%	28%	20%	14%	10%
8.0%	82%	56%	38%	26%	18%	12%	8%
8.5%	82%	54%	36%	24%	16%	11%	7%
9.0%	81%	52%	34%	22%	14%	9%	6%
9.5%	80%	51%	32%	20%	13%	8%	5%
10.0%	79%	49%	30%	19%	12%	7%	5%

(Row label along left side: i_rate)

Figure 4: τ_{phase} versus the timing of the expenses (columns) and the discount rate, $i_r ate$ (rows).

In EnergyScope Pathway, τ_{phase} aims at depreciating the value of expenses done in the future. The discount rate accounted for in this annualisation factor, i_{rate}, is considered as identical for all the technologies of the system. In line with Limpens [16], we set the nominal value to $i_{rate} = 1.5\%$ which is lower than values taken in other studies, between 7.5% and 12% [17–19]. Having a low value of discount rate favours less late expenses compared to a higher value of discount rate.

Stefano - Can you explain the logic of the annualization factor in the pathway model?
Sylvain - p.13: Why no annualizing over the lifetime of the unit? Would that lead to different results?

Accounting for the depreciation of money with time (see previous comment), we considered that the assets are fully paid at the moment they are installed. For this reason, we consider the arithmetic average between the investment cost of the assets at the year starting the phase of installation and the year ending it. This choice was done for two main reasons: potential decommissioning and lack of data beyond 2050. In the Pathway version of EnergyScope, the asset will be used over its whole lifetime unless it is prematurely decommissioned. Therefore, annualising over the entire lifetime of the unit might induce a bias in case of this premature decommissioning. Then, for assets with longer lifetime and/or installed later in the transition, annualising over the lifetime would require to have data beyond 2050. Effort that I have not decided to make.

Regarding the impact on the results, my educated guess is that this impact would be limited as the technologies of a same sector are assumed to have similar trends in terms of the evolution with time of their respective investment costs. Consequently, the major impact would be to end up with a lower total transition costs but the design of the system would be marginally impacted.

Given these further explanations, I have not brought any modification to manuscript in this regard.

Sylvain - p.71 - Differentiated discount rates could be useful.

As written in Chapter 3: "In practice, the discount rate would vary depending on the technology investment risk". Depending on the technology readiness level, private investors would be more or less risk-averse. However, EnergyScope only considers a vision of a central-planner where a single agent makes the investment decisions without differentiating the sources of the capitals, i.e., private and public. Assuming a differentiated discount rate would require to make assumptions about the private-public distribution of the capitals. These further explanations for keeping a single value of discount rate have been added after Eq. (1.3) when discussing the annualised phase factor.

The discount rate accounted for in the annualisation factor is considered as identical for all the technologies of the system. In practice, the discount rate would vary depending on the technology investment risk. Depending on the technology readiness level, private investors would be more or less risk-averse. However, EnergyScope only considers the vision of a central-planner where a single agent makes the investment decisions without differentiating the sources of the capitals, i.e., private and public. Assuming a differentiated discount rate would require to make assumptions about the private-public distribution of the capitals. For this reason, we have decided to keep an identical value of discount rate for all the technologies.

Stefan - Interest rate must be revisited if a paper is published.

See previous comments.

3.1.3 Power grid and transport infrastructure

Sylvain - How do you model the power grid interconnections with the neighbouring countries as well as the transport network of the different energy carriers within the country? p.63 - The model decides to use ammonia instead of SNG → is the transport infrastructure accounted for? p.73 - How is the transport infrastructure accounted for?

Regarding the power grid interconnections with the neighbouring countries, similarly to the import of other energy carriers, there is no representation of those physical routes. The whole-energy system of the country is represented as a single-node and the imported energy commodities are available "at the front door" of the system. It goes the same way for the infrastructures to transport energy carriers within the system. As it is represented assuming a copper-plate approach, all the demands, resources and conversion technologies are concentrated in one single node. This is now explicitly written in a new paragraph of Section 2.2:

Regarding the power grid interconnections with the neighbouring countries, similarly to the import of other energy carriers, there is no representation of those physical routes. The imported energy commodities are available "at the front door" of the system. In terms of spatial resolution of the country itself, it is modelled as a single-node. This is similar to the copper plate model of a power grid. In other words, the infrastructures to transport the energy carriers within the country are not considered. It is assumed that the demands have to be supplied by the production, regardless of the flows between the producers and the consumers. Yet, adapting the networks is accounted for in terms of the required investments. For instance, a high share of VRES

requires an investment to reinforce the power grid (i.e., 368 M€/GW of additional installed capacity of VRES).

Stefano - Can you explain the choice of N=5 for the uncertainty ranges?

As detailed by Moret [20]: "the ranges resulting from the uncertainty characterisation, are defined for a specific point in time in the planning horizon, usually its last year. Therefore, they need to be scaled accordingly when used in the optimisation model. Without this scaling, it would mean assuming that the uncertainty for year N stands for all the years in the planning horizon". In his thesis, Moret considered N = 20 as the duration of the planning horizon between 2015, the year of Moret's work, and the snapshot optimisation of the Swiss case study in 2035. In my case, the planning horizon is 5-year long as the duration of a phase between two representative years of the transition. Referring to Moret [20] for the interested reader, I have explained a bit more the reason for this scaling factor in the second paragraph of Section 2.4:

In this work, following the approach of Moret [20], we have defined ranges of uncertainties for the model parameters. For the operation-type parameters (types II and III), a scaling factor needs to be considered to avoid assuming that the uncertainty for the last year of the planning horizon (N) is representative for all years in the planning horizon Moret [20]. In EnergyScope Pathway, 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.

Stefano - p. 20: "inspired by Guevara et al." → how was their approach used in your work?

Guevara et al. [21] implemented a stochastic process to maintain realism in the evolution of uncertainty through the transition. In this sense, they avoid a parameter to go from the upper bound at year y to the lower bound 5 years later. It allows zigzag from one time step to another. (see Figure 3.2). In my case, once the sample of uncertain parameters is drawn, there is no zigzag ($\alpha = 0$ in [21]) but without especially be at the nominal value. Besides this, the inspiration does not go further. Given this explanation, I have not brought modification to the manuscript in this regard.
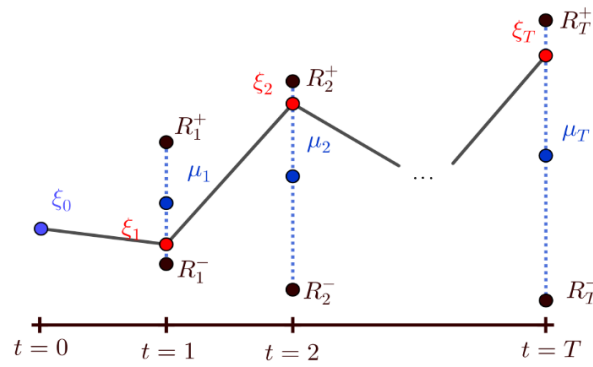
(b) Evolution of the stochastic process $\{\xi_t\}_{t=0}^T$

Stefano - p. 21: footnote. The statement is qualitative, it should be quantitative. What is the minimum number of runs needed to validate your experiments? Did you look into that? How was the surrogate model validated?

The footnote was intentionally qualitative as the quantitative information came later on (in Section 1.2.2). To improve this, I have moved the content of this footnote into the core of the text and after this quantitative information has been brought in Section 1.2.2, after "to achieve a LOO error below 1% for the total transition cost."

As second order PCE is the minimum to ensure accuracy of the surrogate model, selecting and grouping the parameters as presented in Section 1.2.3 is compulsory to alleviate the computational burden. Otherwise, considering thousands of independent uncertain parameters would lead to millions of EnergyScope Pathway runs, if no more. Another alternative to reduce the computational cost of the GSA would be to consider the monthly (instead of hourly) time resolution for the runs of EnergyScope Pathway. However, despite its shorter computation time (i.e., couple of seconds), the main drawback of the monthly model is its poor representation of the integration of VRES [2].

Stefano - p. 23: is PCE an appropriate method for LP / MILP models. Why is PCE needed is EnergyScope is already very fast? There is a good fit (1% LOO error) for the total cost, which is often quite linear, but how about technology choice / sizing?

