Sequential Bayesian experimental design for optimization of detailed combustion kinetics mechanisms

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Developing accurate combustion reaction kinetics models requires informative experimental data. Bayesian Sequential Experimental Design (BSED) offers a systematic approach to iteratively identify optimal experimental conditions by maximizing the expected information gain (EIG). However, its application to computationally intensive nonlinear chemical kinetics has been limited. To overcome this bottleneck, this study presents a novel and accelerated BSED framework. This framework uniquely integrates Artificial Neural Networks (ANNs) for significantly faster simulations, reverse Kullback-Leibler divergence for rapid EIG calculation, and ANN-based Hamiltonian Monte Carlo [1] for efficient Bayesian inference. Furthermore, to enhance practical implementation, we introduce a Gaussian Process Regression (GPR) surrogate for iterative estimation of experimental measurements, defining a new EIG_GPR design target. The effectiveness of this framework is validated through experimental designs targeted at ignition delay time (IDT) and laminar burning velocity (LBV) in ammonia combustion, demonstrating its capability to identify significantly more informative conditions for kinetic parameter estimation. A semi-automated Jet-Stirred Reactor (JSR) platform was developed for comprehensive evaluation. Comparison of JSR experimental design times based on BSED demonstrates that the accelerated framework achieves an order-of-magnitude speedup compared to unaccelerated methods, elevating experimental design efficiency to the level of linear-assumption-based D-optimality. Furthermore, EIG_GPR reduced the overall computation time by a factor of 15 compared to accelerated EIG. This work marks a substantial advancement towards the efficient and accurate development of complex combustion models.

References

[1] Cheng L et al. Artificial neural network-based Hamiltonian Monte Carlo for high-dimensional Bayesian Inference of reaction kinetics models. Proceedings of the Combustion Institute. 2024;40:105590.