Development of an Uncertainty Quantification Predictive Chemical Reaction Model for Syngas Combustion

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Abstract

An automated data-centric infrastructure, Process Informatics Model (PrIMe), was applied to validation and optimization of a syngas combustion model. The Bound-to-Bound Data Collaboration (B2BDC) module of PrIMe was employed to discover the limits of parameter modifications based on uncertainty quantification (UQ) and consistency analysis of the model–data system and experimental data, including shock-tube ignition delay times and laminar flame speeds. Existing syngas reaction models are reviewed, and the selected kinetic data are described in detail. Empirical rules were developed and applied to evaluate the uncertainty bounds of the literature experimental data. The initial H_2/CO reaction model, assembled from 73 reactions and 17 species, was subjected to a B2BDC analysis. For this purpose, a dataset was constructed that included a total of 167 experimental targets and 55 active model parameters. Consistency analysis of the composed dataset revealed disagreement between models and data. Further analysis suggested that removing 45 experimental targets, 8 of which were self-inconsistent, would lead to a consistent dataset. This dataset was subjected to a correlation analysis, which highlights possible directions for parameter modification and model improvement. Additionally, several methods of parameter optimization were applied, some of them unique to the B2BDC framework. The optimized models demonstrated improved agreement with experiments compared to the initially assembled model, and their predictions for experiments not included in the initial dataset (i.e., a blind prediction) were investigated. The results demonstrate benefits of applying the B2BDC methodology for developing predictive kinetic models.