Like in Diederik Coppitters' works [22, 23], the "ultimate" objective of PCE is to build up a surrogate model, $\hat{M}$, to serve a robust design optimisation (RDO) process. For an original non-linear model M, this surrogate model, formed of as a series of polynomials, has the main advantage to run much faster than the original model. In my case, I used PCE as an uncertainty quantification (UQ) tool without going up to the

RDO step. As written in the first paragraph of Section 1.2.2, I (only) aim at getting the statistical moments of the quantity of interest and determine Sobol' indices. Similarly, in Chapter 5, I used PCA to extract main direction of variation when it comes to the design of the system without performing runs using these PCs that are another representation of the original model. Consequently, regarding this objective, PCE is an appropriate method for EnergyScope Pathway.

When the LOO error is higher than 1% (but limited to 20-25%), which is the case when performing the PCE on technology size/choice (i.e., installed capacity of SMR by 2050) or the import of renewable molecules (see Section 3.2.2), the approach remains valid to qualitatively rank the parameters, as discussed in the paragraph "Qualitative ranking based on Sobol' indices" of Section 1.2.2.

Given these explanations and the elements already present in the text, I have not brought further modifications in the manuscript.

Stefano - p. 24: Sobol indices. Can you explain the choice wrt other methods? Difference between factor prioritization and factor fixing?

This comparison with a similar approach like factor fixing and factor prioritization (based on Morris method [24]) is detailed in the paragraph "Comparison with a proven method" of Section 1.2.2. I have extended this paragraph by integrating the table of comparison between the Morris method and PCE. This also avoids the reference to our own work and the reference [48], page 25 (see previous comment).

Besides being an in-house used method, the choice to use PCE is to be able to quickly extract statistical moments of the output of interest, as explained in the first paragraph of Section 1.2.2.

Sylvain - p.21 - How are the groups of uncertainties defined? Is there a table?

Even though the uncertain parameters, their groups and their ranges of uncertainties might be the same for other case studies, they have been especially adapted for the present case study, i.e., Belgium. Consequently, I decided to exhaustively list these uncertain parameters in the chapter dedicated to the case study (see Section 2.4). However, to not leave the reader handing there and wondering if there other parameters and how we have decided to group them, I have added a reference to Section 2.4 at the end of Section 1.2.1 focusing on the characterisation of the uncertainties:

Section 2.4 gathers the list of the uncertain parameters considered in this work.

Sylvain - Table 1.2 - what are the other parameters?

See previous comment.

Sylvain - p. 57: Why a uniform distribution? A gaussian would clearly be more appropriate. Maybe some uncertainties are underestimated (because clipped by uniform distribution).

As already written in the first paragraph of Section 1.2.1, given the scarcity of data to actually define a distribution of uncertainty for the parameters, the common practice is to consider uniform distribution. As detailed by Coppitters [23]: "Distributions are typically defined based on large datasets, which are not always at hand for each parameter. Therefore, when no meaningful information can be extracted on the distribution from a limited dataset, a uniform distribution is typically assumed, which assigns an equal probability to each value within a range. This approach is similar to assigning an interval to a parameter, but takes advantage of the central tendency when uniform distributions are propagated through a system model (i.e., central limit theorem)". Given what is already in the thesis manuscript and these further explanation, no modification has been brought to the manuscript in this regard.

REINFORCEMENT LEARNING

Stefano - p. 31: Can you explain the need of using NN here? Couldn't you just run the energyscope model?

The need of using NN is in the learning phase of the RL approach, not in running EnergyScope. The justification to use NN is already detailed in Section 1.3.2: "Before jumping to the choice of the learning algorithm, it is worth noting that we opted for the combination of RL with Deep Neural Network (DNN), called Deep Reinforcement Learning (DRL). Among others, one of the main drawbacks of traditional RL algorithms, i.e., without the use of Neural Network (NN), is that it suffers from the "curse of dimensionality" when facing problems with continuous action and state spaces (see Chapter 4). By approximating the state-action function with its parameters (i.e., weights and biases), DNN can address this difficulty. "
    Given what is already written in the manuscript, I have not brought modification in this regard.

Sylvain - p. 27 When presenting the advantages of RL, you mention model-free approach. Ok, but you have a representation of the real world available to train the model!

Indeed, we know the input parameters, the constraints and the objective function implemented in EnergyScope to optimise the transition pathway of the whole-energy system. In the RL framework, a model is representation of how the environment will respond to the agent's actions. Unlike other cases such as grid world, the dynamics of

the environment, i.e., the transition from one state to another given the uncertainties and the actions taken by the agent or the consequent reward function, is not known. Going for a model-free approach, we avoid building a model within the agent to inform it about this (complex) dynamics.

This aspect is already explained in Section 1.3.2: "Given the assumed absence of knowledge of the agent about the dynamics of the environment, i.e., its transition or reward functions, we needed a so-called "model-free" learning algorithm." Given what is already written in the manuscript, I have not brought modification in this regard.

PRINCIPAL COMPONENT ANALYSIS

Stefano - p. 32: Why is PCA needed? Wouldn't it be easier to just aggregate similar outputs of interest?

Aggregate similar outputs of interest, without prior knowledge about these "similarities" would be challenging and require assumptions to carry out this aggregation, especially given the size of the problem (113 technologies over 7 representative years). The objective of PCA is to alleviate this effort and automatise this aggregation in order to capture the main variance of the design through the whole transition in a reduced number of principal components. It is reminded in Section 5.1.1: "Even though the following observations could be made by analysing the distribution of installed capacities (see Appendix D.3) or the covariance matrices, the PCA decomposition offers a more visual and summarising representation of the main trends of variation."

Given what is already in the text and these explanations, I have not brought modification to the manuscript in this regard.

Stefano - p. 42: Figure 1.17. What is your definition of robustness? Having a tight distribution but all shifted towards very suboptimal costs seems to fit your definition. Please clarify.

As discussed during the private defense, it is more the spread of variation of the distribution that matters to characterise the robustness rather than the average position. This is now clarified at the end of Section 1.4.2:

It is really the range over which the distribution spans, $2 \cdot \text{MOE}$, that matters to characterise the variability of the projections of a roadmap. Indeed, as $\text{PC}_{\text{transition}}$ are vectors composed of positive and negative coefficients, the average position of the distribution, μ, does not bring insight about the robustness of a roadmap.

Sylvain - p. 39 Why are their outliers in the first case? Isn't a bit arbitrary to set them to a min/max value?

As detailed in Section 1.4.2, even though these points result from the optimisation and make sense mathematically, they are defined as outliers as they fall out of the whiskers of their respective box plot. The way we managed these outliers is arbitrary but is fair trade-off between leaving them as they are which would mislead the direction of PCs and completely removing them. As extensively discussed in Section 5.1.1, this pre-processing step will mostly affect the LT-heat sector where heat pumps running on methane are installed in rare cases, i.e., less than 10% of the 1260 transitions. Given the size of this sector, i.e., between 22% and 27% of the EUD for Belgium, and the LP approach where there is a complete substitution of a technology by another one under certain conditions, these gas-HP can have a major weight in the system. However, to keep the main trends of variation without being "polluted" by outlying results (here, less than 10% of the cases), we proceeded that way.

Given what is already in the text and these explanations, I have not brought modification to the manuscript in this regard.

CHAPTER 2 - CASE STUDY

GENERAL AND INTRODUCTION

Stefano - I am a bit underwhelmed by the many nitty-gritty data in this Chapter. While it is surely important to document everything, couldn't at least part of this be moved to the Appendix?

Most of the data about the Belgian case study have been collected by Limpens [16]. The objective of this Chapter was to focus on my contributions: non-energy demand (NED), electrofuels, SMR, uncertain ranges for the pathway model and CO_2-budget. However, to put these contributions in perspective with similar features in the model, I have decided to keep general information about the end-use demands, the resources and the conversion technologies. Consequently, I have kept the same level of information in Chapter 2 rather than in appendix.

Sylvain - p. 45 How is the range accounted for the characterisation of private mobility technologies?

Indeed, the increase of the range is a consequence of the increased efficiency and battery capacity. Consequently, I have removed the mention to the range at the end of the last paragraph in the contributions of Chapter 2.

