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

A hierarchical multi-objective reinforcement-learning-based approach

Doctoral dissertation presented by
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Contents

Symbols

Acronyms

API	Application Programming Interface
BECCS	Bioenergy with Carbon Capture and Storage
BEMS	Building Energy Management System
BEV	Battery Electric Vehicle
BTX	Benzene, Toluene and Xylene
CAPEX	Capital Expenditure
CCGT	Combined Cycle Gas Turbine
CCS	Carbon Capture and Storage
CHP	Combined Heat and Power
CNG	Compressed Natural Gas
DC	Direct Current
DHN	District Heating Network
DNN	Deep Neural Network
DRL	Deep Reinforcement Learning
ESOMs	Energy System Optimisation Models
ESTD	EnergyScope Typical Days
EUD	End-Use Demand
FC	Fuel Cell
FEC	Final Energy Consumed
GDP	Gross Domestic Product
GHG	Greenhouse Gases
GSA	Global Sensitivity Analysis
GWP	Global Warming Potential
HP	Heat Pump
HT	High-Temperature

HVC	High-Value Chemicals
IAMs	Integrated Assessment Models
ICE	Internal Combustion Engine
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
IQR	Interquatile Range
LCA	Life Cycle Assessment
LCOE	Levelised Cost of Energy
LFO	Light Fuel Oil
LOO	Leave-One-Out
LP	Linear Programming
LPG	Liquefied Petroleum Gas
LT	Low-Temperature
MDP	Markov Decision Process
MMSA	Methanol Market Services Asia
MTBE	Methyl Tert-butyl Ether
MTO	Methanol-to-olefins
NED	Non-energy Demand
NG	Fossil Gas
NN	Neural Network
NRE	Non-renewable Energy
NSC	Naphtha Steam Cracker
OPEX	Operational Expenditure
PC	Principal Component
PCs	Principal Components
PCA	Principal Component Analysis
PCE	Polynomial Chaos Expansion
PDF	Probability Density Function
PV	Photovoltaic
RE	Renewable Energy
RL	Reinforcement Learning
SAC	Soft Actor Critic
SMR	Small Modular Reactor
SVD	Singular Value Decomposition
TRL	Technology Readiness Level
UQ	Uncertainty Quantification
VRES	Variable Renewable Energy Sources

List of publications

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

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

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

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Chapter 1

Robustness assessment of pathway roadmaps

"The more data we have, the more likely we are to drown in it."
Nassim Nicholas Taleb, in *Fooled by Randomness: The Hidden Role of Chance in Life and in the Markets*, 2008

Assessing the robustness of a roadmap driving the transition pathway of a whole-energy system is complex, especially due to the curse of dimensionality. This curse comes from the number of variables of the system (e.g. the installed capacity of technologies), the multiple-year approach specific to the pathway optimisation (i.e. versus the snapshot approach) or the number of uncertain parameters. On top of this, the sector coupling interconnecting the installed capacities and the used resources among the different (non-)energy sectors can make harder the understanding of big trends of such a system. To navigate through this load of uncertain and interconnected data, it is necessary to assess the robustness of pathway roadmaps.

To deal with such uncertainties, decision-makers have several options: (i) resistance; (ii) resilience; (iii) static robustness; and (iv) adaptive robustness [1]. Where resistance consists in planning for the worst-case scenario, resilience aims at a fast recovery whatever the conditions in the future. Finally, in static robustness, one seeks for a roadmap that would perform "satisfactorily" in a wide range of plausible futures, whereas, a roadmap would be dynamically robust if it is prepared to adapt in case of a change in conditions. Where the adaptability of the policy was addressed in Chapter **??**, the objective of this chapter is to apply the method described in Section **??** to deal with the static robustness of pathway roadmaps. Castrejon-Campos et al. [2] assessed policy mix folllowing the same philosophy of "satisfactory level of performance" as [1]. In their work, they mostly focused on the electricity sector, accounting for a variety of stakeholders and related interests using STET (Socio-Technical Energy Transition) models to capture more properly societal and behavioral aspects in relation with policy implementation, enriching purely techno-economy model, like EnergyScope, that usually assume rational choice within an overall cost minimization. However, in the case of the transition pathway of a whole-eenrgy system, the challenges stand here in the definition of the "performance metric" as well as the "satisfactory level of performance". Between the sole total transition cost and the entire set of installed technologies that give too few and too much information, respectively, the performance metric here is defined through the Principal Component Analysis (PCA) approach. Then, when comes the "satisfactory level of performance", we propose a relative level of performance through a comparative analysis of different roadmaps. In other terms, one roadmap will not be robust or not in itself but rather more or less robust than another one.

