### Whole-energy system models: the advisors for the energy transition

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#### 1. What are whole-energy system models?

Climate change is making the transition to more renewable and sustainable energy systems an urgent global priority. Countries and communities around the world are developing their respective long-term energy plans, and deciding on the key resources and technologies required to meet their future energy needs. These developments are guided and supported by energy models.

Energy models are simplified mathematical representations of energy systems. They can consider a global scale—top-down—or they can start from the small scale with finer technical details—bottom-up. These models perform an energy balance: *resources* can be imported or extracted; these resources are transported, stored, and converted by *energy conversion technologies* if necessary, with the ultimate goal of supplying end-use *demand* (electricity, transport, heating, and the production of goods) [1].

Altogether, the number of energy system models is overwhelming (483 in a recent review [2]), with each model answering slightly different questions [3]. We focus here on energy system optimisation models that include all forms of energy-whole-energy-and find the optimal pathways to convert resources into end-use energy demand. Future energy systems will be smart, flexible, highly renewable, and sector-coupled. To study and plan such complex systems, whole-energy system models look at the energy system in its entirety. They are instrumental in understanding the effects of past policies, and in devising scenarios that account for complex interactions and synergies among different technologies, energy vectors, and specific needs [4].

#### 2. It is not only about the power sector

Historically, energy models have been developed for the power sector, being tools for planning and

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dispatch to ensure the power grid stability. As the energy transition requires a large penetration of renewable energy sources—mostly electricity based like solar and wind—the power sector will maintain a key role. However, there is more to consider than just the power sector. Future energy systems will be strongly sector-coupled: mobility and heat are—and will be—high energy consumers even if provided by electricity through heat pumps and electric vehicles (*electrification*). Focusing solely on the power sector will thus not be enough.

wind Solar and are intermittent and non-dispatchable. Therefore, energy storage will be an essential part of the system, even if the demand can become partially flexible, backups are implemented, or we resort to curtailment. This energy storage may not always be in the form of batteries. For example, chemical energy carriers could be our only way to store very large amounts of energy (from 100 GWh) [5].

Storage presents many challenges for research (e.g. what is the rate of storage degradation?), engineering (e.g. how can we make storage more efficient?), and economy (e.g. how can we integrate storage in the market?). But these challenges also offer opportunities. The most significant being the opportunity to couple diverse sectors. For example, renewable electricity can be stored as ammonia (one of the potential chemical energy carriers) and subsequently used in the fertiliser industry—coupling the energy and industry sectors. As another example, electric vehicle smart charging and heat storage solutions can serve as buffers for the electricity grid. Multi-sector multi-vector whole-energy system models aim to account for all of these opportunities.

Electrification is also a matter of timescale: the increase will be gradual. We currently obtain 80% of our final energy through combustion, ignoring this massive share is unreasonable. Combustion will need to improve (pollutant reduction), and to evolve (alternative fuels, some produced from electricity). It will remain to be an important provider of energy during the transition, and the most probable solution for some specific activities (e.g. planes, cement, glass).

Realistic planning will need to integrate all of the dimensions of the energy system without falling

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short of an integrated optimum; this is again the main motivation of whole-energy system models.

#### 3. System thinking vs. isolated thinking

Many projects focus on designing the perfect solution to a given energy problem: they design the most efficient boiler or they introduce innovative urban wind turbines. Yet, these exciting solutions cannot be evaluated in isolation. Their full potential can only be truly assessed and realised when integrated in the whole energy system. This system is usually so complex that many interactions cannot be anticipated, even if they appear obvious in hindsight. The efficiency of the ultimate photovoltaïc cell is not as meaningful until it is integrated within a module, and connected to an inverter. We also cannot disregard how the electricity is to be used (end-use, conversion to fuels, heat pumps, etc).

The optimal conversion route might also depend on the system configuration. As an example, converting biomass to biofuels can allow an overall reduction in terms of greenhouse gas emissions. However, to exploit this potential, it is necessary to link the production of biofuels to a wider deployment of the corresponding efficient end-use technologies. Only an analysis within such a context could point towards the best combination of routes [6].

Still, energy system models require a detailed and exhaustive characterisation of all technologies. Failure to do so properly may lead to biased results. For example, oversimplifying the diversity of alternative fuels into one surrogate could hide their true potential in various applications (e.g. in the chemical industry). As another example, taking the efficiency of heat pumps from laboratory tests, and not in real conditions, could overestimate their usefulness. Therefore, there is a strong need for properly documented data which consists of not only the nominal performance, but includes the whole range of operating conditions-ultimately the goal of the many projects developing these technologies. In this context, several initiatives aim at centralising data from various sources (e.g. the Open Power System Data platform [7]).