> Regarding BEV, while the CAPEX has been kept unchanged, the efficiency and the battery capacity have been increased.

RESOURCES

Sylvain - p. 51 Last paragraph of p. 51 is not clear. Are we talking about the purchase cost or the CO2 content?

There was indeed a confusion in the information to deliver in this paragraph. For the sake of clarity, I have restructured Section 2.2. After the introductory paragraph, the graphs and the following paragraph focus on the cost of purchasing. The two last paragraphs address the aspects of availabilities and global warming potentials, respectively.

CONVERSION TECHNOLOGIES

Stefano - Figure 2.5: What is the purpose of the violet line between "biomass gasification" and "methanolation"?

These were actually two different arrows, one pointing from "biomass gasification for CH3OH" to "Methanol" and the other from "Methanolation" to "Methanol". To avoid this confusion, the figure has been updated and the origin of these arrows are now on different vertical levels (see Section 2.3).

Sylvain - p. 54 Is there a differentiation between ground mounted and rooftop PV?

In the continuity of Gauthier Limpens' works [16], we consider here only rooftop PV. This potential of 59.2 GW corresponds to 250 km^2 of available roof well oriented that exist today. Accounting for ground mounted PV would almost double this potential, as shown in Paolo Thiran's thesis. In future works, it would be interesting to also implement this additional potential, especially for the sake of harmonisation of input data. On the contrary, Elia, the Belgian TSO, foresees a much more limited increase of installed PV, i.e., 18 GW by 2034 [25]. Consequently, for this thesis, I have decided to stick to this intermediate potential of 59.2 GW. For the sake of clarity, I only added "rooftop" in the second paragraph of Section 2.2:

> On the other hand, wind, solar, hydro and uranium are limited by the technical potentials of rooftop PV panels (59.2 GW) [...]
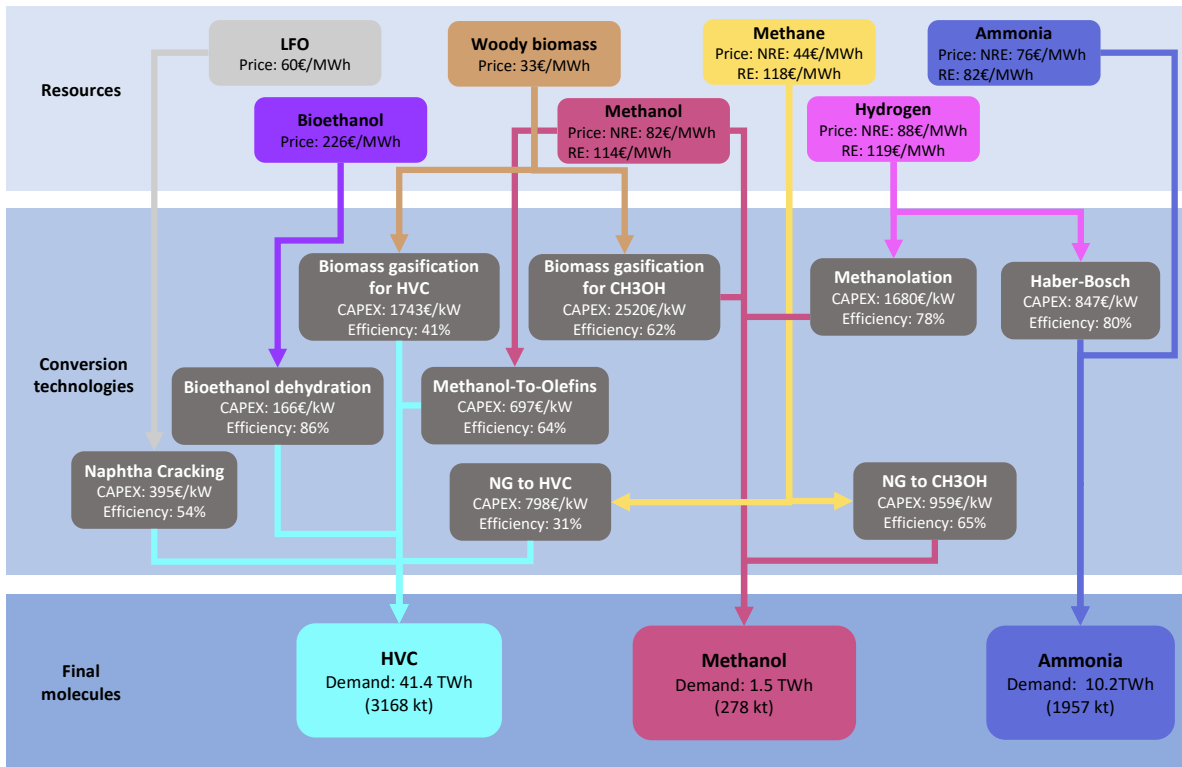
Sylvain - p. 51: Offshore wind max capacity is too low and PV is lower than Bregilab.

Concerning the potential of PV, see previous comment. Regarding offshore wind, we have assumed a conservative potential of 6 GW as the lower bound of the forecast done by the Belgian offshore platform[1]. Similarly to EnergyVille [6], we could have gone up to the upper bound of 8 GW. Going much higher, such as 24 GW for the "Electrification" scenario of EnergyVille, would account for access to a part of the 150 GW offshore wind park project in the North Sea signed betwee Belgium, Germany, Denmark and the Netherlands (the "Esbjerg Offshore Wind Declaration"). Since these potentials have been discussed and detailed in previous works and are not the main topic of my thesis, I have not brought any further modification to the manuscript in this regard.

Sylvain - p. 51 Why investigating SMR?

As discussed during the private defense, we have decided to investigate to role of nuclear energy in the future for two main reasons: hot topic in Belgium and similar study by EnergyVille [6]. First, when presenting the results of our work at conferences/meetings, we have been asked many times how our results, massively rely-

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[1]https://www.belgianoffshoreplatform.be/fr/

ing on imports of renewable molecules, were influenced by the installation of nuclear power plants by 2050. Second, during my thesis, EnergyVille delivered a report PATHS2050 where, among others, they investigated the impact of SMR. As they observed that installing SMR would significantly reduce the need to import renewable molecules, we also wanted to assess this impact in our work. Given these explanations, no further modification has been brought to the manuscript in this regard.

Sylvain - p. 53 4850€/kW is at the lower end of the EnergyVille scenario for SMR (4500€/kW). This is a very optimistic price forecast! Current tenders for 3rd generation are higher than 100€/MWh. There are papers showing that SMRs are not really expected to be cheaper than 3rd generation. How realistic is 41 €/MWh? LCOE of SMRs would be much higher if: - the capital cost was more realistic and, - the Capacity factor was lowered to account for their flexible use.

As discussed during the private defense, similarly to EnergyVille [6], we have considered the same CAPEX for SMR as the one considered for conventional nuclear power plants. Where EnergyVille considers a nominal CAPEX of 7500€/kW (like the current large Gen III design of Hinkley Point in the UK), we considered 4850€/kW like the CAPEX of conventional nuclear units in EnergyScope.

On top of the uncertainty applied to the CAPEX of SMR [-40%, 44%] considered in the thesis, I carried out a test on these assumptions by plotting the LCOE of electricity-production units considering different assumptions for SMR (see Figure 4.3). Even considering 50% more expensive SMR subject to a higher discount rate (5% versus 1.5% for the other technologies), we notice that SMR keeps on being more cost-competitive than other flexible production units, like e-ammonia CCGTs, that are substituted by SMR when the latter can be installed (see Chapter 3). In other words, it means that the optimistic values assumed for SMR in the thesis lead to a cheaper whole-energy system but does not affect its design, i.e., the installed technologies. Consequently, no further modification has been brought to the thesis regarding this comment.

Stefan - SMR must be revisited if a paper is published.

See previous comments.

Sylvain - p. 53 What about fuel cost?

