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Foundational Fuel Chemistry Model 2 — Can data assimilation yield useful insights in reaction rate constants?

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The foundation fuel chemistry model version 2 (FFCM-2) is a recently developed reaction model for C_{0-4} hydrocarbon combustion. In the development of FFCM-2, reaction rate constants, primarily sourced from reaction rate theory and experiments, were evaluated for their uncertainties. The optimization and uncertainty minimization were conducted using a neural-network based, method of uncertainty minimization employing polynomial chaos expansions (NN-MUMPCE), which assimilated over 1,000 sets of legacy combustion property data while ensuring that all rate constants adhered to their associated physical constraints and uncertainty bounds. The current study focuses on an analysis of the optimized reaction rate constants. By comparing the trial and optimized rate constants with literature data, we demonstrate that large-scale data assimilation, when combined with appropriate physical constraints, can effectively minimize rate uncertainties and provide valuable insights into individual rate constants.

Several key examples include the analysis of high-pressure methane ignition; we demonstrate that data assimilation is capable of yielding useful insights about missing reactions and refining the rate constants of the newly discovered reaction pathways. We show that data assimilation is useful in constraining rate constants where literature study has notable uncertainties for three selected rate constants.