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ChemZIP: Accelerated Modeling of Complex Aerothermochemical Interactions in Novel Turbomachines for Sustainable High-Temperature Chemical Processes

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Abstract

A revolutionary new class of turbomachines---called RotoDynamic Reactors (RDRs)---have emerged to decarbonise gas-fired heat within more than 40 high-temperature, carbon-intensive, hard-to-abate industries. For applications in the chemical industry, not only is the flow physics uniquely complex (featuring strong shockwaves, large separations, high turbulence, and sharp curvatures), but there is now an additional challenge chemistry interacting strongly with the flow. This is the first instance in turbomachinery where aerothermochemical interactions along the bladed path are present. Therefore, accurate aerothermochemical modelling tools are necessary to design the machine to maximise valuable reaction products. However, traditional tools for modelling reactive flows are prohibitively computationally costly for design purposes because of the high dimensionality of intense stiffness of the system.

Although several physics- and data-driven computational acceleration approaches (such as flamelets or PCA + non-linear regression) have been successfully developed over the last 15 years, they have mainly focused on numerical combustion modelling. In this work, we introduce a new machine-learning-enhanced multi-fidelity modelling methodology called ChemZIP to efficiently capture endothermic aerothermochemical interactions along the bladed path of turbomachines. Our approach is more universal than flamelet approaches (which are combustion-specific) and can be applied to all types of chemical systems from catalysis to pyrolysis, and it addresses many of the limitations of existing data-driven approaches when applied to non-combustion processes. For example, a novel training data generation process has been developed, which allows rich dynamic responses of the chemical system to be embedded into the training dataset at a fraction of the cost of reacting flow simulations.

For a set of processes-relevant 3-D configurations far removed from the training dataset, ChemZIP's predictive accuracy of the thermochemical state remains within 10% of an industry-standard solver Fluent. Convergence is achieved approximately 50 times faster than state-of-the-art acceleration strategies even for a small mechanism. Therefore, coupled computations are now sufficiently fast that aerothermo*chemical* optimisation is now feasible for the first time in the RDR's design cycle.

Keywords:

Chemical processes, chemical kinetics, reacting flow, scientific machine learning, stiff problems, neural networks, autoencoders, turbomachinery, turbo-reactor, RotoDynamic Reactor.