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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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Abstract

This thesis will be awesome

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

– Antoine de Saint Exupéry, Citadelle, 1948

Remerciements

Thank you, thank you, far too kind

Contents

Symbols

Acronyms

BEV	battery electric vehicle
BTX	benzene, toluene and xylene
CCGT	combined cycle gas turbine
DHN	district heating network
EnergyScope TD	EnergyScope Typical Days
EUD	end-use demand
FC	fuel cell
GHG	greenhouse gases
GWP	global warming potential
HP	heat pump
HVC	high value chemicals
IEA	International Energy Agency
LCOE	levelised cost of energy
LFO	light fuel oil
LOO	leave-one-out
LPG	liquefied petroleum gas
MMSA	Methanol Market Services Asia
MTBE	methyl tert-butyl ether
NED	non-energy demand
NG	natural gas
NRE	non-renewable energy
NSC	naphtha steam cracker
PCE	Polynomial Chaos Expansion
PV	photovoltaic
RE	renewable energy

SDGs	Sustainable Development Goals
SMR	small modular reactor
UQ	Uncertainty Quantification

List of publications

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

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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`

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

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

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

Chapter 1

Methodology: Through a variety of complementary tools

1.1 Contributions

- Apply Stefano's method on the pathway model with a similar approach as Guevara et al.
- Check that PCE was appropriate as a method for such a system (ECOS2020)

Other authors' main contribution statement

On top of the main contributions of this thesis that are aforementioned, three main authors are to be mentioned for having brought a significant part of the methodological work. Based on Stefano Moret's monthly whole-energy system model (i.e. EnergyScope) [1], Gauthier Limpens has developed the hourly version of the snapshot model (i.e. EnergyScope TD) [2], as well as the perfect foresight pathway model [3], to which I personally contributed too. Diederik Coppitters has developed the RHEIA framework allowing to quantify the impact of uncertainties and carry out robust optimisation of energy systems [4]. The current work used this framework for the first of these functionalities. Finally, Stefano Moret extensively assessed the uncertainty characterisation on the Swiss energy system [5]. This thesis follows the same methodology, updating the uncertainty ranges for the pathway model.

1.2 Whole-energy system transition model optimisation: EnergyScope Pathway

On the contrary, this work optimises the entire transition pathway from a known system in 2020 up to 2050 thanks to EnergyScope Pathway [3]. According to pathway models review, EnergyScope Pathway can be categorised as an investment and operation optimisation model that assesses the whole-energy system, has a hourly time-resolution and is open-source documented model. Moreover, it maintains a low computational cost (i.e. around 15 minutes for a 30-year pathway with a hourly discretisation). Presenting here only the main constraints of the model and the main input data in Section **??**, the reader is invited to refer to the extended paper [3] and the documentation [6] for more extensive information.

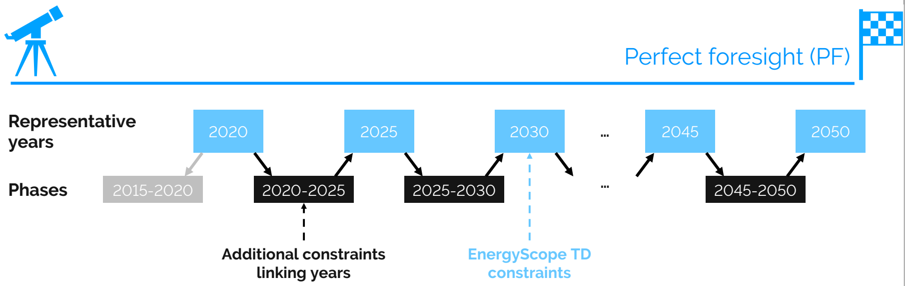

Figure 1.1. Illustration of the pathway methodology based on an existing energy system model. The methodology spans from 2020 to 2050, with one representative year every five years. The model EnergyScope Typical Days (EnergyScope TD) is applied in 7 representative years (light blue boxes). The formulation includes additional constraints (black boxes) that link the years together. The pathway's initialisation assumes that all capacities installed in 2020 were built during the pseudo-phase of 2015-2020 (grey box). The overall problem is defined as the pathway model. Graph adapted from [3].

