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Linear time reduction of large kinetic mechanisms with directed relation graph: *n*-Heptane and iso-octane

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Abstract

The algorithm of directed relation graph recently developed for skeletal mechanism reduction was extended to overall linear time operation, thereby greatly facilitating the computational effort in mechanism reduction, particularly for those involving large mechanisms. Together with a two-stage reduction strategy and using the kinetic responses of autoignition and perfectly stirred reactor (PSR) with extensive parametric variations as the criteria in eliminating unimportant species, a detailed 561-species *n*-heptane mechanism and a detailed 857-species iso-octane mechanism were successfully reduced to skeletal mechanisms consisting of 188 and 233 species, respectively. These skeletal mechanisms were demonstrated to mimic well the performance of the detailed mechanisms, not only for the autoignition and PSR systems based on which the reduced mechanisms were developed but also for the independent system of jet-stirred reactor. It was further observed that the accuracy of calculated species concentrations was equivalently bounded by the user-specified error threshold value and that the reduction time for a single reaction state is only about 50 ms for the large iso-octane mechanism.
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Keywords: Directed relation graph; Reduced mechanism; *n*-Heptane; Iso-octane

1. Introduction

Chemical kinetics of fuel oxidation is an integral component of combustion phenomena. However, because of the complexity and strong nonlinearity of the reaction pathways and the associated reaction rates for the myriad of reactions and species involved, computational simulations with detailed mechanisms have been limited to the simplest fuels such as hydrogen and the lower hydrocarbons in idealized flow fields. The simulation is further complicated by the existence of highly reactive radicals which induces significant stiffness to the governing equations due to the dramatic differences in the time scales of the species. Consequently, there exists the need to develop from these detailed mechanisms corresponding reduced mechanisms of fewer variables and moderated stiffness, while maintaining the accuracy and comprehensiveness of the detailed mechanism.

A major category of previous reduction methods was based on time scale analysis, through which both the number of variables and the stiffness can be reduced by eliminating short time scales associated with quasi-steady-state species or partial equilibrium reactions [1–8]. The method of intrinsic low-dimensional manifold [9] performs eigenvalue analysis of the Jacobian matrix and assumes that the fast subspace van-

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ishes quickly. The frequently reused reaction conditions are handled with the method of in situ adaptive tabulation to reduce the overall simulation cost [10,11]. The theory of computational singular perturbation (CSP) considers the time dependence of the Jacobian matrix, and higher-order accuracy can be obtained [12–16].

While time scale analyses can reduce the number of species and the stiffness by eliminating species or reactions with short time scales, significant overhead in central processing unit (CPU) cost is typically involved in solving the algebraic equations obtained by assuming that the fast species or reactions are exhausted, particularly when the size of the mechanism is large. Therefore, it is frequently necessary to identify and eliminate the unimportant species and reactions, i.e., to perform the skeletal reduction, before reduction based on time scale analysis is conducted.

Various methods for skeletal reduction have been developed. One of the earliest developed methods for skeletal reduction is sensitivity analysis [17–19], which is simple to apply. However, it does not directly provide decoupled information about the reactions and species, and further postprocessing is required. The method of principal component analysis (PCA), based on sensitivity analysis, operates on the sensitivity matrices and systematically identifies the redundant reactions [20]. A major restriction of algorithms based on sensitivity analysis is that they are time consuming to compute the sensitivity matrices for large mechanisms.

Reaction elimination can also be performed using optimization approaches, such as integer programming, aiming to obtain an optimal set of reactions for given constraints [21]. While the optimal set of reactions can be identified, the optimal solution strictly depends on the selection of constraints, which is frequently quite involved. Furthermore, the optimization approach is asymptotically slower than sensitivity analysis, since integer programming is in general an NP-hard problem. Another method, the detailed reduction [22], provides a fast way for the identification of unimportant reactions by directly comparing the reaction rates with a preselected critical value. The restriction of this method is the lack of consideration of species or reaction coupling, because of which a slower reaction is not always unimportant, particularly when it involves crucial radicals. Consequently, significant human interaction and extensive validation may be required.

While skeletal reduction based on reaction elimination has been extensively studied, those methods involving direct species elimination are less established. A method was developed for the identification of unimportant species by resolving species coupling using Jacobian analysis [23]. The coupling among species is formulated with the entries of the Jacobian matrix and the species that are strongly coupled with the major species are identified iteratively. This method is practically faster than those based on sensitivity analysis, although formulation of the species coupling using Jacobian matrix is nontrivial and system-dependent knowledge is frequently required.

In a recent work [24], the method of directed relation graph (DRG) was developed to identify unimportant species by resolving species coupling with high efficiency and minimal requirement of system-dependent knowledge. In the present investigation this method was extended to the reduction of large mechanisms with hundreds of species, namely those for n-heptane and iso-octane [25,26], and the efficiency and accuracy of this extended method were demonstrated and analyzed.

2. Methodology

2.1. DRG method

The skeletal reduction is to identify and eliminate unimportant reactions or species. Typically, the identification of unimportant species is more involved than that of reactions due to the complex coupling of the species. The method of DRG was developed to resolve species coupling efficiently, by starting with direct species coupling, which indicates that the removal of one species B from the mechanism induces immediate error to the production rate of another species A. Such immediate error, noted as r_{AB}, can be expressed as

$$r_{\mathrm{AB}} \equiv \frac{\sum_{i=1,I} |\nu_{\mathrm{A},i}\omega_i \delta_{\mathrm{B}i}|}{\sum_{i=1,I} |\nu_{\mathrm{A},i}\omega_i|},$$

$$\delta_{\mathrm{B}i} = \begin{cases} 1, & \text{if the } i\text{th reaction involves} \\ & \text{species B,} \\ 0, & \text{otherwise,} \end{cases} \tag{1}$$

where the subscripts A and B indicate the species identity, i is the ith reaction, $\nu_{\mathrm{A},i}$ the stoichiometric coefficient of species A in the ith reaction, and ω the reaction rate. The terms in the denominator are the contributions of the reactions to the production rate of species A, and the terms in the numerator are those in the denominator that involve species B. If the relative error r_{AB} is not small compared to a threshold value ε, the removal of species B from the skeletal mechanism immediately induces a nonnegligible error in A. Consequently species B should be kept in the skeletal mechanism if species A is to be retained. Such an immediate requirement of species A to species B is denoted as $\mathrm{A} \rightarrow \mathrm{B}$.

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