Contributions

The main contributions of this chapter is the application of the methodology proposed in Section **??** to the case study of the Belgian energy transition. First, we develop the different steps that lead to the principal components of the transition. We analyse these big trends of variation and highlight the fact that these variations stand for the entire pathway, a group of consecutive representative years or rather on a tipping-year. Then, and most importantly, we assess the robustness of different technological roadmaps by projecting their resulting myopic pathway against these directions of variation. The application of PCA to provide a new metric for robustness applied to the case of Belgium is the added-value of this chapter.

1.1 Definition of the principal components of the transition

As detailed in Section **??**, we have decided to define the directions of variation, i.e. the robustness metrics, based on the installed capacities through the transition in the different end-use sectors, i.e. electricity, High-Temperature (HT) heat, Low-Temperature (LT) heat, passenger mobility, freight mobility, High-Value Chemicals (HVC), ammonia and methanol. These capacities represent the technological roadmaps to supply these End-Use Demand (EUD) while respecting the CO_2-budget. As introduced in Section **??**, the data considered in this method come from the Global Sensitivity Analysis (GSA) carried out on the perfect foresight optimisation of the Belgian transition pathway (see Chapter **??**). This gave 1260 different transitions resulting, for each of them, from the pathway optimisation subject to a sample of uncertain parameters (see Section **??**). Appendix **??** gives the exhaustive distributions of the installed capacities among the different end-use sectors from the GSA.

1.1.1 Principal components of each representative year

After the pre-preprocessing of the raw data (i.e. data scaling and outliers management, see Section **??**), the Principal Components (PCs) of each representative year of the transition, except 2020 as the initialisation year, can be computed.

First of all, before investigating the PCs, it is worth looking at the total variance of each representative year (see Table 1.1). Even though the absolute value of these variances has no physical meaning, we observe that the variations are more important at earlier stages of the transition. In other words, the further goes the transition, the more limited are the degrees of freedom to respect the CO_2-budget.

Table 1.1. Whole-system design variance of the different representative years and their comparison with 2025.

Year	**Design variance** $[10^{-3}]$	**vs. 2025**
2025	10.4	-
2030	12.1	+15%
2035	9.7	-7%
2040	6.1	-42%
2045	5.1	-51%
2050	4.8	-54%

Then, keeping the PCs capturing at least 90% of the total variance of each representative year, this gives between four, in 2035, and seven, in 2050, PCs depending on the year (see Figure 1.1), and a total of 34 PCs. At later stages of the transition, the increasing number of required PCs, in line with their smaller share of explained variance, is another indication that the variance of the system design is more spread over a wider range of technologies and with a more limited amplitude.

Finally, we consider the respective contribution of the different technologies in the different PC_y, i.e. their corresponding component in the different eigenvectors. Highlighting the top-5 technologies for $PC_{y,1}$, $PC_{y,2}$ and $PC_{y,3}$, we observe general trends over the whole transition as well as tipping year where there is a clear trade-off between several technologies (see Figure 1.2). As pointed out in Section **??**, PCA does

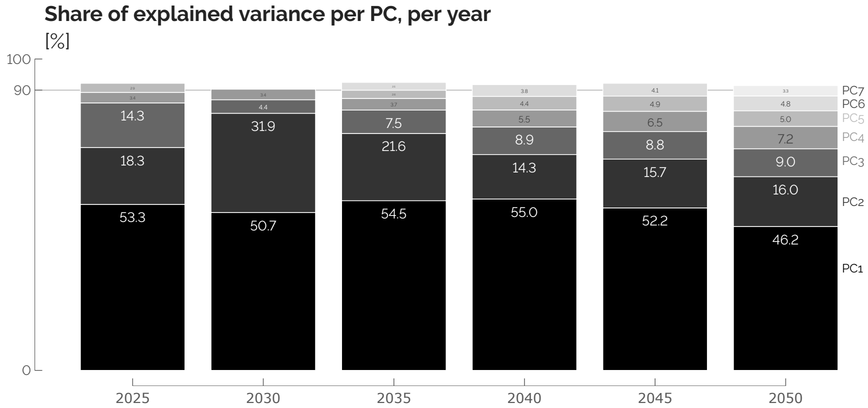

Figure 1.1. PCs capturing at least 90% of the total variance of their respective representative year of the transition.

not make any distinction between a vector of variation and its opposite. This is why $PC_{2025,1}$ and $PC_{2035,1}$ are actually very similar even though there are mostly on the opposite sides of the 0-axis.

