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 came 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.

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.

General comments/questions

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?

Assumptions - Fine tuning

Stefano - 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?

Graphs

Stefano & **Stefan** - Graphs should be better explained. Many axes labels are missing, and the captions are often insufficient to read the figures.

Structure

Stefano - 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.

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.

REFERENCES

Stefano - 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.

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.

INTEREST RATE

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 - 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.

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

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?

Stefano - Can you explain the logic of the annualization factor in the pathway model and the choice of N=5 for the uncertainty ranges?

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.

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.

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

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?

UNCERTAINTY QUANTIFICATION

Stefano - p. 23: is PCE an appropriate method for LP / MILP models. There is a good fit for the total cost, which is often quite linear, but how about technology choice / sizing?

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

Stefano - Why is PCE needed is EnergyScope is already very fast?

REINFORCEMENT LEARNING

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

PRINCIPAL COMPONENT ANALYSIS

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

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.

CHAPTER 2 - CASE STUDY

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?

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

These are actually two arrows pointing from "biomass gasification for CH3OH" to "Methanol" and 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.
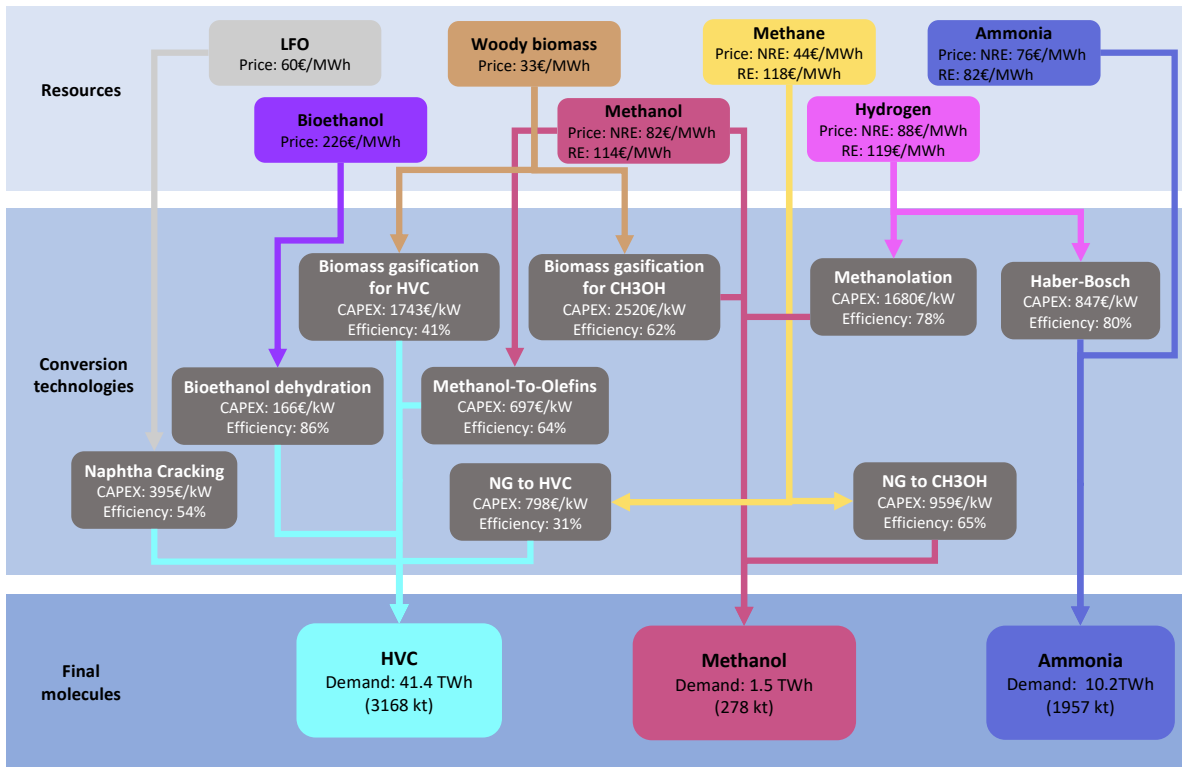
REINFORCEMENT LEARNING

BINDING

Christophe - The concept of binding constraint was not clear.

Besides the information given in Section 4.2.3 of the manuscript (and reminded here below), I do not see further explanations that could clarify 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.