1.3 Uncertainty quantification

1.3.1 Uncertainty characterisation

1.3.2 Polynomial Chaos Expansion

We used Polynomial Chaos Expansion (PCE), an approach for surrogate-assisted Uncertainty Quantification (UQ), to propagate uncertainties in input parameters through the system model. This allowed us to assess statistical moments on the quantity of interest and determine Sobol' indices [7]. To construct a PCE of the EnergyScope Pathway model, we employed the open-source Python framework RHEIA [8, 9]. Where the first part of this section is dedicated to the mathematical definition of this approach, the second details its choice and summarises the comparison made with another approach (i.e. Morris method) in a previous work [10].

Definition

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

$$\hat{M}(\xi) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}^{d,p}} u_{\boldsymbol{\alpha}} \mathbf{\Psi}_{\boldsymbol{\alpha}}(\xi) \approx M(\xi), \tag{1.1}$$

where the vector $\boldsymbol{\xi} = (\xi_1, \xi_2, \dots \xi_d)$ comprises the independent random input parameters (section A.3), d corresponds to the number of input distributions and $\boldsymbol{\alpha}$ is a multi-index, i.e. a vector of non-negative indices of length d, where each index corresponds to the degree of each univariate polynomial that forms the basis of the multivariate polynomial $\mathbf{\Psi}_{\boldsymbol{\alpha}}$. As uniform distributions are considered, the Legendre polynomials are adopted, as they are the associated family of polynomials that are orthogonal with respect to standard uniform distributions [11].

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

$$\mathcal{A}^{d,p} = \left\{ \boldsymbol{\alpha} \in \mathbb{N}^d \, : \, |\boldsymbol{\alpha}| \leq p \right\}. \tag{1.2}$$

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

$$\operatorname{card}\left(\mathcal{A}^{d,p}\right) = \binom{p+d}{p} = \frac{(d+p)!}{d!p!} = P + 1. \tag{1.3}$$

The coefficients $(u_0, u_1, \ldots, u_{P+1})$ are quantified using a regression method applied to orthonormal polynomials [11]. To ensure a well-posed least-square minimisation, it is recommended to have a number of training samples at least twice the number of coefficients [11]. Therefore, $2(P+1)$ samples are evaluated in the system model, and the model response for each quantity of interest is recorded. To generate the training samples, the quasi-random Sobol' sampling technique is employed [12]. As a low-discrepancy sequence, this technique exhibits the main advantage to investigate efficiently and (almost) uniformly the hypercube of uncertainties, unlike uniformly distributed random numbers.

The process of defining the polynomial degree includes incrementally increasing it until a desired level of accuracy is achieved [8]. Starting with $p = 1$, a PCE is constructed and the leave-one-out (LOO) error is evaluated. If the LOO error is below a specified threshold, the corresponding polynomial order is considered sufficient for generating an accurate PCE. However, if the error exceeds the threshold, the order is increased, and additional samples are generated following the rule of Eq. (1.3).

For the specific study of this work, a polynomial order of 2 is necessary (with 1260 training samples as per Eq. (1.3)) to achieve a LOO error below 1 % for the total transition cost.

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

$$\mu = u_0, \tag{1.4}$$

$$\sigma^2 = \sum_{i \neq 0} u_i^2. \tag{1.5}$$

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

$$S_i^T = \sum_{\alpha \in A_i^T} u_\alpha^2 / \sum_{i=1}^{P} u_i^2 \qquad A_i^T = \{\boldsymbol{\alpha} \in A | \alpha_i > 0\}. \tag{1.6}$$

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

Comparison with a proven method

Besides being an in-house used method, an early step of this thesis consisted in assessing PCE with similar approach used in the literature [10].