Assessing the energy system as a whole unlocks the potential for the full deployment of synergies and generates unexpected results. For example, focusing only on the power sector may lead to an oversizing of battery storage, which comes at great expense. (author?) [8] show that by focusing solely on the electric system, 2 TWh of batteries are needed. Whereas by analysing the energy system as a whole and making use of synergies between sectors, the capacity drops down to 0.3 TWh. As another example, in Belgium, the need for batteries is mainly replaced by thermal storage. By oversizing wind and solar power production (65 TWh/year), the surplus production can be converted using heat pumps (30 GW) and stored as heat (4.5 TWh/year), whilst

during low renewable production, heat pumps are switched off, reducing the demand on the electrical system [9].

# 4. The real world is uncertain, a pathway only makes sense if it is robust

Setting a sustainability target has been the goal of many reports and conferences, but we also need to navigate toward it materially. Progressing from the energy system of today, to a more sustainable one of the future, will require more than academic discussion; as importantly, it will require a pathway to implementation that can be realised. Owing to its complexity, the energy-system transition may require disruptive changes that are unlikely to be reached with a linear progression towards the target. For example, we do not know if the contribution of fossil fuels should monotonically decrease, or when to deploy storage to reach high renewable shares in the long term. We also do not know if the transport sector should be transformed first, and how this transformation couples with industry. Many other questions are left unanswered when we move from where to go to how to get there.

Using models enables policy and decision makers to steer towards rational and hopefully optimal solutions. However, when obtaining the optimum, the user is left with "what if" questions: what if the operating conditions change (e.g. the demand); what if the design parameters cannot be precisely controlled (e.g. decentralised PV); or what if the parameters of the models are uncertain (e.g. fuel prices). All these questions must be answered by integrating uncertainty quantification into whole-energy system models. These methods take the input uncertainties into account and propagate them to the output, obtaining thereby a range of possible solutions or even their probability density functions [10, 11]. However, these methods require knowledge about the input uncertainties. In a whole-energy system, this knowledge embraces all sectors, all factors, all energy vectors, and all conversion systems. Yet, this knowledge does not always need to be precise; often, it just needs to be pragmatically included.

Ultimately, the planner needs to optimise a system with uncertainties, performing thereby robust design optimisation [12]. Thus, another optimisation objective is added: to minimise the variance of the performance. Most often, reducing the variance—making the system more robust—conflicts with optimising the performance, such that there is a trade-off—a Pareto front. It leaves the designer with a choice: what should be sacrificed in performance to gain in robustness.

In such a complex and multi-sectorial context with thousands of parameters, there is significant room for uncertainty and a comprehensive analysis can become a daunting task; similarly to combustion chemistry problems where many parameters remain uncertain [13]. For robust optimisation, which compounds optimisation with the uncertainty quantification, the cost can become intractable: it is the *curse of dimensionality*, the high computational cost associated with the large number of parameters. Minimising the cost is crucial, both for the robust optimisation (e.g. with sparse polynomial chaos [14]) and the energy models (e.g. with the use of typical days [15]).

Vested with such information, the planner can make better decisions and compare the merits of different configurations, trying to find a robust pathway: a pathway that would be less affected by uncertainties. Not applying our prior knowledge of the uncertainties, even if limited, could lead to a fragile pathway where the risk of failure would affect our chances to reach the target.

As an illustration, energy models often rely on long-term forecasts for important parameters, such as the price of natural gas. These forecasts are unfortunately seldom accurate [16]. (author?) [17] showed that in the last 20 years, forecasts have underestimated the evolution of European natural gas prices by as much as 300%, and that this stimulated exhaustive investments in gas-fired power plants that eventuated to be too expensive to be operated. This contributed to generating the current situation of overcapacity in the European electricity market, with installed capacities more than doubling peak demand in many countries. The consequences have been dramatic: as an extreme example, in the Netherlands, newly constructed combined cycle power plants were shut down in 2014 since they became non-economically viable to operate. Considering uncertainties in the planning process reduces the overcapacity from 24% of the actual demand to less than 10% [17].

# 5. Conclusion: the energy transition is an interdisciplinary effort

Energy system modelling is a very active research field. It tackles many challenges and tries to answer many questions. Its primary purpose is to guide us through the disruptive changes of the energy transition. As such, it has a key role for the decision and policy makers. Without it, how can one realistically plan an optimal and sustainable energy system? Aiming today at 80%—or 100%—renewable energy is a paradigm shift [18]; it is a significant step forward, where future energy systems may highly contrast that of today.

Searching for a robust pathway towards a sustainable energy system involves navigating in very uncertain waters. There can be various ways to set the objective of this optimisation, but since we are on a race with climate change, we believe there is only one thing that matters: given the many constraints (e.g. market, societal, economic), what would be the most efficient way to reach a sustainable energy system.

Decisions about the energy transition involve much more than technical results [19]. These results need to be integrated within energy market models so they can integrate co-benefits—the synergies we create alongside climate change mitigation [20]—or the many obstacles like the rebound effect. Ultimately, decisions also carry tradeoffs with access to energy, risk, and security. The energy transition is an interdisciplinary effort [21]. Blind technology advancement is most probably not the way forward for the transition towards sustainability. As the world devises long-term energy plans, whole-energy system models can guide us on the pathway towards sustainability.

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