Physics-Based Reduced Order Modelling of Combustion Systems: Design and Applications

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Abstract

Energy transition is unquestionably a priority in modern society. Political institutions are aligning with this goal, implementing policies to decrease reliance on fossil fuels and encourage the use of renewable energy sources. Consequently, the share of renewables in the energy mix is poised to increase significantly within the next few years. However, the intermittent nature of renewable sources necessitates the development of efficient storage techniques for the medium and long term.

Smart Energy Carriers and carbon-free fuels offer a promising path to reducing CO_2 emissions while ensuring reliable energy storage and supply. Among these options, hydrogen and its carbon-free derivatives have garnered growing optimism. These molecules can store excess renewable energy in gas form, which can then be transported and converted into thermal energy via combustion, primarily producing harmless byproducts such as water and nitrogen.

Nevertheless, combustion remains the dominant method of energy conversion, and the different combustion properties of e-fuels present several technical challenges. A key concern is the formation of pollutants like NO_x during high-temperature oxidation, which contributes to environmental issues such as acid rain. It is, therefore, imperative to efficiently adapt current combustion technologies and develop more efficient ones to produce energy through combustion processes that are sustainable, efficient, and extendable to a wide range of fuels.

Numerical modeling and simulations have become strategic tools for industry, helping to optimize the design of new technologies while reducing the need for costly experimental campaigns. Computational Fluid Dynamics (CFD) is a

widely used approach, but its high computational demands make large-scale deployment challenging, especially for high-fidelity simulations.

The primary barrier to widespread CFD use is the high computational cost of high-fidelity modeling. Accurately representing chemical and physical processes requires solving complex partial differential equations on grids consisting of millions of elements. Even for simple fuels, combustion involves intricate chemical reactions, necessitating detailed kinetic mechanisms with numerous species and reactions.

Within the last few years, the development of more cost-effective strategies for numerical modeling has been an important topic for research. In particular, alternative tools, such as Chemical Reactor Networks, represent a strategic way to complement and limit high-fidelity simulations, providing kinetics simulations of realistic combustion systems in a convenient amount of time. Based on the assumption that a complex flow field can be represented through a highly simplified network of connected chemical reactors, they allow for the solution of conservation equations only in a few elements, paving the way for the use of extremely detailed kinetics mechanisms in a highly reduced time frame.

Reactor networks, however, are characterized by a lower degree of fidelity, and their grey-box nature necessitates expertise and careful attention in their design, which must be meticulously tailored for different test cases. Consequently, the correct design and the potential applications of these tools remain active areas of research.

In this work, new methods and procedures for the efficient design of such physics-based reduced-order models are studied and analyzed. The development of more efficient design techniques, including those based on machine learning algorithms, offers reliable models that can be used for parametric design, optimization, and control in a straightforward and cost-effective manner. This approach complements the use of complex simulations and reduces their number, limiting the computational burden and allowing for smarter combustor design processes.