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

A hierarchical multi-objective reinforcement-learning based approach

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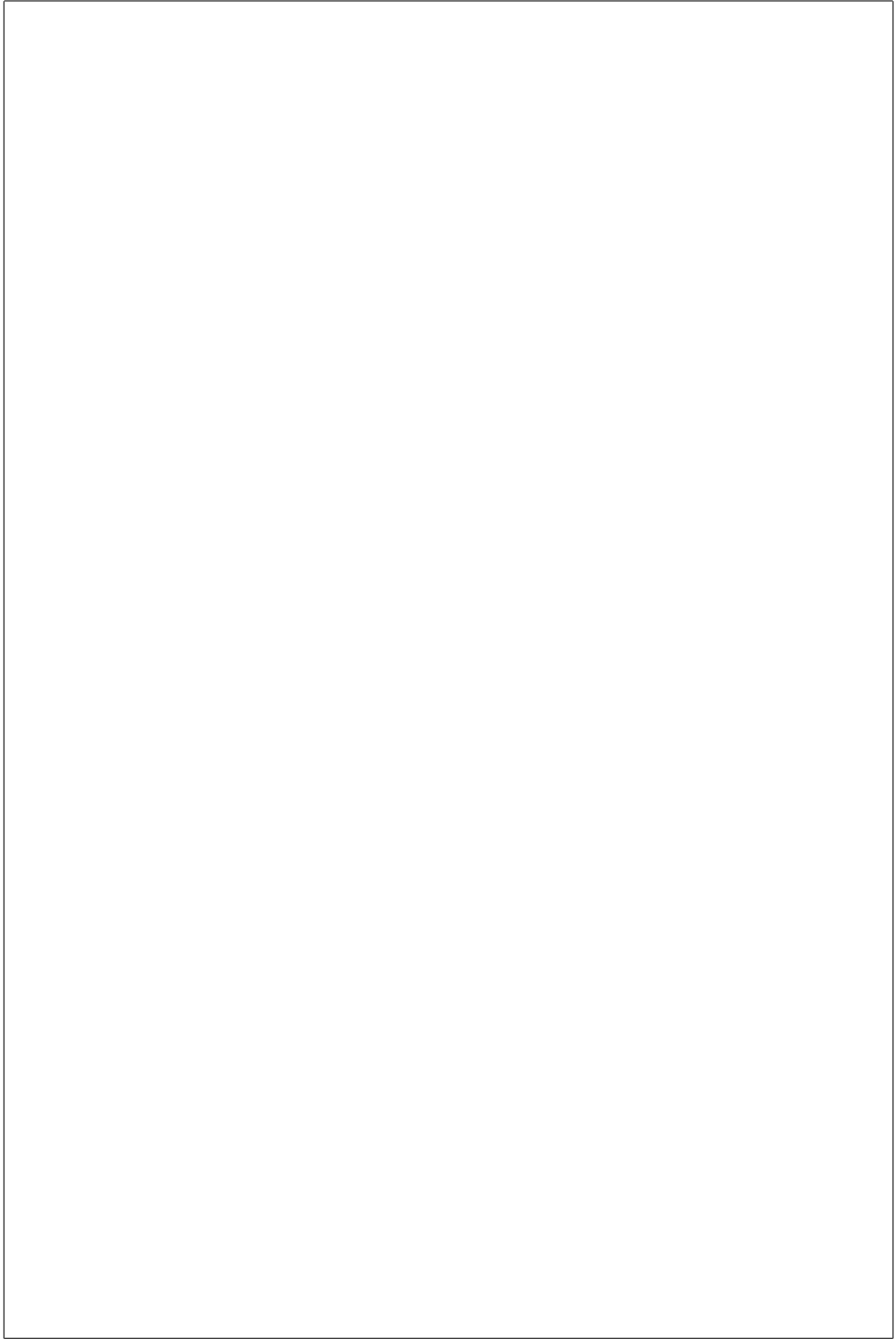
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Symbols

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
ESOMs	energy system optimisation models
EnergyScope TD	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	interquartile range
LCA	life cycle assessment
LCOE	levelised cost of energy
LFO	light fuel oil
LOO	leave-one-out
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
SDGs	Sustainable Development Goals
SMR	small modular reactor
SVD	singular value decomposition
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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Rixhon, X., Limpens, G., Contino, F., & Jeanmart, H. (2021). “*Taxonomy of the fuels in a whole-energy system.*” In *Frontiers in Energy Research, Sec. Sustainable Energy Systems*, (Vol. 9). URL: <https://doi.org/10.3389/fenrg.2021.660073>

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Chapter 1

Reinforcement Learning CO₂-policy investigation

“For the things we have to learn before we can do them, we learn by doing them.”