Even though the cost of purchasing uranium was already presented in Figure 2.3 of the thesis, I have added this value in Table 2.1:
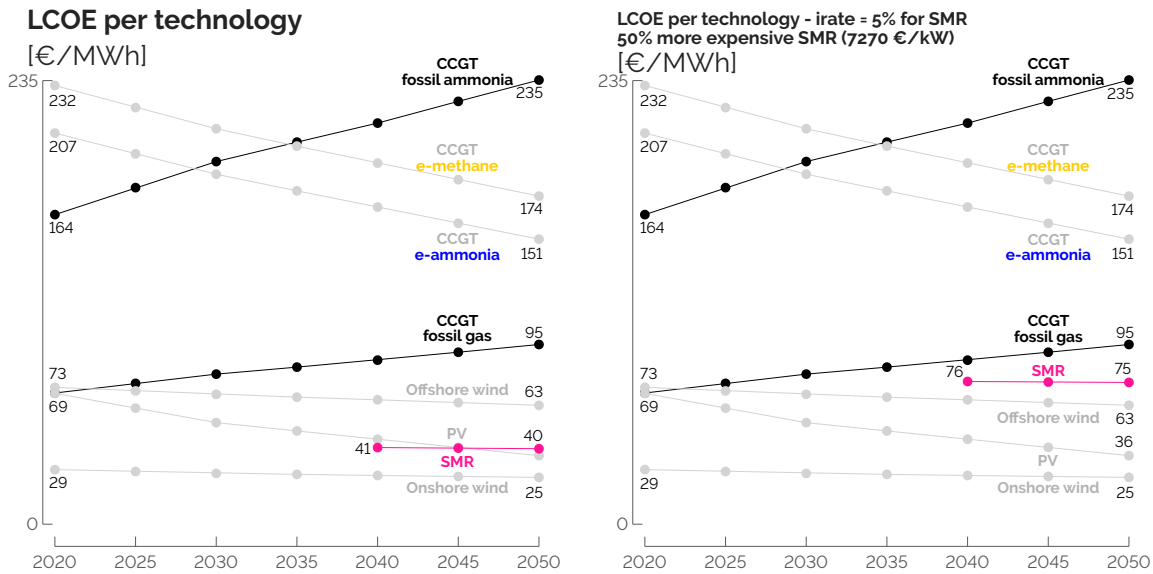
Figure 5: LCOE per technology producing exclusively electricity considered in the thesis (left) and same LCOE but, this time, with a higher CAPEX (7270€/kW versus 4850€/kW in the thesis and a discount rate of 5% on this technology. Even considering these less favourable assumptions for SMR, it still outcompetes other flexible production units like CCGT running on e-ammonia.

Table 2: 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.

Feature	Value	Unit
CAPEX	4850	€/kW
Annual OPEX	103	€/kW/year
Lifetime	60	year
Cost of purchasing uranium	**4**	**€/MWh**
Efficiency	40%	-
Maximum capacity	6	GW
Annual availability	85%	-
Operational year	2040	-
Flexibility	Full	-

Sylvain - p. 55 - Figure 2.5 - Coupled with heat for endogenous and exogenous reactions?

Indeed, the potential consumption/production of heat and/or electricity for each conversion process is considered in the model. For instance, the Methanol-To-Olefins (MTO) process consumes 1.24 GWh of methanol and 0.33 GWh of high-temperature heat to produce 1 GWh of HVC, which makes a 64% efficiency. To clarify this point, the caption of Figure 2.5 has been extended:

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). **The efficiencies account for the potential consumption/production of heat and/or electricity within each conversion process.** Values stand for 2035. Graph from [11].

Sylvain - p. 56 Are modal shares exogenously set?

In line with Limpens et al. [1], modal shares are indeed exogenously set. This aims at keeping some realism and ensures the need of less cost-competitive options like private versus public transport or decentralised versus DHN heating. To clarify this point, it is now explicitly written in Section 2.4:

[...] (ix) other parameters like the discount rate or the **exogenous** modal share change in different key sectors.

Chapter 3 - Atom-vs-molecules

General

Stefano - Would it be fair to say that the scope of this Chapter is adding one technology (SMR) to the model? Is this a significant contribution?

Besides having added SMR to the model which is one of the contributions regarding the case study (Chapter 2), the main contributions of this chapter is the global sensitivity analysis (GSA) performed on the optimisation of the transition pathway of a whole-energy system with 34 uncertain parameters. When applied to the case study of Belgium, this analysis also allowed to highlight the competition between SMR and some of the imported electrofuels (mostly e-ammonia and e-methane) by 2050.

To make it clearer from the beginning of the Chapter, I have extended the contributions of Chapter 3:

This GSA applied to a model optimising the transition pathway of a whole-energy system with these many uncertain parameters is the main contribution of this chapter. Through this analysis, we also managed to point out the impact of integrating SMR in the Belgian energy system as well as the main drivers of the import of e-hydrogen, e-methane, e-ammonia and e-methanol by 2050.

Stefano - What is the learning of this chapter? I was underwhelmed by the long list of results. What is the take-away?

The results are deeply detailed in Sections 3.1 and 3.2. These sections address the impact of adding SMR in the deterministic solution (i.e., uncertain parameters at their respective nominal value) of the Belgian energy transition and global sensitivity analyses on different outputs of interest, respectively. The purpose of these two sections is to give numerical substance to the main conclusions and take-aways that are listed in Section 3.3:

- If available, SMR is installed and mostly affect the electricity and high-temperature sectors;

- To minimise the variation of the total transition cost, the key parameter is the cost of purchasing electrofuels where parameters related to SMR (availability and CAPEX) have much lower impact;

- E-ammonia and, to a lesser extent, e-methane imports by 2050 are impacted by the availability of SMR whereas e-hydrogen and e-methanol are rather influenced by variation related to transport technologies and non-energy demand, respectively;

- Even though SMR and electrofuels are in competition, they do not limit the deployment of VRES in Belgium. In other words, investing in wind and solar is a must-do for the Belgian energy transition;

- Given the set of assumptions, especially considering the end-use-demands and the local potential of VRES, Belgium will need to import molecules in the near future. On top of investing into VRES, it seems reasonable to invest in the imports of these electrofuels as betting on SMR means letting the short-term emissions go up and, potentially, requiring significant (and quick) adjustments in case the technology is not ready on time to still respect the CO_2-budget.

Given these explanations and what is already written in the text, I have not brought further modification to the manuscript in this regard.

Stefano - p. 74 - Figure 3.8: this graphs looks potentially interesting but it is not sufficiently well explained.

The objective of this set of figures is to point out the key parameters that drive the variation of some outputs of interest. Taking the case of Figure 3.8, we focus on the import of e-methanol in 2050. On the x-axis, we represent the value taken by the uncertain parameters in the different samples. As the range is not the same for all the parameters, we have limited this axis from "Min" to "Max". The y-axis represents the feature of interest. The drawn lines represent average trend lines between the output of interest and one specific parameter. For the case of Industry EUD, for samples of the GSA where this uncertain parameter is at 35% of its range, the mean value of methanol imported in 2050 is roughly 50 TWh. The distributions present on the extreme left and right of the graphs correspond to the distributions of the output of interest for the samples of the GSA where the considered parameter takes a value in the bottom (left) or top (right) 15% of its range.

To improve the readability of this figure, I have updated the text zones to specify that these lines and distributions represent results of some specific samples of the GSA. Additionally, I have added a text zone to remind that the value between brackets is the Sobol' index of the considered parameter regarding this specific output of interest, and added this information in the caption of the figure:
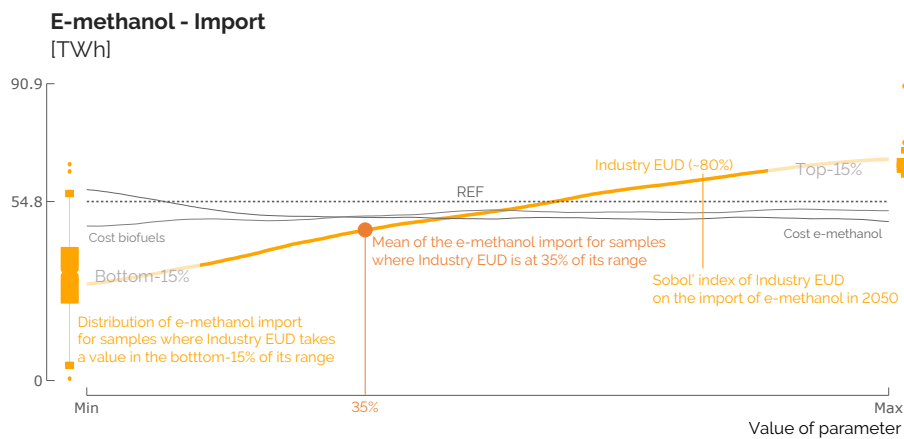

Figure 6: Trend lines of the key parameters (and their Sobol' index) on the import of e-methanol in 2050. Around these lines, box plots point out the distribution of the output of interest for the extreme values (either bottom-15% or top-15%) of some parameters. The grey dashed line gives the value of the output of interest in the REF case.