After characterising the uncertainty ranges, Moret et al. [5] quantified the impact of these uncertainties on the snapshot model of EnergyScope, i.e. ranking them, using the Morris method [13]. This method, as a statistical analysis, relies on individually randomized one-factor-at-a-time designs. Given the d model parameters $\vec{\xi} = (\xi_1, \xi_2, ..., \xi_d)$, the first step of the method consists in generating independent random samples of $\vec{\xi}$ in a standardised and discretised p-level *region of experimentation*, ω. In this *region of experimentation*, each ξ_i, varying in the interval $[\xi_{i,min},\ \xi_{i,max}]$, can take a random discrete value as follows :

$$\xi_i = \xi_{i,min} + j \cdot \frac{1}{p-1}\left(\xi_{i,max} - \xi_{i,min}\right) \quad \text{with } j \in \{0, 1, ..., p-1\} \tag{1.7}$$

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

$$EE_i = \frac{M(\xi_1, \xi_2, ..., \xi_i + \Delta, ..., \xi_d) - M(\vec{\xi})}{\Delta} \tag{1.8}$$

where M is the objective function, $\vec{\xi} \in \omega$, except $\xi_i \leq 1 - \Delta$ and Δ is a set multiple of $1/(p-1)\left(\xi_{i,max} - \xi_{i,min}\right)$. As in other studies [5, 14, 15], we consider p as even and $\Delta = p/[2(p-1)]\left(\xi_{i,max} - \xi_{i,min}\right)$.

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

Beyond the original Morris method, we used the standardized elementary effects, SEE_i, formulation [14], given by

$$SEE_i = EE_i \cdot \frac{\sigma(\xi_i)}{\sigma(M)}. \tag{1.9}$$

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

$$\mu_i^* = \mu(|SF_i|) \tag{1.10}$$

to rank parameters among each other. In (1.10), SF_i is the distribution formed by the r standardized elementary effects, as done in Moret [15].

In [10], we have assessed the PCE approach, comparing the Top-14 most impacting parameters obtained from this approach with the one provided by the improved Morris method based on μ_i^*. Even if the output of each method does not have the same physical meaning, both methods can rank the parameters by their impact on the total annual cost of the energy system. Both rankings were very similar which validates the use of PCE in the rest of this work.

1.3.3 Preliminary screening and selection

1.4 Reinforcement learning

1.5 Principal Components Analysis

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Appendix A

Case study: the Belgian energy system

A.1 Belgian energy system in 2020

The Belgian whole-energy system of 2020 was largely based (88.6% of the primary energy mix) on “conventional fuels"(i.e. oil and oil products (38.2%), natural gas (29.5%), uranium (16.3%) and solid fossil fuels (4.6%) while the rest mainly accounts for 26.7 TWh of lignocellulosic and wet biomass, 12.8 TWh of wind and 5.1 TWh of solar [16]. Given the data available in the literature (mostly for the power sector) and, when not available, following the assumptions made by Limpens et al. [17], Table A.1 gives the major technologies used in 2020 to supply the different demands of **??**.

A.2 CO_2-budget versus linear decrease of emissions

Figure A.1 shows the yearly emissions attributed for each sector in the REF case (i.e. imposed CO_2-budget) and a case where the CO_2-trajectory is constrained instead. Interestingly, these two transition pathways end up in a similar carbon-neutral whole-energy system in 2050. The two main sectors that significantly reduce their emissions in the REF case are the production of high value chemicals (HVC) and the high-temperature heat. In the former, this is linked to the extended use of oil products through naphtha-cracking. The latter is produced by industrial coal boilers for longer, until 2040. Overall, ending up to the same level of emissions in 2050, the REF case represents a 60% reduction of the cumulative emissions compared to the linear decrease, for a 7.5% more expensive transition.

Table A.1. Major technologies used to supply the 2020-demands of **??** in terms of share of production and installed capacity.

