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Title

Assessment of neural network-based predictions of chemical production rates in CFD solvers

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Abstract

The numerical simulation and analysis of chemically reacting flows often requires the evaluation of detailed reaction mechanisms. This is the case, for example, with lifted flames in combustors or with complex mixtures such as the engine, gas generator and ambient air combination in a rocket base flow.

In the case of hydrocarbons in particular, chemistry is complex, mathematically stiff and requires many reactions and species to be considered. This requires significant additional CPU resources which are considerably larger than those needed for the solution of the fluid transport equations alone.

Popular options to reduce the CPU demand of reacting flow simulations are the application of simplified combustion models such as flamelet or eddy breakup models or the use of reduced skeletal or global reaction mechanisms. However, this results in a limited range of applicability concerning the complexity of the gas mixtures, the range of thermodynamic states or the ability to predict kinetics driven lift-off or extinction phenomena.

Another possibility to reduce the CPU cost and stiffness of the evaluation of the chemical source terms is the application of neural networks. The input of the network would be the mixture composition and the thermodynamic state and the output are the rates of change of species concentrations (source terms). Training data can be easily obtained from the exact evaluation of the law of mass action in conjunction with the reaction rates. However, the mathematical stiffness of the problem imposes a severe challenge for the applicability of neural networks.

The paper outlines different implementation strategies of neural networks for the prediction of chemical source terms in CFD solvers and discusses their limitations based on the solution of generic reactor problems.

Further, a robust and consistent neural network-based method to optimize existing global mechanisms for given thermodynamic conditions is introduced. This method is tested using generic reactor problems and the CFD analysis of a lifted methane air flame.