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# Enhancing Chemical Kinetic Mechanism Optimization Using Independent Component Analysis

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In detailed chemical kinetic mechanisms, which are essential for the accurate simulation of combustion phenomena, the Arrhenius parameters ($A$, $n$, $Ea$) are assigned to define the rate constants of various reactions. During mechanism optimization, these parameters are adjusted independently to identify combinations that both satisfy uncertainty constraints for reaction rate constants and accurately predict various combustion characteristics. However, strong correlations between the Arrhenius parameters make it difficult to select valid parameter sets that meet the uncertainty criteria. This challenge becomes particularly severe when optimizing multiple reactions simultaneously, as the number of adjustable parameters increases greatly. Ensuring that all reaction parameters satisfy the uncertainty constraints requires a large number of search iterations, significantly reducing optimization efficiency.

To address this issue, the present study introduces Independent Component Analysis (ICA) for refining Arrhenius parameter space during chemical kinetic mechanism optimization, thereby improving both efficiency and accuracy. ICA is a statistical technique that transforms a correlated parameter space into a space of statistically independent variables. By applying ICA to the space of "valid" Arrhenius parameters, an independent component space containing only valid parameter combinations is generated. Since parameters selected in this independent component space inherently satisfy the uncertainty constraints of Arrhenius parameters, the accuracy of selecting valid Arrhenius parameter sets is greatly improved.

In this study, the conventional evolutionary algorithm-based optimization framework [1,2] is enhanced by incorporating ICA. The approach is applied to the optimization of 24 reactions and 72 Arrhenius parameters in the $NH_3$ reaction mechanism developed by Stagni et al. [3], targeting ignition delay times, species concentration profiles, and laminar flame speeds. As a result, the ICA-based method improved the probability of selecting valid parameter sets by approximately 80% compared to the conventional method, achieving lower objective function values with fewer optimization iterations. These results demonstrate that refining the Arrhenius parameter space using ICA significantly improves both the quality and efficiency of mechanism optimization.

**References**

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