SMR

Stefano - p. 70: "in other words, the variation of the parameter $f_{max,SMR}$...". I am not sure that this sentence is equivalent to the previous one. Please clarify.

The Sobol' index is the ratio between the variance of the total transition cost due to the variation of one parameter and the total variance of the total transition cost. If $f_{max,SMR}$ takes a value between 0 and 0.59, the impact on the system, and, consequently, on its total transition cost, is the same: no SMR installed. A wide range of variation of the parameter leading to zero variation of the output of interest is one of the reasons to explain why the Sobol' index of this parameter is low. To clarify this point, I have rephrased the sentence in Section 3.2.1:

Given the uncertainty characterisation presented in Section 2.4, there are 60% chance that no SMR could be installed. **When $f_{max,SMR}$ takes a value between 0 and 0.59, the variation of the total transition cost is only due to the variation of the other parameters.**

Stefano - p. 71, Table 3.1: isn't the low impact simply due to the low assumed potential? Is this finding meaningful?
Sylvain - p. 70 - But that's because the CAPEX is way too low. With more realistic values, the Sobol would be much higher.

These assumed low potential and CAPEX are indeed some reasons why the SMR-related uncertain parameters have a limited impact on the variation of the total transition cost as already stated in the first paragraph of Section 3.2.1: "However, given its limited deployment, up to 6 GW, SMR-related parameters have a lower impact on the variation of the total transition cost.". However, this is not the only reasons as detailed earlier in the same paragraph: the late potential availability (2040 at the soonest) as well as the "cheap and low-emitting fuel, the long lifetime leading to lower annualised CAPEX and higher salvage value.".

Given these explanations and what is already written in the manuscript, I have not brought further modification to the manuscript in this regard.

Sylvain - p. 67 - It really depends on what is considered primary energy in the case of nuclear

As specified in the table about SMR features (see previous comment), the considered fuel for SMR is uranium, as it is the case for conventional nuclear power plants. Given this, I have not brought modification to the manuscript in this regard.

Sylvain - p. 78 - Why this threshold? Shouldn't it follow the potential capacity?

The threshold locates at 60% of the uncertain parameter $f_{max,SMR}$ which represents the potential capacity of SMR. As presented in Section 2.4, this threshold corresponds to the possibility to install up to 6 GW of SMR in 2050. As already written in Section 3.2.2: "For the installed capacity of SMR, it is the availability of the technology that drives its installation (Figure 3.12). Not shown here but all the samples of the GSA highlight that SMR is installed to its maximum capacity, i.e., 6GW, as soon as possible." To smooth the trend curves of the different uncertain parameters, I have applied a rolling average. For this reason, the 60%-threshold does not appear on the Figure as sharp as it actually is.

Given these explanations and what is already present in the text, I have not brought further modification to the manuscript in this regard.

PV AND WIND

Sylvain - p. 64 - 15 GW of PV in 2025. Realistic?

In the continuity of Gauthier Limpens' thesis and in line with the rest of the research field, the objective of this thesis is to "illustrate the priorities to be taken in each of the sectors and the efforts to make in one sector to facilitate the integration of certain technologies into other sectors" [16]. This work highlights the "must-do" or "no-regret investments" to respect the (very) ambitious CO_2 budget imposed to the model. In this sense, besides the maximum potential of 59 GW solar-PV, we have not made assumption on the rate of deployment. 15 GW of PV in 2025 can be considered as very optimistic and Elia forecasts to have these 15 GW by 2030 [25]. I agree that not limiting the rate of deployment of PV (and wind turbines) is a strong assumption. For this reason, in the perspectives of this work (see Conclusion), I have already pointed this out as "a future work would be to constrain the deployment of local renewables.

Given these explanations, I have not brought further modification to the manuscript in this regard.

Sylvain - p. 69 - No curtailment at all? It would be nice to have the exact number.

There is indeed some curtailment, which remains very limited compared to the total production of solar-PV: 0.3 TWh versus 61 TWh. This information has been added in the paragraph dedicated to "High-temperature heat" of Section 3.1.3:

In the REF case, industrial electric heaters are mainly used to absorb the "over-production" of the 59 GW solar-PV when fully deployed, in the sunny days, and limit the yearly curtailment to a maximum of 0.3 TWh, 0.5% of the yearly 61 TWh produced by solar-

PV.

Sylvain - p. 69 - Very strange. Should be the same as for industrial boilers. No smart charging?

The difference between BEV and industrial electric heaters is that BEV is already a preferred option for electrification, even the REF case. BEV completely substitute diesel and gasoline-cars as soon as possible in the transition and there cannot be more cars as private mobility is limited to supply up to 50% of the demand of passengers mobility. Unlike high-temperature heat, there is no modal swap due to the installation of SMR.

Given these explanations, I have not brought further modification to the manuscript in this regard.

OTHERS

Sylvain - p. 63 What does efficiency change in the installed capacity?

Indeed, the efficiency only has an impact on the amount of primary uranium needed to produce the electricity. Consequently, I have removed this part of the sentence in the first paragraph of Section 3.1.1.

Overall, given the restriction on yearly availability and the slightly higher electrification [...]

Sylvain - p. 72 - Battery trucks are gaining momentum. Is the hydrogen route really the way to go?

In general, the model gives fuel-cell trucks as the favoured option for the future of road freight transport given more cost-competitive options for electrification like private mobility and low-temperature heat. However, as illustrated in the ROB roadmap (see Section 5.2.1), battery trucks seem to be the cost-optimal solution to transition between diesel and either hydrogen trucks, when fossil and electrofuels are assumed to be expensive.

In the Global Sensitivity Analysis, electric trucks are the favoured option for a limited set of samples, about 10% (see Appendix D.3).

Given these explanations and what is already present in the text, I have not brought further modification to the manuscript in this regard.

GENERAL

Stefano - p. 85, Figure 4.1: Does it mean we can run "infinite energy transitions"? Is this realistic? Isn't the "learning" supposed to happen during the different stages?

Even though Reinforcement Learning can be applied to problems with infinite time-horizon discounting reward coming further in the future, it is not the case in my thesis. Indeed, each episode (i.e., the transition) is finite. The purpose of Figure 4.1 was to focus on the reward function and how it articulates in the action-state-reward process. As already represented in this figure, three situations can terminate an episode: (i) infeasible optimisation, (ii) overshot CO_2-budget before 2050 or, (iii) reaching 2050. This is now clarified in the caption of Figure 4.1:

Reward function, R. Before reaching 2050, the episode is prematurely ended and a negative reward is given if the optimisation is infeasible or if the CO_2-budget is exceeded. If the optimisation provides a solution and the CO_2-budget is not exceeded, the episode continues. Finally, if the episode goes until 2050, the reward is a weighted sum between the capped cumulative emissions and the total transition cost, and the episode terminates. After terminating an episode, the process starts over at the initial state, i.e., 2020.

Stefano - How can you account for pivotal events/shocks in the system?

Given the limited foresight of the myopic approach, we can implement, pivotal events/shocks can be implemented through uncertain parameters. For instance, this is how we have implemented the potential to install SMR in 2040 at the soonest. Given the probability described in Section 2.4, the technology can (or not) be installed. However, as detailed in Section 1.2.1, for the other uncertain parameters, they keep the same value relatively to their type and range for the whole transition. In other words, we do not allow zig-zag where, for instance, a cost of purchasing an energy carrier was low for the first half of the transition and, suddenly, in 2040, becomes very high.