End-use demand	**Major technologies**	**Share of supply**	**Installed capacity**
Electricity	Nuclear	39%	5.9 GW
	CCGT	21%	3.9 GW
	Wind turbines	14%	5.0 GW
Heat High-Temp.	Gas boiler	36%	3.3 GW
	Coal boiler	30%	2.3 GW
	Oil boiler	20%	1.5 GW
Heat Low-Temp. (DEC)[a]	Oil boiler	48%	21.4 GW
	Gas boiler	40%	17.5 GW
	Wood boiler	10%	4.4 GW
Heat Low-Temp. (DHN)	Gas CHP	59%	0.3 GW
	Gas boiler	15%	0.3 GW
	Waste CHP	15%	0.1 GW
Private mobility[b]	Diesel car	49%	93.5 Mpass.-km/h
	Gasoline car	49%	94.7 Mpass.-km/h
	HEV	2%	5.9 Mpass.-km/h
Public mobility	Diesel bus	43%	3.6 Mpass.-km/h
	Train	43%	3.9 Mpass.-km/h
	CNG bus	5%	0.8 Mpass.-km/h
Freight mobility	Diesel truck	74%	62.7 Mt.-km/h
	Diesel boat	15%	10.8 Mt.-km/h
	Train	11%	2.5 Mt.-km/h
HVC	Naphtha/LPG cracking	100%	4.6 GW
Ammonia	Haber-Bosch	100%	1 GW
Methanol	Import	100%	-

[a]The decentralised heating units provide 98% of the low-temperature heat demand.
[b]The private mobility accounts for 80% of the passengers mobility.

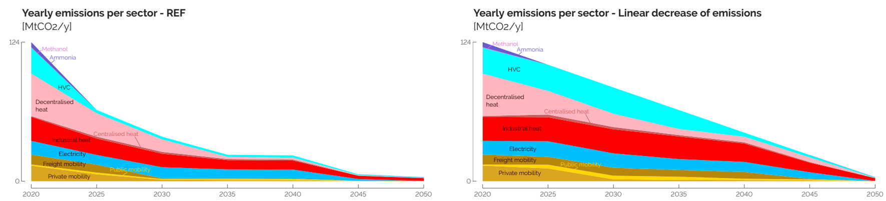

Figure A.1. Respecting the CO_2-budget imposed in the REF case drastically cuts the emissions of the system, especially in the production of high value chemicals (HVC) and the high-temperature heating sector.

A.3 Uncertainty characterisation for the 5-year steps transition

Table A.2 summarises the uncertainty ranges for the different groups of technologies and resources, for the year 2025. Refer to [5, 15] for the methodology and sources. As the model optimises the system every 5 years, $N = 5$ has been selected to get the final ranges of uncertainties of type II and III, based on the work of Moret [15]. For type III uncertainties (i.e. uncertainty ranges increasing with time), a 50% increase has been set arbitrarily between the ranges for 2025 and these same ranges for 2050. In other words, for these specific uncertainties, the ranges for 2050 are 50% larger than for 2025.

Rixhon et al. [18] analysed the impact of these parameters on the total cost of the snapshot Belgian whole-energy system in 2050 subject to different global warming potential (GWP) limits. Based on this work, we have selected a subset of impacting uncertainties, added others due to the pathway formulation (e.g. $\Delta_{\text{change,pass}}$), and listed them in Table A.2. The uncertainty characterisation gives the uncertainty ranges per parameter or group of parameters (category).

This work considers nine groups of uncertain parameters: (i) the cost of purchasing imported energy carriers; (ii) the investment cost (i.e. CAPEX) of some technologies, mostly related to the mobility sector and the integration of renewables; (iii) the maintenance cost (i.e. OPEX) of every technology; (iv) the consumption of electric and fuel cells vehicles in the mobility sector; (v) the potential installed capacity of renewables; (vi) the hourly load factor of renewables accounting for variability of solar irradiance or wind speed; (vii) the availability of resources considered as limited (i.e. biomass and electricity); (viii) the end-use-demands split per sector of activities (i.e. households, services, passenger mobility and industry) and (ix) other parameters like the interest rate or the modal share change in different key sectors. For the specific case of small modular reactor (SMR), the parameter $f_{\text{max,SMR}}$ will influence the maximum capacity (i.e. 6 GW) to install to translate somehow the readiness of this technology. If it is (i) smaller than 0.6, there is no possibility to install SMR during the transition; (ii) between 0.6 and 0.8, these 6 GW can be installed only in 2050; (iii) between 0.8 and 0.9, these can be installed from 2045 onward and; (iv) higher than 0.9, the prescribed maximum capacity can be installed from 2040 onward.