Aristotle, in *The Nicomachean Ethics*, IVth century BC

Uncertainties about the future along with a large variety of integrated assessment models (IAMs) yield to an even larger variety of greenhouse gases (GHG) emissions reduction pathways [1]. For instance, several studies [2, 3] advocate for actions to take in the near future, especially to keep on track with the 1.5°C (if not, 2°C) increase of global temperature by the end of the century. On the contrary, using their top-down model DICE, Nordhaus [4] state that immediate and drastic actions are not compulsory to meet the ambition of climate change mitigation. This is even more valid when models assess a myopic transition pathway subject, with limited foresight through the future with progressively unveiled uncertainties.

To address this issue, several approaches have been used. Among them, multi-stage stochastic programming is often put forward as a promising method. Stochastic programming formulates the problem as a mathematical program with probabilistic constraints or objective functions. These models explicitly consider the uncertainty by incorporating probability distributions for the uncertain parameters. The goal is to find an optimal decision that minimizes/maximizes the expected value of the objective function while satisfying the probabilistic constraints, modelled as a scenario tree. At each stage of the problem, here the transition pathway of a whole-energy system, the model has the possibility of recourse, i.e. to adapt the decisions made at earlier stages, in the response to unveiled uncertainties [5]. Using MARKAL model [6], Kanudia and

Loulou [7] assessed a multi-stage stochastic optimisation of the 5-year steps transition of Quebec between 1995 and 2035 accounting for high/low mitigation action plan and high/low growth scenarios. The authors found that hedging strategies, adapting with the future uncertainties, were outperforming the perfect foresight and deterministic optimisation of the different scenarios. However, stochastic programming is usually applied to limited number of uncertainties, i.e. up to 10, and relies on probability distribution that are often difficult to define properly. Increasing the number of these uncertainties in stochastic programming usually leads to a computational burden that limits the use of such a method in IAMs [1]. Based on the approach of Bertsimas and Sim [8], and similarly to Moret [9], Nicolas et al. [1] rather opted for the robust optimisation of the global pathway up to 2200 given different temperature deviation targets, i.e. 2 or 3°C by 2200 via the use of uncertainty budget, Γ , in the TIAM-World model [10]. Considering 9 climate parameters and their respective lower and upper bounds, the idea behind the uncertainty budget stems from the improbability of all parameters simultaneously reaching one of their two extreme values.

In the exploration of the myopic transition pathway under uncertainties, we decided to investigate the reinforcement learning (RL) approach to benefit from its policy optimisation mechanism. Indeed, policymaking for transitioning a whole-energy system can be viewed as an iterative process of learning from policy implementation efforts, involving ongoing analysis of energy policy challenges and experimenting with various solutions [11]. RL exhibits two main advantages: its effectiveness to handle uncertainties and the model-free approach where an accurate representation of the real world is not needed to optimize the policy [12]. Besides the environment, i.e. the myopic transition pathway of the whole-energy system via EnergyScope Pathway (see Chapter ??), the first part of this chapter presents the three key features of interaction between the agent, optimizing its policy, and the environment: actions, states and reward. Then, the results of this policy optimisation point out strategies to follow, i.e. *sweet spots*, in the transitions under uncertainties as well as *no-go zones* where the chances of succeeding the transition, i.e. respecting the CO₂-budget, are very limited. Finally, these results are compared with references, i.e. the perfect foresight and the myopic optimisation of the transition under the same uncertainties but without the trained RL-agent that can support this transition thanks to its learned policy.

Contributions

Applying the RL approach to the optimization of the myopic transition pathway of a whole-energy system presents several novelties. First of all, as introduced in Section

??, when applied to energy systems, RL is more dedicated either to smaller scale systems (e.g. building energy management system (BEMS), vehicles and energy devices) or to sector-specific, often the power sector, problems (e.g. dispatch problems, energy markets and grid) [12]. In our case, the sector-coupling, the long-term goal at the end of a multiple-steps transition and the number of uncertain parameters make this application new for RL.