Even though the following observations could be made by analysing the distribution of installed capacities (see Appendix **??**) or the covariance matrices, the PCA decomposition offers a more visual and summarising representation of the main trends of variation. Due to their intermittency, integrating more PV panels leads to the installation of other technologies to benefit from free and renewable electricity when it exceeds the electrical EUD. Therefore, we observe that the variation of installed PV is directly linked with the variation of installed industrial electrical resistors and, to a smaller extent, of decentralised and District Heating Network (DHN) electrical HP. These variations cover the whole transition as the main varying factors given their significant contributions to the PC_1. Where this was an example for correlated technologies, we can also identify some key modal shifts where one technology is either substituted by others or in balance with another one. First, about the LT heat sector, the early stages of the transition, i.e. 2025-2030, sees the shift from mainly decentralised oil and gas boilers towards decentralised and DHN electrical HP. Later in the transition, there seems to be a tight competition between (bio)diesel and Fuel Cell (FC) trucks that drive the design variance to a smaller extent as they mostly appear in the second and third PCs of the representative years. Not capturing a significant share of variance, there are other modal shifts (e.g. Battery Electric Vehicle (BEV) substituting diesel and gasoline cars) that are not visible through the PCs. Besides these modal

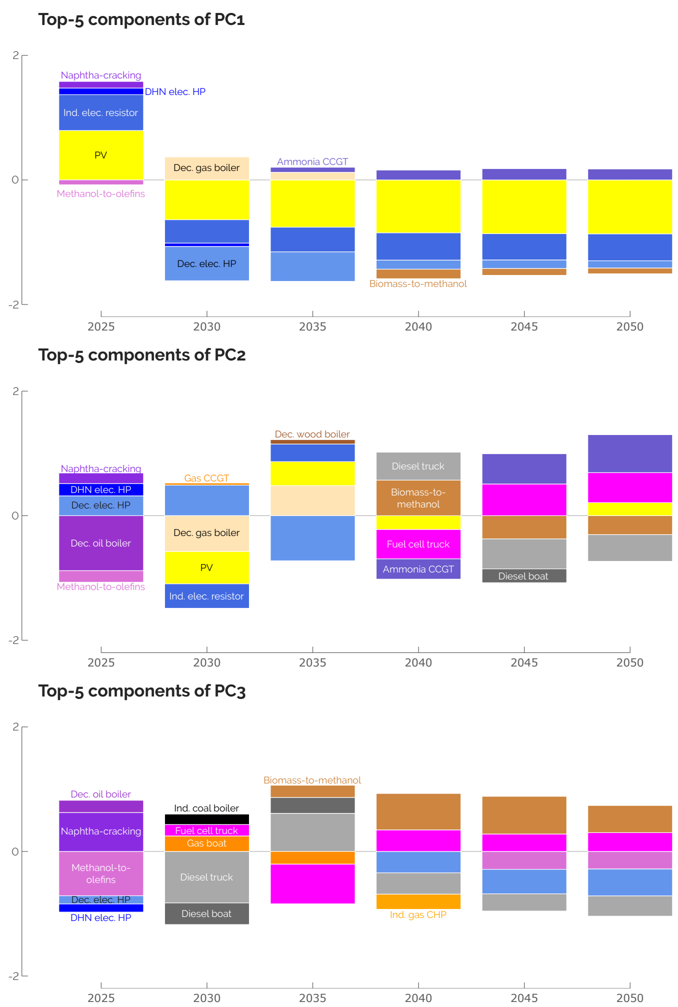

Figure 1.2. Contribution of the top-5 technologies to the first three PCs over the different representative years. Where the variation of Photovoltaic (PV) panels supported by the electrification of the HT heat via industrial electric resistors is the main varying drivers over the whole transition, there are tipping years like 2025 for the production of HVC (i.e. naphtha-cracker to Methanol-to-olefins (MTO) or 2025-2030 for the production of LT heat (i.e. from oil and gas boilers to electric Heat Pump (HP).

shifts spread over several representative years, 2025 is the tipping year concerning the shift from naphtha-cracker and methanol-to-olefins to supply HVC. Finally, there are also technologies contributing to PCs because they are the main producing assets of their respective end-use sector and the demand varies significantly, e.g. biomass-to-methanol.