Table A.2. Application of the uncertainty characterization method to the EnergyScope Pathway model for the year 2025.

Category	Parameter	Meaning	Type[a]	Relative variation[b]	
				min	max
Cost of purchasing	$c_{\text{op,fossil}}$	Purchase fossil fuels	II	-64.3%	179.8%
	$c_{\text{op,elec}}$	Purchase electricity	II	-64.3%	179.8%
	$\boldsymbol{c_{\text{op,electrofuels}}}$	**Purchase electrofuels**	**II**	**-64.3%**	**179.8%**
	$c_{\text{op,biofuels}}$	Purchase biofuels	II	-64.3%	179.8%
Investment cost	$c_{\text{inv,car}}$	CAPEX car	I	-21.6%	25.0%
	$c_{\text{inv,bus}}$	CAPEX bus	I	-21.6%	25.0%
	$c_{\text{inv,ic\_prop}}$	CAPEX ICE	I	-21.6%	25.0%
	$c_{\text{inv,e\_prop}}$	CAPEX electric motor	I	-39.6%	39.6%
	$c_{\text{inv,fc\_prop}}$	CAPEX fuel cell engine	I	-39.6%	39.6%
	$c_{\text{inv,efficiency}}$	CAPEX efficiency measures	I	-39.3%	39.3%
	$c_{\text{inv,PV}}$	CAPEX PV	I	-39.6%	39.6%
	$c_{\text{inv,grid}}$	CAPEX power grid	I	-39.3%	39.3%
	$c_{\text{inv,grid\_enforce}}$	CAPEX grid reinforcement	I	-39.3%	39.3%
	$\boldsymbol{c_{\text{inv,nuclear\_SMR}}}$	**CAPEX SMR[c]**	**I**	**-40.0%**	**44.0%**
Maintenance cost	$c_{\text{maint,var}}$	Variable OPEX of technologies	I	-48.2%	35.7%
Consumption	$\eta_{\text{e\_prop}}$	Consumption electric vehicles	I	-28.7%	28.7%
	$\eta_{\text{fc\_prop}}$	Consumption fuel cell vehicles	I	-28.7%	28.7%
Potential installed capacity	$f_{\text{max,PV}}$	Max capacity PV	I	-24.1%	24.1%
	$f_{\text{max,windon}}$	Max capacity onshore wind	I	-24.1%	24.1%
	$f_{\text{max,windoff}}$	Max capacity offshore wind	I	-24.1%	24.1%
Hourly load factor	$c_{\text{p,t,PV}}$	Hourly load factor PV	II	-22.1%	22.1%
	$c_{\text{p,t,winds}}$	Hourly load factor wind turbines	II	-22.1%	22.1%
Resource availability	$avail_{\text{elec}}$	Available electricity import	I	-32.1%	32.1%
	$avail_{\text{biomass}}$	Available local biomass	I	-32.1%	32.1%
End-use demand	HH_EUD	Households EUD	III	-13.8%	11.2%
	$services\_EUD$	Services EUD	III	-14.3%	11%
	$pass\_EUD$	Passenger mobility EUD	III	-7.5%	7.5%
	$industry\_EUD$	Industry EUD	III	-20.5%	16.0%
Miscellaneous	i_{rate}	Interest rate	I	-46.2%	46.2%
	$\%_{\text{pub,max}}$	Max share of public transport	I	-10%	10%
	$\Delta_{\text{change,freight}}$	Modal share change freight mobility	-	-30%	30%
	$\Delta_{\text{change,pass}}$	Modal share change passenger mobility	-	-30%	30%
	$\Delta_{\text{change,LT\_heat}}$	Modal share change LT-heat	-	-30%	30%
	$\boldsymbol{f_{\text{max,SMR}}}$	**Potential capacity SMR**	**-**	**0**	**1**

[a]Per [15], "I: investment-type, II: operation-type (constant uncertainty over time), III: operation-type (uncertainty increasing over time)".

