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Sensitivity analysis and sequential parameter optimization of soot formation in shock tube methane pyrolysis

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Accurate modeling of soot formation during combustion is often challenging due to uncertainties present at different stages of the process [1]. These uncertainties can grow and propagate as the carbon mass flux moves from small hydrocarbons and polycyclic aromatic hydrocarbons (PAHs) to early-stage particles and eventually to large agglomerates. Understanding and quantifying these uncertainties and their effects on the final results of the soot models are crucial for assessing the reliability of the predictions made by the soot models.

In this study, time-resolved data on soot volume fraction and primary particle diameter from pyrolysis of a 5% CH_4-Ar mixture in a shock tube [2] were used to optimize the Omnisoot model parameters related to soot inception, surface growth, and carbonization. First, a Morris sensitivity analysis was conducted to assess how each parameter impacts the soot model's prediction of volume fraction and particle diameter. Based on this analysis, the parameters were separated into two groups. The first group included PAH inception and adsorption prefactors, which had strong, interactive effects. The second group comprised hydrogen abstraction acetylene addition (HACA) and carbonization prefactors, showing relatively weaker, consistent impacts.

Since the parameters of the second group showed minimal interactive effects, they were optimized first using the shock tube data of volume fraction and primary particle diameter. After that, the parameters of the first group were optimized by constructing two-dimensional response surfaces and applying a least-squares method to minimize discrepancies between the model predictions and the experimental data. After optimizing the parameters, the effect of using different kinetic mechanisms was studied through a combination of sensitivity analysis and reaction pathway analysis, tracking the carbon mass flux from fuel to the key soot precursors. Our results suggest useful directions for selecting appropriate target species for mole fraction measurements, aiding future improvements in numerical simulation of combustion and soot formation.

References

[1] Su, Xingyu, et al. "Uncertainty analysis of soot formation in laminar flames simulated with a sectional method" *Combustion and Flame*. 2024;265:113430.

[2] Clark, Gibson, et al. "A Combined Multi-Speciation, Particulate Formation, and Particulate Morphology Study of Methane Pyrolysis in Shock-Tubes" *14th U.S. National Combustion Meeting*. March 16–19, 2025.