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

Diederik Coppitters, Panagiotis Tsirikoglou, Ward De Paepe, Konstantinos Kyprianidis, Anestis Kalfas, and Francesco Contino

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

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 actual performances. 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 actual performances. Consequently, alternative design solutions were proposed that provide the least sensitive performance to the random environment. To ensure the computational tractability of RDO, 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 of 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).

Coppitters et al. (2022). RHEIA: Robust design optimization of renewable Hydrogen and dErived energy cArrier systems. Journal of Open Source Software, 7(75), 4370. https://doi.org/10.21105/joss.04370.
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References

Abraham, S., Raisee, M., Ghorbaniasl, G., Contino, F., & Lacor, C. (2017). A robust and efficient stepwise regression method for building sparse polynomial chaos expansions. *Journal of Computational Physics*, 332, 461–474. https://doi.org/10.1016/j.jcp.2016.12.015

Chatterjee, T., Chakraborty, S., & Chowdhury, R. (2017). A Critical Review of Surrogate Assisted Robust Design Optimization. *Archives of Computational Methods in Engineering*, 1–30. https://doi.org/10.1007/s11831-017-9240-5

Coppitters, D., De Paepe, W., & Contino, F. (2019). Surrogate-assisted robust design optimization and global sensitivity analysis of a directly coupled photovoltaic-electrolyzer system under techno-economic uncertainty. *Applied Energy*, 248, 310–320. https://doi.org/10.1016/j.apenergy.2019.04.101

Coppitters, D., De Paepe, W., & Contino, F. (2020). Robust design optimization and stochastic performance analysis of a grid-connected photovoltaic system with battery storage and hydrogen storage. *Energy*, 213, 118798. https://doi.org/10.1016/j.energy.2020.118798

Coppitters, D., De Paepe, W., & Contino, F. (2021). Robust design optimization of a photovoltaic-battery-heat pump system with thermal storage under aleatory and epistemic uncertainty. *Energy*, 120692. https://doi.org/10.1016/j.energy.2021.120692

De Paepe, W., Coppitters, D., Abraham, S., Tsirikoglou, P., Ghorbaniasl, G., & Contino, F. (2019). Robust Operational Optimization of a Typical micro Gas Turbine. *Energy Procedia*, 158, 5795–5803. https://doi.org/10.1016/j.egypro.2019.01.549

Eriksson, E. L. V., & Gray, E. M. A. (2017). Optimization and integration of hybrid renewable energy hydrogen fuel cell energy systems – A critical review. *Applied Energy*, 202, 348–364. https://doi.org/10.1016/j.apenergy.2017.03.132

Feinberg, J., & Langtangen, H. P. (2015). Chaospy: An open source tool for designing methods of uncertainty quantification. *Journal of Computational Science*, 11, 46–57. https://doi.org/10.1016/j.jocs.2015.08.008

Giorgetti, S., Coppitters, D., Contino, F., Paepe, W. D., Bricteux, L., Aversano, G., & Parente, A. (2020). Surrogate-Assisted Modeling and Robust Optimization of a Micro Gas Turbine Plant With Carbon Capture. *Journal of Engineering for Gas Turbines and Power*, 142(1). https://doi.org/10.1115/1.4044491

Orosz, T., Rassõlkin, A., Kallaste, A., Arsénio, P., Pánek, D., Kaska, J., & Karban, P. (2020). Robust design optimization and emerging technologies for electrical machines: Challenges and open problems. *Applied Sciences*, 10(19), 6653. https://doi.org/10.3390/app10196653

Pfenninger, S., & Pickering, B. (2018). Calliope: A multi-scale energy systems modelling framework. *Journal of Open Source Software*, 3(29), 825. https://doi.org/10.21105/joss.00825

Rixhon, X., Limpens, G., Coppitters, D., Jeanmart, H., & Contino, F. (2021). The Role of Electrofuels under Uncertainties for the Belgian Energy Transition. *Energies*, 14(13), 4027. https://doi.org/10.3390/en14134027

Coppitters et al. (2022). RHEIA: Robust design optimization of renewable Hydrogen and dErived energy cArrier systems. *Journal of Open Source Software*, 7(75), 4370. https://doi.org/10.21105/joss.04370.
Tsirikoglou, P., Abraham, S., Contino, F., Bağci, Ö., Vierendeels, J., & Ghorbaniasl, G. (2017). Comparison of metaheuristics algorithms on robust design optimization of a plain-fin-tube heat exchanger. 18th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, 3827. https://doi.org/10.2514/6.2017-3827

Verleysen, K., Coppitters, D., Parente, A., De Paepe, W., & Contino, F. (2020). How can power-to-ammonia be robust? Optimization of an ammonia synthesis plant powered by a wind turbine considering operational uncertainties. Fuel, 266, 117049. https://doi.org/10.1016/j.fuel.2020.117049