Then, applying to this optimisation environment, i.e. EnergyScope myopic Pathway, rather than a simulation environment, allows building a hierarchical multi-objective optimisation framework. In this agent, while the objective of the environment remains the minimisation of the total “transition” cost (on the concerned limited time window), the agent optimises its strategy to respect the CO₂-budget.

Finally, comparing the RL-based results with more conventional approaches, i.e. perfect foresight, if not myopic, optimisation without learning process, highlights the added-value brought by the optimised policy.

1.1 Definition of the actions, states and rewards

As already introduced in Section ??, the environment with which the RL-agent interacts is the optimisation of the transition pathway whole-energy system on a specific time window, e.g. 2020-2030 then 2025-2035 and so on, until 2040-2050 (see Figure ??). In a nutshell, starting from the initial state of the environment (i.e. the whole-energy system in 2020), the agent takes a set of actions that influence the environment. Then, the window 2020-2030 is optimised via EnergyScope. Some of the outputs of this optimisation feed the agent with either the new state of the system or the reward, i.e. telling the agent how good the actions were at the state he took it. Based on these two pieces of information, i.e. the new state and the reward, the agent takes another set of actions and the window 2025-2035 is optimised. This goes on until eventually reaching 2050. The main purpose of this section is to define the shape of the reward as well as the sets of actions and states.

Actions

Defining the levers of action, the core of the policy, to support the transition of a country-size whole-energy system is challenging, especially when accounting for political and socio-technical aspects [13]. In our work, focusing only on the techno-economic aspect, we assume that the actions taken by the agent are directly implemented and impacting the environment, without “misfire”. In other words, considering only the techno-economic lens, there is no moderation nor contest towards the agent’s

actions, as the objective is to assess how far and when within the transition to push the different levers of action. Given the overall objective of the agent to succeed the transition, i.e. respecting the CO₂-budget by 2050, we have defined the actions in this sense. The first action, $\text{act}_{\text{gwp}} \in [0, 1]$, aims at limiting the emissions at the representative year ending the concerned time window, $\mathbf{GWP}_{\text{tot}}(y_{\text{end of the window}})$, between the level of emissions in 2020, i.e. $\mathbf{GWP}_{\text{tot}}(2020) = 123 \text{ Mt}_{\text{CO}_2, \text{eq}}$, and carbon-neutrality:

$$\mathbf{GWP}_{\text{tot}}(y_{\text{end of the window}}) \leq \text{act}_{\text{gwp}} \cdot \mathbf{GWP}_{\text{tot}}(2020) \quad (1.1)$$

Out the total GHG emissions in Belgium in 2020, oil (i.e. so-called light fuel oil (LFO) in the model), on the one hand and, on the other hand, fossil gas, account for roughly 40% and 31%, respectively. Then, even though its use in 2020 is much more limited compared to the two formers, i.e. 28 TWh of solid fossil fuels (i.e. so-called COAL in the model) versus 159 and 142 TWh for oil and fossil gas, respectively, coal is a cheap, about 0.017€/GWh, and highly-emitting resource, 0.40 kt_{CO₂,eq}/GWh. For these reasons, three additional actions to support the strict limitation of overall emissions of the first action: limiting the consumption of these three fossil resources up to the level of consumption in 2020, $\mathbf{Cons}_{\text{fossil gas}}(2020)$, $\mathbf{Cons}_{\text{LFO}}(2020)$ and $\mathbf{Cons}_{\text{coal}}(2020)$, over the entire concerned time window, except the first one as this year is the initial condition of the time window and cannot be optimised any more:

$$\mathbf{Cons}_{\text{fossil gas}}(y) \leq \text{act}_{\text{fossil gas}} \cdot \mathbf{Cons}_{\text{fossil gas}}(2020) \quad \forall y \in \text{time window} \quad (1.2)$$

$$\mathbf{Cons}_{\text{LFO}}(y) \leq \text{act}_{\text{LFO}} \cdot \mathbf{Cons}_{\text{LFO}}(2020) \quad \forall y \in \text{time window} \quad (1.3)$$

$$\mathbf{Cons}_{\text{coal}}(y) \leq \text{act}_{\text{coal}} \cdot \mathbf{Cons}_{\text{coal}}(2020) \quad \forall y \in \text{time window} \quad (1.4)$$

where $\text{act}_{\text{fossil gas}}$, act_{LFO} and act_{coal} can take values between 0 and 1. These complete the action space of the agent, $A \in \mathbb{R}_{[0,1]}^4$.