1.1.2 Principal components of the transition

Based on the PCs of each representative year, PC_y, the PCs of the transition, i.e. the metrics to assess the robustness of roadmaps, can be computed. Before aggregating and averaging similar PC_y, it is necessary to rank them to ensure capturing most of the transition variance in the subsequent $PC_{transition}$.

Based on the design variance captured by each PC_y in their respective representative year, we can rank them (see Table 1.2). Summing all of these variances over the different years results in a "pseudo" total variance of the transition. To construct the PCs of the transition, $PC_{transition}$, we keep the PC_y that captures at least 80% of this total variance of the transition (see Section **??**). This results in keeping 14 PC_y: the first and second PCs of each representative year and the third PC of 2025 and 2035. Even though the 80%-threshold is reached with the first 11 PCs, $PC_{2045,2}$, $PC_{2050,2}$ and $PC_{2035,3}$ are accounted for as they are similar to $PC_{2040,2}$. Consequently, aiming at capturing at least 80% of the total transition variance,

Given the similarity between PC_y (see Figure 1.2), some $PC_{transition}$ result from the aggregation and averaging of the components of several PC_y (see Table 1.3). This aggregation step has a double objective: limiting the dimension of the robustness metrics and avoiding ineffective redundancy in terms of $PC_{transition}$ where several of them would otherwise point towards similar directions of variation.

Averaging the components of similar PC_y allows constructing the $PC_{transition}$ (see Figure 1.3). These directions of variation form the robustness matrix on which it is possible to project the results of transition roadmaps tested under uncertainties and myopic pathway optimisation.

1.2 Robustness assessment of pathway roadmaps

Now that the performance metric is defined, we can assess the robustness of different roadmaps. These roadmaps are defined as the technological mix given by the deterministic optimisation of the perfect foresight pathway under certain conditions. The two first roadmaps are the **REF** and **SMR** cases (see Chapter **??**). All the uncertain pa-

Table 1.2. Ranking of PCs per design variance captured in their respective representative year and cumulative share of the captured total variance of the transition

Ranking	**Year**	**PC**	**Design variance** $[10^{-4}]$	**Cumulative share of total variance** [%]
1	2030	PC_1	61.1	13.9
2	2025	PC_1	55.7	26.5
3	2035	PC_1	52.7	38.4
4	2030	PC_2	38.4	47.2
5	2040	PC_1	33.4	54.7
6	2045	PC_1	26.5	60.7
7	2050	PC_1	22.2	65.8
8	2035	PC_2	20.9	70.5
9	2025	PC_2	19.1	74.8
10	2025	PC_3	15.0	78.2
11	2040	PC_2	8.7	**80.2**
12	2045	PC_2	7.9	82.0
13	2050	PC_2	7.7	83.7
14	2035	PC_3	7.3	85.4
⋮	⋮	⋮	⋮	⋮
34	2050	PC_7	1.6	100

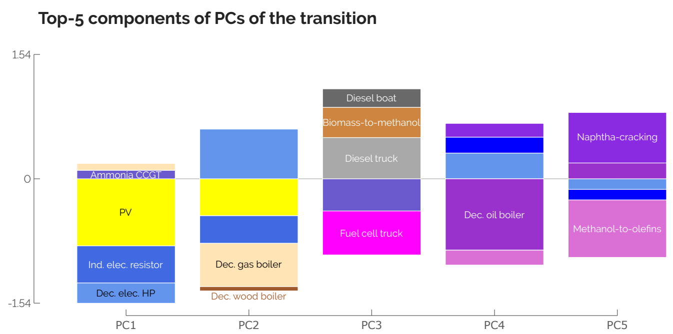

Figure 1.3. Contribution of the top-5 technologies to the different $PC_{transition}$.

