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Advancing sustainable fuel models: Data Assimilation Techniques for combustion chemical kinetics

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Chemical kinetics modeling is a critical component of combustion science, with the accuracy of rate parameters directly impacting the quality of predictions. This study investigates the Augmented Ensemble Kalman Filter (AEnKF) as an advanced data assimilation technique for integrating experimental measurements into kinetic models. In contrast to conventional optimization methodologies that necessitate predefined loss functions, AEnKF employs an iterative process to update model parameters while inherently preserving the dynamics of the system. We illustrate this methodology by examining the oxidation kinetics of ammonia, a carbon-free fuel candidate of increasing significance. This study utilizes time-resolved species concentration profiles derived from shock tube experiments to elucidate the dynamics of the reaction. By systematically identifying and estimating parameters for key reaction steps, it is demonstrated that the AEnKF effectively captures the nonlinear dynamics of ammonia combustion while maintaining physical consistency. Through comprehensive parameter studies evaluating ensemble size and assimilation frequency effects, it is shown that the algorithm efficiently operates across various configurations. Furthermore, the framework is extended to simultaneously assimilate multiple experimental cases across different operating conditions, thereby achieving a more robust parameter estimation process by leveraging diverse datasets. This multi-case approach enables the better constraint of the parameter space and improved model transferability. These results underscore the AEnKF's potential as a powerful tool for parameter estimation in intricate reaction networks, especially in the context of incorporating dynamic experimental data into next-generation combustion models for sustainable fuels.