Neural Network Approximation of Chemical Kinetics with Variable Time and Physics-Enriched Dataset

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We present a neural network approach for accelerating the simulation of hydrogen-air combustion kinetics using a compact neural network architecture with fully connected layers and residual connections adapted for multidimensional time series prediction. The method incorporates logarithmic data renormalization to enhance sensitivity to small concentration changes near zero, coupled with standard scaling, and introduces a recurrent training strategy where multi-step predictions (up to 30 steps) are embedded into the loss function to minimize error accumulation during autoregressive inference. The time step is treated as an input variable, enabling the model to generalize across different temporal discretizations and pressure ranges without retraining. We also demonstrate that enriching the training set with states near temperature inflection points identified via second derivatives reduces mean squared error by 45% (from 1.8×10^{-3} to 1.0×10^{-3}) without increasing dataset size or model complexity. The resulting lightweight network (5 layers, $32,000$ parameters) achieves accurate approximation of species concentrations and temperature evolution for hundreds to thousands of integration steps ahead. This approach demonstrates significant potential for integration into multidimensional computational fluid dynamics simulations of reacting flows.

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