Table 1.3. Aggregation of PC_y to construct the $PC_{transition}$ and share of the captured total variance of the transition by each $PC_{transition}$.

$\mathbf{PC_{transition}}$	$\mathbf{PC_y}$	**Share of total variance** [%]
$PC_{transition,1}$	$PC_{2025,1}$ $PC_{2030,1}$ $PC_{2035,1}$ $PC_{2040,1}$ $PC_{2045,1}$ $PC_{2050,1}$	57.0
$PC_{transition,2}$	$PC_{2030,2}$ $PC_{2035,2}$	13.4
$PC_{transition,3}$	$PC_{2040,2}$ $PC_{2045,2}$ $PC_{2050,2}$ $PC_{2035,3}$	7.2
$PC_{transition,4}$	$PC_{2025,2}$	4.3
$PC_{transition,4}$	$PC_{2025,3}$	3.4

rameters are considered at their nominal value in these two cases. The only difference consists in allowing Small Modular Reactor (SMR) from 2040 onward in the **SMR** case. On top of these two cases, we add a so-called "robust" case, **ROB**, in the same sense as in the works of Bertsimas and Sim [3] or Moret [4] accounting for a "protection parameter". Then, we assess the robustness of these three roadmaps via a similar "three-step rolling horizon approach" as in the work of Moret et al. [5]: (i) setting the initial investment strategies provided by the roadmaps and, (ii) assessing the variation of investments needed through myopic pathway optimisation under uncertainties and, (iii) projecting the strategies from the myopic optimisations on the robustness metrics defined via PCA.

1.2.1 A robust roadmap?

Rather than considering all the uncertain parameters at their worst values as in the work of Soyster [6], we follow here the robust approach of Bertsimas and Sim [3] and Moret [4]. In their works, the authors consider a factor $\Gamma_{obj} \in [0, d]$ that represents a "protection parameter" of the objective function where d is the total number of uncertain parameters (see Section **??**). If $\Gamma_{obj} = 0$, where all the uncertain parameters are at their nominal value, we obtain the deterministic solution of the **REF** case. If $\Gamma_{\text{obj}} = d$, this means considering the "fully robust" solution where all the uncertain parameters are their worst value, as in Soyster [6]. Between these two extreme cases, the uncertain parameters to account for at their worst values follow the ranking given by the GSA (see Chapter **??**). In practice, $\Gamma_{\text{obj}} = 1$ means considering the cost of purchasing electrofuels at its worst value. $\Gamma_{\text{obj}} = 2$ adds the industry EUD at its worst value in the lot, and so on. In the present analysis, we consider the "robust" roadmap by setting $\Gamma_{\text{obj}} = 6$. Consequently, costs of purchasing electrofuels, fossil fuels and biofuels as well as the industry EUD, the interest rate and the variable OPEX of technologies are considered at their worst values, i.e. the upper bound of their respective range. In practice, this means that, in the ROB case, imported energy carriers, except electricity, are 179.8% more expensive, the industrial demand is, by 2050, 23.9% higher[1], the interest rate is 46.2% (i.e. 2.2% versus 1.5% in the REF case) and the variable OPEX of technologies, c_{maint}, is 35.7% higher. The following paragraphs investigate the differences in the different sectors between the ROB and the REF cases, similarly to the comparison carried out with the SMR case in Chapter **??**.

Power sector

Given the more expensive imported energy carriers, the model opts for an earlier electrification of the system and more efficiency. Consequently, the power sector is one of the most impacted ones (see Figure 1.4). At the earlier stages of the transition, the model opts for the full deployment of local Variable Renewable Energy Sources (VRES) as soon as possible and importing more electricity (i.e. +8.7 TWh, +52%) from abroad in 2025. This earlier and bigger integration of VRES is supported by the higher electrification of HT and, to a smaller extent the LT, heating sector as well as in the mobility sectors. It is mostly the industrial electric heaters that absorb the abundant and intermittent electricity produced by PV panels and wind turbines. In the mobility sectors, BEV substitutes gasoline cars from 2025 onward and electric trucks make the transition from diesel to FC trucks. On the supply side, besides the local VRES and the direct import of electricity from abroad, Combined Heat and Power (CHP) units, mostly industrial, are favoured given their higher efficiency at the expense of ammonia-Combined Cycle Gas Turbine (CCGT). In the ROB case, by 2050, these CHP units produce 43.3 TWh, i.e. 23% of the total electricity production, versus 21.9 TWh in the REF case. These observations are in line with the work of Moret et al. [5] focusing

[1] As detailed in Chapter **??**, the industrial demand encompasses the whole Non-energy Demand (NED) and LT heat demand, as well as the industrial share of electricity and LT heat demands.

on the problem of overcapacity in the European power sector. The authors highlighted that the robust strategy diversified the supply sources of electricity between VRES, import of electricity and more efficient technologies like CHP and HP.