Given these explanations and what is already written, I have not brought modification to the manuscript in this regard.

Stefano - Overall, I suggest adding a diagram to Chapter 4, detailing what are the actions available to the decision-maker.

Complementary to the text in the core of the manuscript, I have added a diagram to detail the agent's actions and how they impact the model: taken at the beginning of

the time-window to optimise (year Y), the four actions impact (i) the emissions of the system at the end of the time-window (year $Y + 10$) and, (ii-iv) the consumption of fossil gas, LFO and coal at years $Y + 5$ and $Y + 10$.

Figure 7: Actions available to the decision-maker. Taken at the beginning of the time-window to optimise (year Y), the four actions impact (i) the emissions of the system at the end of the time-window (year $Y + 10$) and, (ii-iv) the consumption of fossil gas, LFO 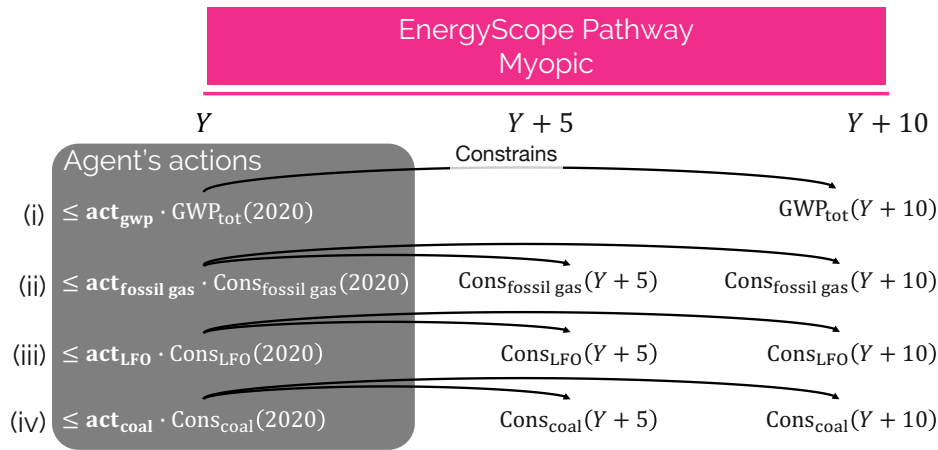and coal at years $Y + 5$ and $Y + 10$. Unlike the first action that sets a target for the end of the time-window, the last three aim at limiting the consumption of these fossil resources over the whole time-window.

Stefano & **Sylvain** - How does this approach compare, for example, to stochastic programming?

This work will be done for the subsequent paper on RL. The strategy would to implement a simplified case study (i.e., smaller system, fewer uncertain parameters and more limited time horizon) where it would be "computationally more affordable" to test the stochastic programming approach and compare it with the optimal policy delivered by the RL approach. Consequently, regarding this comment, there has not been further modification brought to the manuscript.

Stefano - p.91, Table 4.2: how do you differentiate between actions that depend on the agent and exogenous uncertainties? More in general: how is uncertainty integrated in the RL framework?

Both, agent's actions and exogenous uncertainties, change the value of some parameters of EnergyScope Pathway. However, where the sample of uncertainties is drawn once and for all at the beginning of the episode as explained in Section 1.2.1, the agent's actions are taken at the beginning of each 10-year time window. This is now

clarified at the beginning of Section 1.3.2 and the updated version of Figure 1.7, and its caption (see Figure 8 in the present document):

Before starting an episode, a sample of uncertain parameters is drawn and affects the environment, EnergyScope Pathway, according to the methodology detailed in Section 1.2.1.
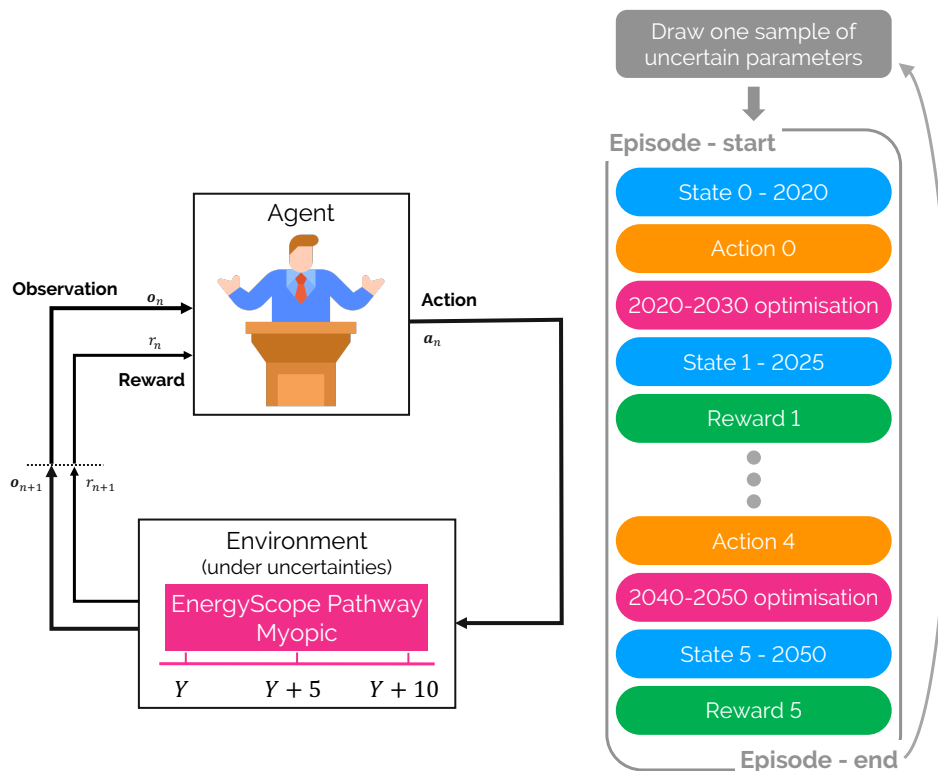

Figure 8: The Reinforcement Learning (RL) framework applied to the myopic optimisation of the energy transition pathway between 2020 and 2050. Here, the agent interacts with its environment, i.e., the energy-system model on a limited decision window of 10 years. At the beginning of each episode, one different sample of uncertain parameters is drawn and affects the environment, EnergyScope Pathway, according to the methodology detailed in Section 1.2.1.

Stefano - Explain more in details the different steps in the RL approach.

Besides the general concepts/fundamentals detailed in Section 1.3.1, the application of the RL approach on the myopic optimisation of the energy transition of a whole-energy system is detailed in Section 1.3.2. Now, Figure 1.7 has been updated to clarify the difference between the uncertainty of parameters and the agent's actions as

well as the interactions between the RL code (action, state, reward) and EnergyScope Pathway (optimisation of the concerned 10-year time-window). I have also added a diagram to explain the impact that the agent's actions have on some parameters of the model.

Given what was already in the manuscript and the aforementioned modifications, I have not added further information to detail the different steps of the RL approach.

GRAPHS AND RESULTS

Stefano - Work on the graph of slide 19 (there is a misunderstanding on the fact that the grey curve is labelled as failure but they are failures in the future)

To clarify this point, I have extended the caption of the related figures (see previous comments) and added two sentences in Section 4.2.2:

Since infeasible cases or those that overshoot the CO_2-budget are discarded before reaching 2050 (see Section 4.1.2), the number of attempts that reach further steps in the transition progressively decreases. Consequently, the share of successful transitions compared to failures progressively increases with time.

Stefano, **Stefan** & **Sylvain** - Graphs like the ones presented during the private defense (slides 22 and 24) should be better explained. In general, improve the presentation of the results, especially for the RL chapter.

Beside extending the captions and clarifying the reasons why the number of total attempts decreases when going down the graph, as detailed in the previous comment, I have brought smaller modifications into the text to improve the presentation of the results, especially in the RL chapter.

Stefan - What is the potential of what we can learn from the results of the innovative methods like RL? We could go further in the analysis as we know we have to phase out coal, install renewables.

First, I focus here below on each of the results sections of Chapter 4 highlighting the key conclusions already in the manuscript:

- **4.2.1 Reward and success**: (i) We have convergence of the learning process; (ii) Limiting success rate given the wide uncertainty ranges of some key parameters and the set of actions given to the agent; (iii) Near-term actions are needed.