To identify the actions that have an actual impact on the environment, we can check if they are binding or not. In a LP problem, constraints represent hyperplanes in the domain of variables. In a two-dimension space, these are straight lines (see Figure 1). When the problem is bounded and feasible, these lines are the edges of a convex polygon: the domain of feasibility. The optimal solution, $\mathbf{x}^*$, is the combination of variables leading to the optimal value of the objective function. Besides being within

Resources

LFO — Price: 60€/MWh

Woody biomass — Price: 33€/MWh

Methane — Price: NRE: 44€/MWh, RE: 118€/MWh

Ammonia — Price: NRE: 76€/MWh, RE: 82€/MWh

Bioethanol — Price: 226€/MWh

Methanol — Price: NRE: 82€/MWh, RE: 114€/MWh

Hydrogen — Price: NRE: 88€/MWh, RE: 119€/MWh

Conversion technologies

Biomass gasification for HVC — CAPEX: 1743€/kW, Efficiency: 41%

Biomass gasification for CH3OH — CAPEX: 2520€/kW, Efficiency: 62%

Methanolation — CAPEX: 1680€/kW, Efficiency: 78%

Haber-Bosch — CAPEX: 847€/kW, Efficiency: 80%

Bioethanol dehydration — CAPEX: 166€/kW, Efficiency: 86%

Methanol-To-Olefins — CAPEX: 697€/kW, Efficiency: 64%

Naphtha Cracking — CAPEX: 395€/kW, Efficiency: 54%

NG to HVC — CAPEX: 798€/kW, Efficiency: 31%

NG to CH3OH — CAPEX: 959€/kW, Efficiency: 65%

Final molecules

HVC — Demand: 41.4 TWh (3168 kt)

Methanol — Demand: 1.5 TWh (278 kt)

Ammonia — Demand: 10.2 TWh (1957 kt)

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the domain of feasibility, it is proven that this optimal solution, when unique[a], locates on a vertex of the domain [1]. The constraints intersecting at this vertex are considered as binding, actually limiting the objective function to be more optimal. In other words, binding constraints, when tightened, aggravate the objective value function. If these are inequality constraints, as represented in Figure 1, it means that their left and right sides of the equation are equal.

[a]There are cases where the objective function has the same optimal value along an entire edge. In this case, there is an infinity of solutions and the problem is indeterminate.

PRINCIPAL COMPONENT ANALYSIS

CONFUSION WITH THE WORD PC

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, com-
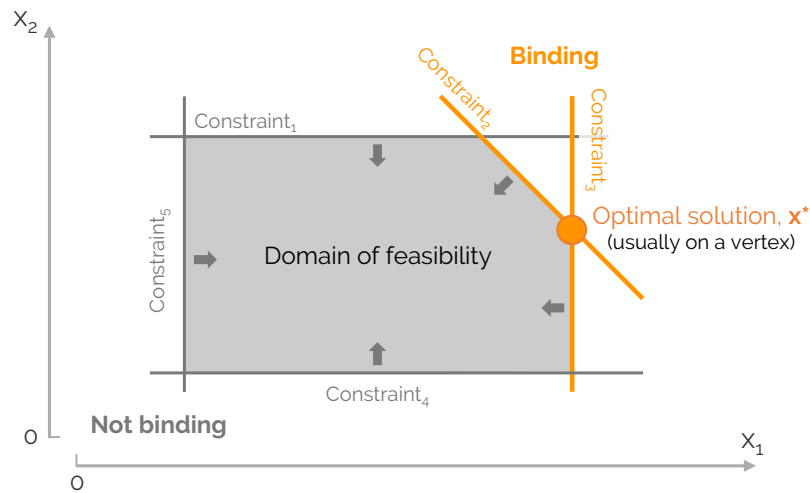
Figure 1: Binding versus non-binding constraints. In LP where the feasibility domain is non-empty and bounded, the constraints defined a convex feasibility domain in the space of variables (here, x_1 and x_2). The optimal solution usually locates on a vertex of this domain, i.e., the intersection of several constraints (here, constraints 2 and 3) limiting the solution. These constraints are considered as binding, i.e., having a limiting impact on the optimal solution.

posed 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.

BIBLIOGRAPHY

[1] D. Bertsimas, J. N. Tsitsiklis, Introduction to linear optimization, volume 6, Athena Scientific Belmont, MA, 1997.