Reward

Properly defined the reward fed by the environment to the agent is crucial in RL for several reasons. If the reward is not properly defined, the agent may optimize its policy for an unintended objective, leading to undesired or suboptimal behavior, i.e. the so-called misalignment of the learning objective [14]. Even worse, it can lead to reward hacking (or reward tampering) where the agent exploits loopholes in the reward function to achieve higher rewards without actually performing the desired task [15]. On the contrary, a proper definition of the reward function increases the sample efficiency, i.e. requiring less episode to converge to the optimal policy. It also makes the policy more stable and able to withstand variations and uncertainties in the environment [16].

Through its maximisation of the expected return (see Section ??), a RL-agent is as sensitive to positive reward, i.e. the carrot, as negative reward, i.e. the stick. When the former encourages desired behaviours, the latter can be seen as a penalty or a punishment and discourages the undesirable behaviours [17]. In our case, we have decided to combine these two approaches (see Figure 1.1).

First of all, taking a set of actions at a certain state might lead to an infeasible optimisation problem. In other words, as actions have a direct impact on some constraints of the problem, they might limit too much the feasible domain to the point where no solution can be found. For instance, the extreme case of aiming at carbon-neutrality, i.e. $\text{act}_{\text{gwp}} = 0$, and forbidding the use of the three aforementioned fossil fuels, i.e. $\text{act}_{\text{fossil gas}} = \text{act}_{\text{LFO}} = \text{act}_{\text{coal}} = 0$, from the beginning of the transition makes the optimisation impossible to solve. In this case, the episode is prematurely ended and the reward is “highly” negative, -300. If EnergyScope is able to provide a solution to the time window to optimise and the end of the transition, i.e. 2050, is not reached, a test on the cumulative emissions so far. On the one hand, if these cumulative emissions exceed the CO₂-budget, 1.2 Gt_{CO₂,eq} (see Section ??), the episode is also ended and a penalisation is given to the agent. This penalisation is proportional to the difference between the CO₂-budget and the actual cumulative emissions. On the other hand, the episode continues with a zero reward if the CO₂-budget is not exceeded. Eventually, if reaching 2050, we decided to tweak the reward function in capping the share of the cumulative emissions and integrating the transition cost. Given the main objective of the agent to respect the CO₂-budget and not to be more ambitious “CO₂-ambitious”, we cut short the contribution of the cumulative emissions as soon as they are lower or equal to the CO₂-budget. Moreover, to make the agent sensitive to the cost-impact of its policy, we added the total transition cost in the reward function where the $\text{Trans. cost}_{\text{ref}}$ on Figure 1.1 is equal to $1.1 \cdot 10^3$ b€. This value comes from the mean of the total transition costs obtained through the global sensitivity analysis (GSA) performed on the perfect foresight transition pathway optimisation (see Section ??). In this final form of the reward, one will notice that overshooting cumulative emissions are more penalising than an overshooting transition cost, i.e. weight of 200 for the emissions versus 100 for the cost. The values of these weights are the results of a trial and error. This way, we observed that the agent first targeted the respect of the CO₂-budget and then, to a lesser scale, avoided reaching over-costly transitions.