[b]The nominal values of each of the parameters is 0, meaning no variation compared to the nominal values of the impacted parameter in the model.

[c]This range has been inferred from the local sensitivity analysis performed by EnergyVille [19].

Appendix B

EnergyScope Pathway: More details on its choice and its formulation

B.1 EnergyScope Pathway: The right model to choose

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

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

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

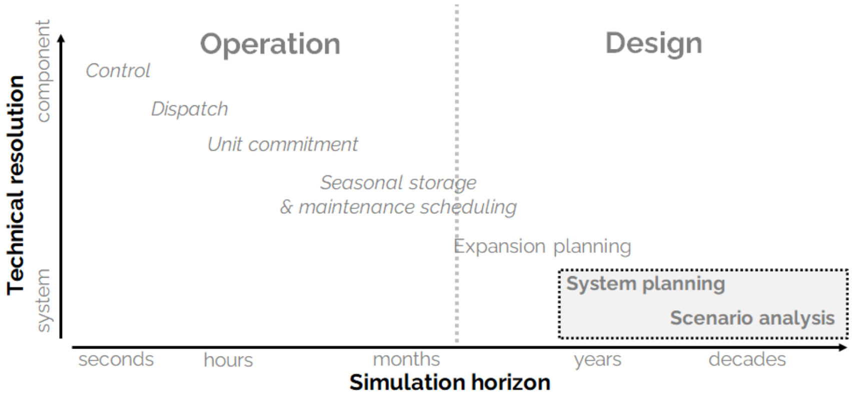

Figure B.1. Model can be classified by their core focus: **Operation** or **Design**. These categories can be broken down into subcategories. This paper focuses on the system planning and scenario analysis models. Inspired from [20].

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

These requirements can be transposed into criteria that a model should match: (i) it should have an hourly resolution spanning a one-year time horizon; (ii) it should encompass the entire energy system, including all types of demands (such as heat, electricity, mobility, and non-energy), as well as all resources, conversion processes, and storage technologies; (iii) it should optimise the system design, accounting for all the options; (iv) it should have a long-term investment horizon, spanning several decades; (v) its computational time should be reasonable, typically less than one hour on a personal laptop; (vi) it should be open-source, with accessible data and comprehensive documentation. These requirements are commonly found in reviews of energy system models. In 2010, Connolly et al. [21] reviewed 68 tools, considering similar criteria: (i-iv) and (vi), along with others such as the number of users and market equilibrium. In 2019, Prina et al. [22] reviewed 12 “*most established*" models, focusing on criteria (i-ii) and (iv). This review was followed by a classification where criteria (i-iv) were taken into account [23]. In 2021, Chang et al. [24] conducted a survey-based review of 42 models for energy transition modelling, covering all criteria except computational time. Based on these reviews, Table B.1 compares models based on all the previous criteria except the computational time (v). Indeed, the latter is hard to compare as models are not apply to the same case study and the information is rarely given. The table includes only the models that achieved partially at least four out of the five criteria. The authors endeavored to refresh the model's information by consulting the model's website and repository, yet there is a possibility that some information might have been overlooked or omitted inadvertently.

