**An automatic framework for continuous model development**

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In the field of chemical kinetics, the growing complexity of predictive models—especially for combustion and fuel behavior—demands reliable and standardized validation methods. Too often, models are assessed through subjective visual comparisons or point-by-point errors, which can miss deeper structural mismatches between simulations and experiments. In this work, we introduce a methodology that helps overcome these limitations by offering *structured, quantitative metrics* for model validation. Our approach is based on Curve Matching (CM), a technique from functional data analysis that transforms both experimental and simulated data into smooth curves. This allows us to compare not just numerical values but also trends, shapes, and even subtle differences in derivatives. Crucially, the method incorporates experimental uncertainties and highlights where and how predictions deviate most significantly from reality, assessing also the goodness of the provided metrics in a quantitative way. This methodology has been applied to validate kinetic models for oxymethylene ethers (OMEs), an emerging class of alternative fuels, across different reactor setups and operating conditions. The analysis reveals specific reaction families in need of refinement—such as those influencing high-temperature ignition delays—while ensuring consistency across related chemical structures. By embedding this process into a broader data ecosystem, named SciExpeM, we make it possible to automate the analysis and provide model developers with actionable insights, replacing subjective interpretation with reproducible, data-driven evaluation. This contributes to building a more robust foundation for predictive modeling in combustion science.

**Keywords**: *Chemical Reaction Engineering, Chemical Kinetics, Combustion*