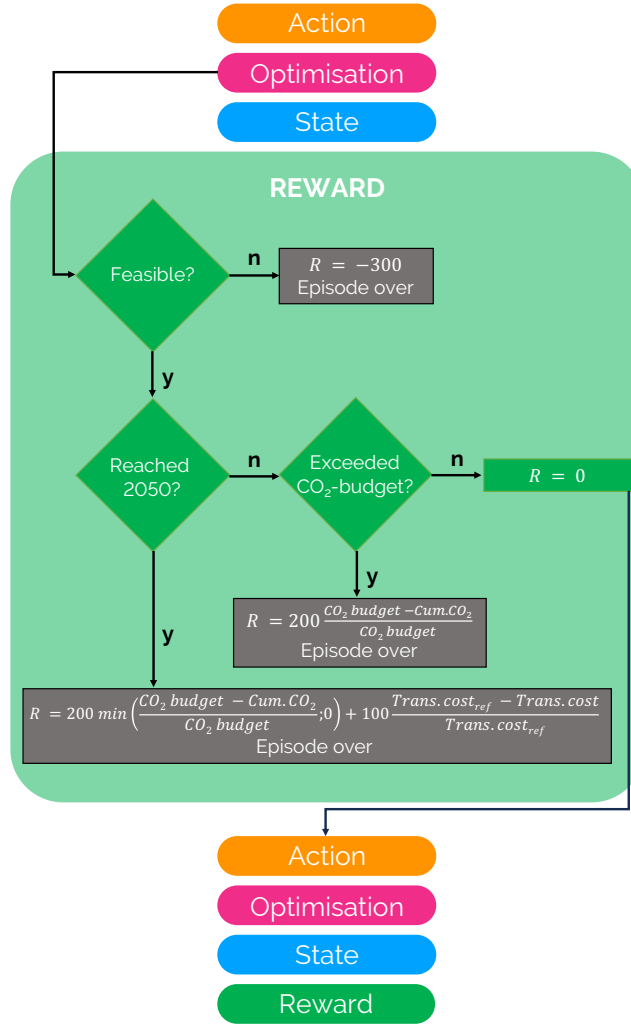


Figure 1.1. Reward, R , function scheme. Before reaching 2050, the episode is prematurely ended and a negative reward is given if the optimisation is infeasible or if the CO₂-budget is exceeded. If the optimisation provides a solution and the CO₂-budget is not exceeded, the episode continues. Finally, if the episode goes until 2050, the reward is a weighted sum between the capped cumulative emissions and the total transition cost.

States

Besides the reward, states are the other piece of information provided by the environment to the agent. In RL, the purpose of states are to represent the current situation or configuration of the environment in which the agent operates. The primary function of states in RL is to provide the necessary context for the agent to choose appropriate actions based on its current observations and goals [17]. The challenge in the definition of the states is to provide enough information but not too much to avoid overwhelming the agent with non-informative features.

Consequently, after another process of trial and error, we have converged to a four-dimension state space characterizing the energy system at the end of the optimised time window. The first dimension is directly related to the main objective of the agent: respecting the CO₂-budget until 2050. Therefore, the cumulative emissions emitted so far in the current step of the transition is the first dimension of the states. Similarly, the cumulative cost of the transition so far constitutes the second dimension of the states to inform the agent about the cost-impact of its actions on the environment. Finally, to enrich the level of details, we have added two other dimensions representative of the key-to-the-transition indicators identified by in Renewable Energy Directive (RED) III of the European Commission [18]: the share of renewables in the primary energy mix and, the energy efficiency. The former is computed as the share of local renewables (i.e. wind, solar, hydro and biomass) and imported renewable energy carriers (i.e. biofuels and electrofuels) in the total consumption of primary energy. Even though energy efficiency is usually defined as the ratio between the final energy consumed (FEC) and the primary energy mix, we decided to define this efficiency with a focus on the end-use demand (EUD), like in the rest of this thesis. Where electricity, heat and non-energy EUD are expressed in terms of energy content, we needed to convert passenger and freight transports into their respective FEC to integrate them in the ratio.

1.2 Results - As in Smart Energy Systems Conference

Confirm here with what is said in [19]: Importantly, our results also show that near-term policy stringency is an important driver of cumulative Res-FFI-CO₂ in climate change mitigation scenarios. If strengthening of NDCs fails, Res-FFI-CO₂ will be even higher, not only because of additional near-term emissions, but also due to a decrease of economic mitigation potentials in the longer term caused by further carbon lock-in. Delaying the strengthening of mitigation action will increase the world's dependence on CDR for holding warming to well below 2°C, and is likely to push the 1.5°C target out of reach for this century.

1.3 Discussion

Potentially interesting to implement reward shaping to accelerate learning or guide the agent towards achieving the desired behaviour more efficiently. In our case, the agent receives a sparse reward signal, indicating success or failure at the end of an episode. However, this sparse reward signal may not provide enough information for the agent to learn effectively, leading to slow convergence or difficulty in learning the optimal policy. Reward shaping addresses this issue by providing additional, intermediate rewards during the learning process based on various heuristics, domain knowledge, or problem-specific insights. These intermediate rewards can help guide the agent towards desirable states or actions, making the learning process more efficient and effective. However, reward shaping should be applied with caution, as poorly designed reward functions can lead to unintended consequences such as suboptimal policies, reward hacking, or overfitting to the shaped rewards rather than learning the underlying task (see Section 1.1).

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