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Neural Network-Augmented Reduced Kinetics for Shock-tube Ignition Delay Predictions

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Data assimilation is an effective tool for generating accurate and reduced-cost models to replace or augment existing models used in partial differential equations (PDEs). Training can be done with reference to high-fidelity simulation and/or experimental data with the optimization and testing performed in-situ using a PDE-constrained, adjoint-based optimization approach [1]. We apply this method to a one-dimensional Navier-–Stokes model of U.S. Air Force Academy shock-tube experiments for stoichiometric ethylene–air autoignition at subatmospheric pressures [2, 3]. We optimize a neural network for the Arrhenius kinetic parameters of a semiglobal (eight-species, three-step) chemical-kinetic model to match the space-time species evolution predicted by analogous one-dimensional calculations using a more detailed (23-species, 66-reaction) chemical-kinetic model. The optimization is first performed on individual chemical kinetics predictions, always starting from target data, and later expanded to optimizing predictions of the chemical kinetics for the entire time horizon. This two step optimization procedure enables the model to rapidly approach a better solution when started from the initial suboptimal three-step parameters. We compare the model to detailed calculations and experimental targets for out-of-sample ignition conditions and discuss the challenges of adjoint-based optimization over nonlinear ignition trajectories.

References

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