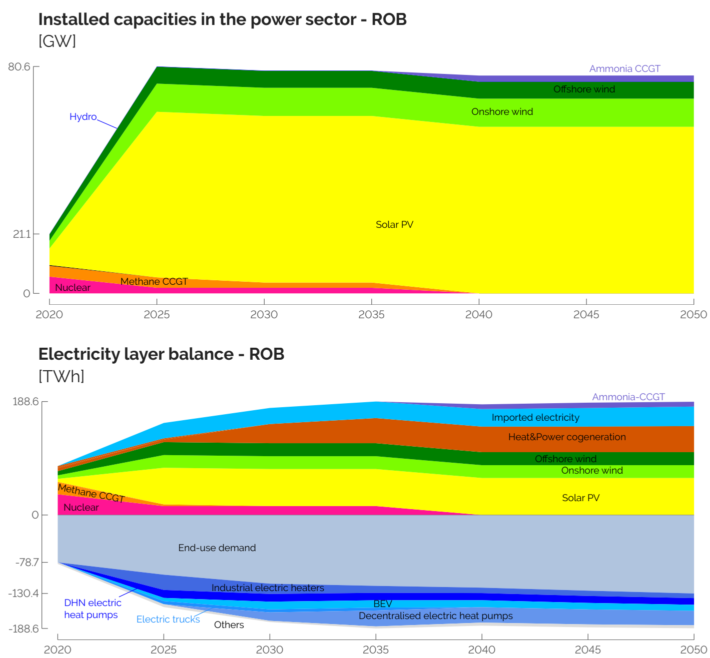

Figure 1.4. Installed capacities and layer balance of the power sector in the ROB case. Compared to the REF case, local VRES are deployed as soon as possible supported by an earlier electrification of the heat and transport sectors. CHP units also represents a higher share of the electricity supply given their higher efficiency at the expense of other flexible production units like ammonia-CCGT.

Heating sectors

By 2050, the additional 23.9% of industrial EUD directly impacts the technological mix to supply the HT heat, i.e. +13.6 TWh as direct HT heat EUD on top of the extra 3.4 TWh consumed by the MTO process. As aforementioned, at earlier stages of the transition, up to 20.9 GW of industrial electric heaters supply the additional demand and support the integration of solar PV. However, in the mid-term, 27% of these heaters are prematurely decommissioned where 24% are not renewed after reaching the end of their lifetime. Instead, up to +3.5 GW of industrial CHP units are installed to efficiently use e-methane that is considered more expensive in the ROB case to supply electricity and 52% of the HT heat demand. About the LT heat sector, the principal impact is the bigger installation of DHN and decentralised electric HP, up to +2.1 GW and +0.8 GW respectively.

Mobility sectors

In the transport of freight, the ROB roadmap transitions from diesel to FC trucks with the temporal use of electric trucks from 2025 to 2035. Similarly to the industrial electric heaters, it is a way to integrate the early installation of solar PV and absorb part of its intermittent electricity. Freight transport via trains and boats are not different from the REF roadmap. About the passenger mobility, compared to the REF case, the shift from Internal Combustion Engine (ICE) cars to BEV occurs earlier in the transition, in line with the increased production of intermittent electricity from VRES.

Non-energy

Technologically speaking, by 2050, the ROB case accounts for an additional 1.2 GW of MTO to supply the extra 10.3 TWh of HVC. Besides this, the extra 2.5 TWh and 0.4 TWh of e-ammonia and e-methanol are supplied by the import of their respective energy carrier.

