Mechanism reduction strategies for gasoline surrogate fuels

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A detailed reaction mechanism for a four-component gasoline surrogate, developed by Lawrence Livermore National Laboratory, showed good agreement with engine experiments and fundamental combustion properties measured in engine-relevant conditions using the target real gasoline. However, with 1389 species and 5935 reversible reactions, the mechanism is far too large to use in practical engine simulations. Therefore, reduction of this surrogate mechanism was performed. First, the directed relation graph with error propagation and sensitivity analysis (DRGEPSA) method was used to generate skeletal mechanisms at varying levels of detail. This step can produce significantly compact skeletal mechanisms, but those with tight error limits were still too sizable for practical use. Therefore, a second reduction step was employed, using the quasi-steady-state (QSS) approximation based on computational singular perturbation analysis. The QSS species concentrations were solved analytically, rather than through an iterative solution approach. For error constraints of 10% and 30%, the final reduced mechanisms consist of 245 and 178 species, respectively. Both reduced mechanisms and the corresponding skeletal mechanisms were validated with homogeneous autoignition, perfectly stirred reactor, and premixed laminar flame simulations over a wide range of conditions.