From Table B.1, four models almost check all the boxes (partially the pathway one): Calliope, GENeSYS-MOD, PyPSA and TIMES. The TIMES model, short for The Integrated MARKAL-EFOM System, is a well-established framework renowned for its capacity to generate comprehensive energy models. It encompasses a rich array of features, including support for multi-cell modeling, pathway analysis, full-scale representation of energy systems, and the consideration of market equilibrium dynamics, all of which facilitate thorough scenario exploration. This model has a widespread adoption and has been utilized by worldwide institutions such as the International Energy Agency (IEA) or technical ones such as VITO (Vlaamse Instelling voor Technologisch Onderzoek) research institute in their research endeavors. Notably, TIMES was reported commercial in 2010 [21]. A more recent survey conducted in 2020-2021 confirmed that the model was using a commercial interface [24]. Recent developments by the IEA-ETSAP have resulted in a version that is compatible with open-source solver CBC. In various studies conducted in different regions, including Canada, Sweden, the EU, and Denmark, TIMES has been shown to utilize 12 to 32 time-slices annually [23]. It is noteworthy that Haydt et al. [54] conducted a study focusing on the electrical sector, using 288 time slices, equivalent to a 12-day time resolution, highlighting the sensitivity of results to time resolution. Regarding data accessibility, while some publications partially present the dataset used, the overall accessibility of TIMES data remains an area of ongoing inquiry [53]. Calliope is a '*tool that makes it easy to build energy system models´* at different geographical scale. Even if the framework offers the possibility of modelling multi-year systems, the authors didn't find a relevant publication on this topic. In fact, the model is typically employed for scenario analysis with a specific focus on the electricity system. Previous studies have used the model to investigate the phasing out of fossil and nuclear energies in a multi-regional UK power system [55]. More recently, the model has been applied to analyse a scenario of a multi-energy district in Switzerland [56]. Moreover, the model has been used with

Table B.1. Comparison of existing models that partially satisfy at least four of the six criteria (in alphabetical order). Legend: ✓criterion satisfied; ✓ criterion partially satisfied; ✗ criterion not satisfied. Data from [21–24].

Model	**Ref.**	**Hourly**	**Whole-energy**	**Optimis. invest. & operation**	**Pathway**	**Open-source**
Calliope	[25, 26]	✓	✓	✓	✗[a]	✓
COMPOSE	[27]	✓	✓	✓	✓	✓[b]
DER-CAM	[28, 29]	✓	✓[c,d]	✓	✗[e]	✓[f]
DIETER	[30]	✓	✓[d,g]	✓	✗[e]	✓
E2M2	[31]	✓	✓[c,d,h]	✓	✓	✗[i]
EMPIRE	[32]	✓	✗[c,d,g,h]	✓	✓	✓[b]
Ener. Trans. Model	[33]	✓	✓	✗[j]	✓	✓
EnergyPLAN	[34]	✓	✓	✗[k]	✗[l]	✓[f]
energyRt	[35]	✓	✓	✓[m]	✓	✓
EnergyScope TD	[2]	✓	✓	✓	✗[l]	✓
Enertile	[36]	✓	✓[d]	✓	✓	✗[n]
ESO-XEL	[37]	✓	✗[c,d,g,h]	✓	✓	✓
GENeSYS-MOD	[38]	✓	✓	✓	✓[o]	✓
H2RES	[40]	✓	✗[p]	✓[p]	✓	✓
iHOGA	[42]	✓	✗[c,d,g,h]	✓[m]	✓	✓[b]
IMAKUS	[43]	✓	✓[c,d]	✓	✓	✗[i]
OpenDSS	[44]	✓	✓	✗[k]	✓	✓
Plexos	[45]	✓	✓[q]	✓	✓	✗[i]
PyPSA	[47, 48]	✓	✓	✓	✓[r]	✓
RamsesR	[50]	✓	✓[c,d,h]	✓	✓	✓
ReEDS	[51]	✗[s]	✓[d,g,h]	✓	✓	✓[b]
TIMES	[52]	✓	✓	✓	✓	✓[t]