In conclusion, the two main assumptions impacting the ROB roadmap strategy compared to the REF one were the higher cost of purchasing imported energy carriers (except electricity) and higher industrial EUD.More expensive imported energy carriers lead to, on the one hand, an earlier full deployment of local VRES (i.e. PV, wind onshore and offshore) supported by a higher electrification of the heating and transport sectors. On the other hand, it increases the share of the total OPEX due to the consumption of resources (i.e. excluding the OPEX of the technologies) in the total transition cost: i.e. 56% versus 38% in the REF case. This, combined with the increase of industrial EUD, encourages a more efficient use of the resources, i.e. CHP and HP. The increased interest rate and variable OPEX of technologies have a more negligible impact on the roadmap strategy as they identically affect the entire set of technologies.

1.2.2 Projection on robustness metric

After defining the robustness metric and describing the roadmaps to assess (i.e. REF, SMR and ROB), the final step consists in testing these roadmaps under uncertainties in a myopic pathway optimisation. This aims at assessing the adaptation of the roadmaps as uncertainty gradually unfolds over time [5], which brings more realism than perfect foresight [7]. The three roadmaps are tested 500 times fixing the installed capacities $f_{\text{max}} \geq \mathbf{F} \geq \mathbf{F}^*$ for all the end-use technologies, and taking values of the 34 uncertain parameters (see Section **??**) following the Sobol' sequence. However, uncertain parameters limit the potential installed capacity, f_{max}, of PV panels, onshore and offshore wind turbines and SMR. For these, in case the installed capacity prescribed by the roadmap is higher than the maximum potential affected by the value of the uncertain parameter, the actual installed capacity is set to this new limit. In reality, this would be similar to revise to a smaller extent the expected roadmap due to external events (e.g. smaller public acceptance [8, 9], lower Technology Readiness Level (TRL) or longer installation time than expected).

No tested roadmap is more robust than the others on all the PCs of transition (Table 1.4). Overall, the roadmaps follow the same trend over the different PCs of transition: they span over the most narrow range for PC 3 and over the widest range for PC 2. In practice, it means that roadmaps resulting from perfect foresight optimisation, when tested through a myopic process, would be more robust towards the variations driven by the freight transport sector (i.e. FC and diesel trucks and diesel boat) and less robust towards the variation driven by the decentralised heating sector (i.e. decentralised HP and wood and gas boilers) and PV.

Table 1.4. 95% confidence range of projected data from roadmaps tested in myopic optimisation [$\cdot 10^{-3}$]. Values in brackets give the relative difference with the REF roadmap. There is no "best overall" roadmap.

PC	**95% confidence range**		
	REF	SMR	ROB
1	4.2	4.2 (=)	3.7 (**-12%**)
2	5.7	5.6 (-2%)	6.1 (**+8%**)
3	2.2	2.3 (+3%)	1.9 (**-17%**)
4	4.5	4.4 (-2%)	4.5 (+1%)
5	2.7	3.1 (**+15%**)	2.6 (**-4%**)

The SMR roadmap spans over similar ranges as the REF case. The most significant difference concerns PC 5. This PC is driven by the variations in the HVC sector. As detailed in Chapter **??**, one of the impacts of the installation of SMR from 2040 onward is the delayed substitution of naphtha-crackers by MTO. Consequently, in the near-term, the SMR roadmap presents more variation in terms of installed capacity of MTO.

The ROB roadmap is more robust than the REF case on PCs 1, 3 and 5, by 12%, 17% and 4% respectively. About PC 1, it is driven by the variation of installed capacities of PV. In the ROB case, the earlier full deployment of solar PV makes this roadmap more robust towards these variations. Concerning PC 3, this higher robustness is explained by variations in the installed capacities of diesel trucks, biomass-to-methanol and ammonia-CCGT that are 32%, 30% and 15% smaller than in the REF case, respectively. Finally, as the ROB roadmap accounts for additional capacities to supply the potential additional demand of HVC, it is more robust towards the variations in this sector.

On the contrary, the ROB roadmap is less when considering PC 2, driven by the variations in the LT and HT heat sectors. The biggest impact comes from the variations of industrial resistors. In the ROB case, even though they are more installed at earlier stages of the transition to support the integration of PV, a part of them are either prematurely decommissioned or not renewed. This makes this roadmap more sensitive to additional industrial heaters needed in the myopic optimisation at the latest stages of the transition.

1.3 Discussion

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