- **4.2.2 States**: (i) Validation of the formulation of the reward function (first respect the CO_2-budget then minimise the cost); (ii) Reminder of the need for near-term actions; (iii) No-go zones in terms of share of renewables in the primary mix; (iv) Efficiency of the system does not give effective information for the agent to act upon.

- **4.2.3 Actions**: (i) Limiting GWP and consumption of fossil gas are the keys; (ii) Even in a myopic perspective, limiting LFO is ineffective as it is phased out by the cost-driven model; (iii) Unlike coal that would still be part of the mix if the agent did not limit its consumption.

- **4.3 Comparison with PF**: (i) Following CO_2-trajectory prescribed by PF would likely lead to failing the transitions with limited knowledge into the future; (ii) Succeeding myopic transitions relies more often on importing more electrofuels, mostly e-ammonia.

Phasing out coal is, of course, necessary as it is a highly-polluting resource. However, what this work shows is that, whatever the stage in the transition, a policy limiting the use of coal will always be effective, whereas one could think that coal should be limited only at early stages to get rid of coal-driven technologies once and for all for the rest of the transition. Consistency towards banning coal through the whole transition is needed. To insist on this aspect, this has been added at the end of Section 4.2.3:

Whatever the stage in the transition, a policy limiting the use of coal will always be effective, whereas one could think that coal should be limited only at early stages to get rid of coal-driven technologies once and for all for the rest of the transition. Consistency towards banning coal is needed.

About the installation of renewables, not only it is (obviously) necessary to maximise the chance to succeed the transition (see Chapters 3 and 4) but it also provides robustness towards additional investments to make when deploying a roadmap through a (more realistic) myopic transition (see Chapter 5). This conclusion was already drawn by Moret et al. [26] for the snapshot model and targeting the power sector only. Here, we extend this work and validate this conclusion for the whole transition pathway and addressing the additional investments in all the sectors.

Through the application of RL on the optimisation of the transition pathway, we are able to assess the effectiveness of a policy, which could be of interest to other researchers. This has been added at the end of the conclusions of Chapter 4:

This framework allows future research to test other policies on other case studies and identify the key actions and the timing to take them through the transition.

In conclusion, besides the results coming from the application to the specific case study of Belgium, a major added-value of this work is also to validate innovative approaches (RL and PCA) when applied to explore and optimise transition pathways under uncertainties. For instance, Section 4.2.2 shows that the reward function was properly defined to aim first at respecting the CO_2-budget then minimising the cost. It also provides innovative ways to visually present results in the field of the optimisation of transition pathway under uncertainties that suffers from the (overwhelming) curse of dimensionality. Via distributions or principal components, this work summarises a lof of information into graspable visuals that allow drawing effective conclusions such as the identification of sweet-spots and no-go zones.

Given these explanations and what is already written in the manuscript, I have not brought other modification to the text.

Stefano - p. 89: Figure 4.3 seems to deliver an important message (early action is needed to ensure we meet climate goals), but it is not clearly explained. Improve captions / add axes. Where do I see the "tipping points" in this figure?

Like other figures in this Chapter, Figure 4.3 represents distributions of features spreading over the x-axis. In this case, these are distributions of the rewards collected by the agent at the end of each episode of its learning process. For this reason, labelling the axis does not seem obligatory as the x-axis is nothing else than the feature (here, the reward) and the y-axis has no physical meaning expect representing how often the feature of interest took a certain value/range of values. Compared to the other similar figures of the chapter, I have not labelled the x-axis as, for Figure 4.3, the reward is the only feature represented whereas two or more features are gathered on the same figure.

With this in mind and what is already written in the caption of the figure and the core of the text, we can infer from the right hand side that 2040 is the "tipping year" as it represents the year at which the failures occur more often, compared to the other representative years.

Given these explanations and what is already in the text, I have not brought modifications to the manuscript in this regard.

Stefano - p. 90: What does it mean to succeed/fail in 2030? And why are the number of attempts reduced going down in the graph?

As discussed during the private defense, the grey curves represent the distribution of occurrences failing (i.e., infeasible optimisation or overshooting CO_2-budget) by

2050 at the latest. The number of remaining attempts reduce as prematurely ended episode are removed from the further counts. The purpose of displaying these numbers of "Total attempts" is to explain why the areas below the orange curves increase relatively to the grey curves. These two aspects are now explicitly explained in the caption of Figure 4.4 and the other similar figures:

> Exploration of the state space over the learning process: distribution of occurrence of cumulative emissions (left) and costs (right). **Number of remaining attempts decrease with time since infeasible problem and solutions overshooting the CO_2-budget are discarded prematurely, i.e., before reaching 2050. Besides infeasible problems, distributions labelled as "Failure" represent the attempts that overshot the CO_2-budget by 2050 at the latest.** The majority of successful transitions have cumulative emissions much lower than the CO_2-budget and are cheaper than the REF case.

Stefano - p. 94: Figure 4.6 seems to be less revealing than other figures. Also the figure caption seems to contradict the first statement following the figure. It would be important to clarify: which are the actions that emerge to actually matter?

Indeed, Figure 4.6 is less revealing as it shows no big trend in terms of neither impacting actions nor their timing in the transition. It is detailed in the first paragraph of Section 4.2.3 after which the figure should appear in the manuscript. I have worked to make Figures as close as possible to their related paragraph. However, in some cases, several other paragraphs come between them. To identify the actions that emerge to actually matter, we need to check if they are binding or not, as detailed in the subsequent paragraphs and in Figure 4.7.

Given these explanations and what is already present in the text, I have not brought further modification to the manuscript in this regard, except minor adjustment to get Figure 4.6 as close as possible to its related paragraph.

OTHERS

Sylvain - p. 87 - What is a step?

In the context of Reinforcement Learning, a step consists in taking an action, collecting a reward based on the previous state and the taken action and ending in a new state. Even though it was already mentioned in Chapter 1, the fact that the results come further from the methodology part makes it harder for the reader to remember the meaning of a step. It is now more explicitly defined in the first paragraph of Section 1.3.2:

> From this state, the agent takes a step: action, reward, new state.

and reminded in the first sentence of Section 4.2.1:

> The learning phase has been split into batches of 500 steps,i.e., 500 sequences of state-action-reward-new state.

Sylvain - p. 96 - The early constraints on generation avoid lock-in situations correct?

Correct. This confirms what Vogt-Schilb et al. [27] detailed in their works. To emphasise on this point, I have added one sentence in Section 4.2.3:

> In line with Vogt-Schilb et al. [27], the early constraints on generation and the sharper decrease of the emissions avoid lock-in situations.

Stefan & **Sylvain** - p. 97 - The agent can reach systems that are cheaper than any other solution obtained by the perfect foresight approach. How can this be possible?

This was observed on the annual system cost which is not the objective function of the Pathway model. It is more relevant to look at the total transition cost which is, logically, lower for the PF approach compared to myopic when facing the same sample of uncertain parameters. To clarify this aspect, I have removed the paragraph (and the graph) about the comparison of the annual system cost and added instead a paragraph (and a graph) about the comparison of the total transition cost in Section 4.3:

> Looking at the total transition cost, the combination of the agent's actions and favourable economic conditions (see Section 4.2.2) make the myopic transitions cheaper, on average, than the PF cases (see right side of Figure 9). This is also due to the fact that the perfect foresight approach always finds a solution even in worst conditions such as high cost of purchasing resources and high EUD. This explains the wider variability of the results too. However, with the same sample of uncertain parameters, given the assumed full knowledge over the whole time horizon, PF naturally results in a cheaper transition than its myopic equivalent.

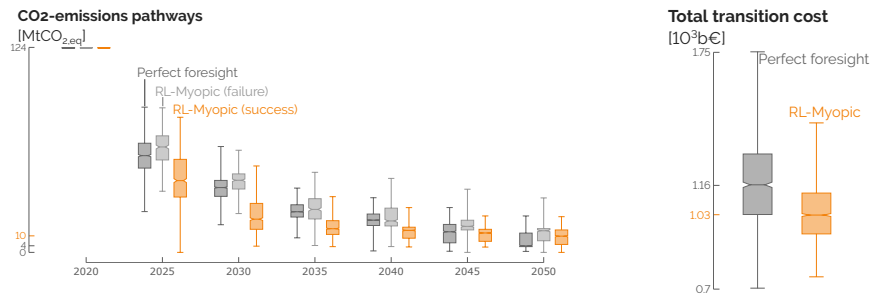**Sylvain** - p. 100 - What/where are the no-go zones? Is there a narrative to describe them ?

