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RHEIA: Robust design optimization of renewable Hydrogen and dErIved energy cArrier systems

Diederik Coppitters[1, 2], **Panagiotis Tsirikoglou**[3], **Ward De Paepe**[4], **Konstantinos Kyprianidis**[5], **Anestis Kalfas**[6], **and Francesco Contino**[1]

1 Institute of Mechanics, Materials and Civil Engineering, Université catholique de Louvain **2** Fluid and Thermal Dynamics, Vrije Universiteit Brussel **3** Limmat Scientific AG **4** Thermal Engineering and Combustion Unit, University of Mons **5** Department of Automation in Energy and Environment, School of Business, Society and Engineering, Malardalen University **6** Department of Mechanical Engineering, Aristotle University of Thessaloniki

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Summary

Climate change is a constant call for the massive deployment of intermittent renewable energy sources, such as solar and wind. However, to cover the energy demand at all times, these sources require energy storage over more extended periods. In this framework, renewable energy storage in the form of hydrogen is gaining ground on leading the transition of today's economy towards decarbonization. Among others, hydrogen can be integrated into multiple energy sectors: hydrogen can be converted back into electricity (power-to-power), it can be used to produce low-carbon fuels (power-to-fuel), and it can be used to fuel hydrogen vehicles (power-to-mobility). The performance of these hydrogen-based energy systems is subject to uncertainties, such as the uncertainty on the solar irradiance, the energy consumption of hydrogen-powered buses and the price of grid electricity. Disregarding these uncertainties in the design process can result in a drastic mismatch between simulated and real-world performance, and thus lead to a *kill-by-randomness* of the system. The *Robust design optimization of renewable Hydrogen and dErIved energy cArrier systems* (RHEIA) framework provides a robust design optimization pipeline that considers real-world uncertainties and yields robust designs, i.e., designs with a performance less sensitive to these uncertainties. Moreover, RHEIA includes models to evaluate hydrogen's techno-economic and environmental performance in a power-to-fuel, power-to-power and power-to-mobility context. When combined, RHEIA unlocks the robust designs for hydrogen-based energy systems. As RHEIA considers the system models as a black box, the framework can be applied to existing open-source and closed-source models. To illustrate, an interface with the EnergyPLAN software is included in the framework.

Statement of need

Incorporating hydrogen is still an anomaly in design optimization studies of renewable energy systems (Eriksson & Gray, 2017). Moreover, the optimization is often performed under the assumption of deterministic parameters (i.e., fixed, free from inherent variation). Considering fixed values for model parameters in design optimization yields designs that might be sensitive – the real issue is that we cannot know– to real-world uncertainties and results in a drastic mismatch between simulated and actual performances. In fields different from energy systems, e.g., structural mechanics, aerospace and automobile applications, Robust Design Optimization (RDO) yielded robust designs by minimizing the variance on the performance (Orosz et al., 2020). Consequently, alternative design solutions were proposed that provide the least sensitive performance to the random environment. To ensure the computational tractability of RDO, surrogate modelling techniques achieve a promising computational efficiency to quantify the mean and variance on the performance. Nevertheless, applications of such surrogate-assisted robust design optimization techniques are limited (Chatterjee et al., 2017). To fill these research gaps, RHEIA provides a multi-objective RDO algorithm, for which the uncertainty quantification is performed through a Polynomial Chaos Expansion (PCE) surrogate modelling technique. In addition, RHEIA includes Python-based models for relevant valorization pathways of hydrogen: power-to-fuel, power-to-power and power-to-mobility. The significant techno-economic and environmental uncertainties for these models are characterized based on scientific literature, and a method is included to gather climate data and demand data for the location of interest. Finally, RHEIA allows connecting your own models to the RDO and uncertainty quantification algorithms as well.

Simulation models that include the evaluation of hydrogen-based energy systems exist, e.g., INSEL, EnergyPLAN and TRNSYS. Despite their extensive component model libraries, these simulation models lack an optimization feature. HOMER Energy includes an optimization algorithm to design hybrid microgrids, including hydrogen system component models. In Python, Calliope (Pfenninger & Pickering, 2018) considers the optimization of multi-scale energy system models, where hydrogen is regarded as a fuel in advanced gas turbines. However, neither multi-objective problems nor uncertainties during design optimization can be considered.

Coppitters et al. applied the RDO framework to Python-based hydrogen-based energy systems: A directly-coupled photovoltaic-electrolyzer system (Coppitters et al., 2019) and a photovoltaic-battery-hydrogen system (Coppitters et al., 2020). In addition, Verleysen et al. used the framework to optimize an Aspen Plus model of a power-to-ammonia system (Verleysen et al., 2020). Other Aspen Plus models have been optimized as well through RHEIA: a micro gas turbine with a carbon capture plant (Giorgetti et al., 2020) and a micro gas turbine (De Paepe et al., 2019). Finally, Rixhon et al. performed uncertainty quantification on an EnergyScope model (Rixhon et al., 2021).

Future work

Among others, we will make the following improvements in future versions of RHEIA:

- Including a sparse PCE algorithm, developed in our research group at the Vrije Universiteit Brussel, to handle the curse-of-dimensionality for high-dimensional problems (Abraham et al., 2017). The sparse PCE algorithm has been proven effective in RDO for a photovoltaic-battery-hydrogen application (Coppitters et al., 2020). To ensure a smooth inclusion of this sparse PCE algorithm in RHEIA, we built the `pce` module, instead of adopting an existing PCE package in Python, such as ChaosPy (Feinberg & Langtangen, 2015).
- Including optimization algorithm alternatives (e.g., Particle Swarm Optimization, Firefly Algorithm, Cuckoo Search), following our experience gained over the last years on using these algorithms in a surrogate-assisted RDO context (Tsirikoglou et al., 2017). Moreover, optimization schemes that can handle mixed-integer problems are also of vital interest. The latter will enable RHEIA to address design and optimization problems closer to the industry.
- Adding additional models on hydrogen-based energy carrier production and utilization (e.g. ammonia, biomethane) in power-to-gas applications.
- Including an adapted PCE to perform uncertainty quantification with imprecise probabilities, to distinguish between the importance of epistemic and aleatory uncertainty on a parameter. For example, we performed an RDO with imprecise probabilities on a photovoltaic-battery-heat pump system(Coppitters et al., 2021).

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