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Automated Validation of Combustion Kinetic Mechanisms through Curve Matching: A Functional Data Analysis Approach for Large and Incomplete Datasets

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In this work, we present a systematic methodology for automating the validation of combustion kinetic mechanisms using Curve Matching (CM), a functional data analysis approach particularly suited for large and incomplete experimental datasets. Unlike traditional validation methods that rely on point-wise comparisons or subjective visual assessment, CM transforms discrete experimental and simulated data into continuous functions to compare not only magnitude differences but also curve shapes and their derivatives. Our approach incorporates experimental uncertainties through bootstrapping procedures and provides quantitative metrics identifying where model predictions deviate significantly from experiments. We demonstrate the application of this methodology several datasets for validating oxymethylene ether (OMEs) kinetic mechanisms across various reactor types and operating conditions. Through pattern detection and interval analysis techniques, we identify specific reaction classes requiring refinement, such as those affecting high-temperature ignition delay predictions. The physics-driven nature of this approach maintains the self-consistency of reaction rate rules across the related molecular structures, as demonstrated in the recent development of a lumped kinetic model for $OME_{2\text{-}5}$ oxidation, where the methodology successfully preserved coherency among reaction classes. By implementing this approach within a data ecosystem framework, we enable automated analysis that provides modelers with actionable insights for mechanism improvement while avoiding subjective assessments. This represents a significant advancement in standardizing model validation procedures, extracting systematic knowledge from experimental data, and supporting more efficient development of accurate combustion kinetic mechanisms.