International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

Fast optimization of combustion mechanisms through model and experimental data reduction

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Bioalcohols are promising alternatives to reduce dependence on fossil fuels. While bioethanol is widely used, its properties limit its compatibility with current petrol engines. Longer-chain alcohols, such as biobutanol and biopentanol, are more suitable and can be used in existing vehicles. It has been shown by Bolla et al.[1] that among several combustion mechanisms developed for the four butanol isomers, the mechanism of Sarathy et al. [2] shows the best overall performance when evaluated against a huge data collection, but there it still has significant room for improvement. This work focuses on improving its predictivity through kinetic parameter optimization using the Optima++ code[3,4] to improve performance for a large set of combustion data.

Parameter optimization can be very challenging in the case of large combustion models and/or large experimental data collections. Recently, Horváth et al. proposed the Mechanism Reduction Assisted Parameter Optimization and Model Development (RAPOD) method [5] to overcome the challenge of optimizing the n-pentanol chemistry model in the large multifuel NUIGMech 1.1 combustion mechanism against a small data collection. According to RAPOD, a reduced mechanism is developed first that can very accurately reproduce the simulation results of the detailed model, and then its parameters are optimized and reintroduced into the full model. In the case of butanol, due to the huge size of the data collection, it is not feasible to perform the parameter optimization of the Sarathy model even when using a reduced model. In this work, the RAPOD approach has been extended to reduce the large data collection as well. The optimized model shows similar improvements in accuracy for the entire data set.

In this study, we downloaded the experimental ignition delay data (835 IDT) collected for butanol isomers by Bolla et al. [1], from the ReSpecTh information system [6]. First the Sarathy butanol mechanism was reduced considering a small number of representative scenarios covering the relevant conditions. Then, representative data points were selected from the data collection using an automated procedure during the optimization. The extended RAPOD method allowed for faster optimization of two orders of magnitude.

References

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