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Improving Chemical Reactor Networks via Machine Learning techniques

A. Remiddi[1,2,3]*, A.T. Inciardi[1,2,4], A. Procacci[1,2], A. Parente[1,2,3]
arianna.remiddi@ulb.be
[1] Aero-Thermo-Mechanics Department, Université libre de Bruxelles, Brussels, Belgium
[2] Brussels Institute for Thermal-Fluid Systems and Clean Energy (BRITE), Université Libre de Bruxelles and Vrije Universiteit Brussel, Belgium
[3] WEL Research Institute, Wavre, Belgium
[4] UCL, Institute of Mechanics, Materials, and Civil Engineering, Louvain-la-Neuve, Belgium

In the context of the pressing need for a transition towards a carbon-neutral economy, the adoption of novel energy sources and combustion technologies is progressively becoming mandatory. Such a technological transition requires a new paradigm of innovative approaches to prototyping and modeling, that can be supported by the newest data-driven approaches. Among these, Chemical Reactor Networks (CRNs) provide a cost-effective alternative to traditional Computational Fluid Dynamics (CFD) simulations, enabling the simulation of complex combustion systems and the prediction of their operations and performance within shorter timescales while maintaining high accuracy on the chemical description. Operatively, this method takes as an input the result of a low-detailed CFD simulation, simplifies the numerical domain clustering it into a discrete set of regions, and represent each of them as a canonical 0D reactor with an highly detailed thermochemical description [1]. The method presented in this work already benefits of some data-driven approaches, such as using the Principal Component Analysis (PCA) [2] to automate the main features extraction from the CFD and the clustering process. However, the construction and predictive capability of a CRN, as well as its generalizability, directly depend on the availability and quality of the input dataset. To address a potential scarcity of the dataset, machine learning techniques can be employed to leverage existing data and support interpolation or extrapolation. This works aims to investigate the ways in which machine learning approaches such as neural networks can enhance the generalizability of a CRN across a broad range of operating conditions, for instance by predicting its main parameters, allowing the CRN to represent new operating conditions and unseen scenarios.

References

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