Figure 9: Comparison of CO_2-emissions pathways (left) and total transition cost (right) from the perfect foresight optimisation under uncertainties and the RL-based myopic optimisation. Myopic transitions succeed with a more drastic reduction of emissions in the short-term and, on average, more favourable economic conditions.

No-go zones are introduced in the second paragraph of Chapter 4: "[...] as well as no-go zones where the chances of succeeding the transition, i.e., respecting the CO_2-budget, are very limited." It is then detailed at the end of Section 4.2.2: "Below the near-term threshold of ~60%, this is the "no-go zone" where succeeding the transition becomes unlikely, except if betting on the future installation of SMR. " and in the caption of the related figure. Given the information already present in the manuscript, no modification has been brought in this regard.

Christophe - The concept of binding constraint was not clear.

Besides the information given in Section 4.2.3 of the manuscript, I do not see further explanations that could clarify more the concept of binding constraint in a Linear Programming (LP) problem. Consequently, regarding this comment, there has not been further modification brought to the manuscript.

Sylvain - p. 96 - Why 10 years if the step is 5?

Because the action limits the emissions of the system at the end of the 10-year time-window whereas limiting the consumption of fossil gas, LFO and coal is done over the whole time-window, as detailed in Section 4.1.1. Given what is already written in the manuscript, I have not brought modification to the manuscript in this regard.

CHAPTER 5 - PRINCIPAL COMPONENT ANALYSIS

Stefano - p. 101 - you mention different definitions of "robustness": which one do you use in your work?

This work assesses the robustness of the decision-making process in two different ways. On the one hand, using a Reinforcement Learning (RL) approach, it allows highlighting the key actions to take to support a myopic transition and maximise the chances to respect the emissions-budget. On the other hand, after drawing a robustness-metric based on a Principal Component Analysis (PCA) approach, this work investigates how much a planned roadmap is sensitive to additional investments required in a myopic transition with progressively unveiled uncertainties. In other words, we use two different definitions of robustness: (i) the ability of a policy to maximise the chances to succeed a myopic transition under uncertainties to meet a CO_2-budget, (ii) the ability of a technological roadmap to limit the investment into additional capacities when tested in myopic conditions.

These two definitions are now clearly introduced in the introduction of the manuscript:

Chapter 4 focuses on the robustness of a policy as its ability to maximise the chances to succeed a myopic transition under uncertainties to meet a CO_2-budget.

Chapter 5 assesses the robustness of different technological roadmaps as their ability to limit the investment into additional capacities when tested in myopic conditions.

at the end of the introductory paragraph of Chapter 1:

Finally, an agent-based Reinforcement Learning (RL) approach is detailed to address the robustness of a policy in uncertain transitions with limited vision in the future. This chapter ends with a PCA-based approach to draw a robustness metric and assess the ability of technological roadmaps to limit the investment into additional capacities.

in the second to last paragraph of the contributions of Chapter 1:

The third principal methodological contribution is the use of Principal Component Analysis (PCA) to assess the robustness of a technological roadmap. Given the uncertainties and the timespan of the transition, this approach allows highlighting the main "directions" of variation of the system design (i.e., the installed capacities). After this step of identification, strategies can be projected on these directions to see how robust they are to the need of additional capacities.

In the second paragraph of Chapter 5, we list different definitions of robustness. In this work, we consider indeed "static" robustness as we aim at either getting a policy that maximises the chance to succeed the transition or a technological roadmap that limits the need to invest into additional capacities. It is now clarified in the second paragraph of Chapter 5:

Where Chapter 4 addressed the static robustness of a policy as its ability to maximise the chances to succeed a myopic transition, the objective of this chapter is to apply the method described in Section 1.4 to deal with the static robustness of pathway technological roadmaps, defined as their ability to limit the need to invest into additional capacities.

Finally, I have gone through the manuscript and made sure that RL-based approach was addressing the robustness of **policies** (i.e., sequences of actions) whereas the PCE-based approach rather focuses on the robustness of **technological roadmaps**.

Stefano - p. 109 - how is Gamma-robustness implemented here? It seems like it is in some sense "manually" forced? Explain better how the ROB solution is derived.

To my understanding, the Γ-robustness consists in considering a number, Γ, of uncertain parameters taking their worst-case value simultaneously and "evaluate how the solution of the optimisation problem changes when varying Γ" [26]. Inspired by this approach, we have arbitrarily set this value to $\Gamma = 6$ to consider the six first uncertain parameters impacting the most the variation of the total transition cost. Consequently, the ROB technological roadmap is obtained from the deterministic optimisation of the perfect foresight pathway accounting for these six parameters (i.e., costs of purchasing electrofuels, fossil fuels and biofuels as well as the industry EUD, the interest rate and the variable OPEX of technologies) at their respective worst-case value. As it does not exactly follow the robust approach of Bertsimas and Sim [28] and Moret [20], I have changed the first sentence of Section 5.2.1:

Rather than considering all the uncertain parameters at their worst values as in the work of Soyster [29], we follow a **method inspired by** the robust approach of Bertsimas and Sim [28] and Moret [20].

Moreover, the facts that this $\Gamma = 6$ is arbitrarily set and that the ROB roadmap, like the REF and SMR ones, results from a deterministic optimisation of the perfect foresight pathway are now clarified:

In the present analysis, we label the roadmap as "robust" (ROB) by arbitrarily setting $\Gamma_{obj} = 6$. The ROB roadmap results from the deterministic optimisation of the perfect foresight pathway where the following six parameters are set at their worst-case value (upper bound of their range): costs of purchasing electrofuels, fossil fuels and biofuels as well as the industry EUD, the discount rate and the variable OPEX of technologies.

Christophe - When using the word "component", there seems to be a confusion and it is not always easy to understand if you refer to the vector or the coefficient related to one of the original variable.

The confusion probably comes from the fact a Principal Component (PC) actually represents an eigenvector of the covariance matrix. This vector is, by definition, composed of **components**, each of them being a coefficient related to a specific original variable. Parts where the word "component" is not directly linked to "vector", "eigenvector" or "PC" are those that could mislead the reader. Modifications have been brought to these parts.

   End of second paragraph of section 1.4.1:

Moreover, this means that **the coefficient** α_{ki}, i.e., the component of $\boldsymbol{\alpha_k}$ related to the ith original variable, x_i, gives its weight in the kth PC, i.e., z_k.

CONCLUSION

Stefano & **Sylvain** - p. 119 - the statement mentioning the "major added value of the perfect foresight" approach seems surprising and needs to be clarified. The decreasing CO_2 emissions trajectories shouldn't be a S-shaped (logistic) curve?

I agree that this sentence and what came next focused on the perfect foresight approach whereas the rest of the paragraph rather targets the RL-based myopic results. Therefore, I have reformulated the end of this paragraph and focused on the shape of the decreasing CO_2 trajectories. These are indeed S-shaped curves but that are sharper for the myopic approach than in the PF results.

This work also highlighted a major difference between the perfect foresight (PF) approach and the agent-based myopic transitions. Given the assumed full knowledge on the future, the trajectories to decrease the CO_2 emissions resulting from perfect foresight are more progressive, and foreseen to be more applicable, compared to a sharper drop at the early stages of the transition, like in the myopic approach.

Stefan - The conclusion is a summary and should rather be a discussion.

I decided to split the conclusion into four blocks of paragraphs. The first two (from page 117 to the top of page 120, in the version of the manuscript submitted before the private defense) are indeed a summary of (1) what we have done in this thesis (case study and methodology) and (2) the results we have got. The two last blocks,

however, take a step back from the results and aim at drawing main conclusions, discussing them and providing decision-makers with further insightful information and methods to plan the energy transition. Consequently, I have not brought modification to the manuscript in this regard.

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