[a] Topic is being discussed in the chat of their repository but not yet included in their documentation.
[b] '*Free under some special conditions´*.
[c] Transport not accounted.
[d] Industry not accounted
[e] Not specified but time horizon is 1 year.
[f] Freeware.
[g] district heating network (DHN) not accounted.
[h] individual heating not accounted.
[i] Commercially (paid) licensed.
[j] The ETM is a simulation model with a simple merit order 'optimisation' for electricity, flex and heat.
[k] Simulation model.
[l] Yearly horizon without pathway.
[m] EnergyRT optimises investments only, while iHOGA conducts optimisation and simulation without specifying timing or scope.
[n] Only for internal use.
[o] Löffler et al. [38] applied a pathway transition, but the time resolution was increased to 12h and it uses 3 typical days over a year. [39] performed a multi-regional pathway (16 nodes) for the case of Germany from 2020 to 2050 with a time step of 5 years. However, the time resolution is 16 time slices representing 4 hours per day and one day per season.
[p] In their review in 2021, [41] classified H2RES as a simulation model on power sector only. In their work [40] presented a new version of H2RES claiming to optimise the power system and partially represent other sectors. Their study applied the model to a transition pathway for Croatia. In the conclusion, it is claimed '*H2RES offers practically unlimited potential for functionality expansion since it is an open-source program´* which open the doors for future developments to encompass new features.
[q] Does not account for all sectors but allow to implement them according to [46].
[r] [49] applied PyPSA to a whole energy system split in 37 nodes. Using a myopic approach, the model optimises the energy transition with a 3-hours resolution).
[s] Seasonal time slice.
[t] Model is now open-source with limited access to data [53].

decades of weather data. However, its application has been limited to assessing the impact of inter-year variability in wind and PV on the results, rather than evaluating a transition pathway [57]. Similarly GENeSYS-MOD presents some limitations. This model is an application of the open-source energy modelling system (OSeMOSYS), itself represented as a model with a poor time discretisation and a heavy computational burden according to [22]. Löffler et al. [38] applied the model to the world by splitting it into 10 regions and most of the energy demand sectors. The time disaggregation can be chosen by the user, for their application they used representative years with three days and two time slice per day. Among the open-source models with an active community, PyPSA is one of the best-performing, with a large and active community, development at the state of the art, worldwide applications, and usage not only limited to academia. A study conducted by Bartholdsen et al. [39] centered on Germany employed a representation comprising 16 time slices for representative years. This choice was substantiated by the work of Welsch et al. [58], which demonstrated that this level of temporal granularity yields consistent results in comparison to hourly time resolution over a year. However, it is noteworthy that the utilization of a limited number of time slices may simplify the optimization of storage technologies, especially those designed for inter-month energy storage. This simplification can be viewed as a pragmatic approach to reduce the computational burden while over-simplifying the challenge of accurately integrating intermittent renewable energy sources. Furthermore, PyPSA, a modeling framework recognized for its robustness and active user community, has also been employed to investigate scenarios related to myopic transitions [49]. Hence, it is worth noting that while Calliope, OSeMOSYS, PyPSA and TIMES frameworks have the potential to be used for evaluating a transition pathway, the authors have not come across any publication that explicitly demonstrates their application to such cases with an hourly time resolution over significant time slices.

Hence, it appears that none of the models of Table B.1 fully meet all five criteria outlined in the table, topped with the additional consideration of acceptable computational time. This observation is consistent with the findings presented in [22] who identified two approaches for optimising the energy transition pathway based on the six criteria. The first approach involves running a snapshot model multiple times using an algorithm that optimises the transition path and validates the system's operability. The second approach aims to extend a snapshot model to represent the entire transition pathway. However, they excluded this option due to the lack of models that met the requirements of being fast enough and easily adaptable. Therefore, they developed a new model based on the first methodology, named EPLANoptTP. It uses a multi-objective evolutionary algorithm to optimise the EnergyPLAN model [34]. To manage computational time, the number of decision variables is limited to three: photovoltaic (PV), wind turbine and battery capacities. Thus, the model does not investigate all the options (i.e. criteria (iii)).