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Application of CSP/CEMA to the Identification of Key Chemical Species and Reactions Driving the Ammonia Autoignition Process

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Combustion reactions are complex phenomena that evolve in a high-dimensional thermodynamic state space. To achieve effective combustion control such as reducing the emissions of NO_x and N_2O, it is crucial to identify the appropriate control variables that govern these complex reaction processes. In this context, identifying key species and reactions that drive the system dynamics becomes essential, motivating the application of methods such as Computational Singular Perturbation (CSP) theory and Chemical Explosive Mode Analysis (CEMA). CSP theory and CEMA, both based on chemical kinetic ordinary differential equations, have been widely used to identify quasi-steady-state species and characterize flame behavior. We highlight the broader applicability of CSP/CEMA as universal tools capable of extracting dominant and physically intuitive features from complex reaction systems. We revisit two key indices introduced in the CSP/CEMA framework [1,2], the Explosion Index (EI) and the Participation Index (PI). We clarify their derivation and physical interpretations, which have received limited discussion. Based on these indices, we investigate ammonia combustion, a carbon-free fuel that is currently undergoing active kinetic modeling, to identify the dominant reaction structures. Using a recent ammonia kinetic model [3], which shows good agreement with experimental data, we extract the representative structures of ammonia combustion under various conditions, including low to high temperatures and lean to rich mixtures. Finally, by comparing these results with those obtained from earlier-generation kinetic models, we highlight substantial differences in the updated kinetic model and provide insights into the ongoing refinement of ammonia kinetic modeling.

References

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