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A dynamic adaptive chemistry scheme with error control for combustion modeling with a large detailed mechanism

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ABSTRACT

A new error controlled dynamic adaptive chemistry (EC-DAC) scheme is developed and validated for ignition and combustion modeling with large, detailed, and comprehensively reduced *n*-heptane and *n*-decane mechanisms. A fuel oxidation progress variable is introduced to determine the local model reduction threshold by using the mass fraction of oxygen. An initial threshold database for error control is created according to the progress variable in a homogeneous ignition system using a detailed mechanism. The threshold database tabulated by the fuel oxidation progress variable is used to generate a dynamically reduced mechanism with a specified error bound by using the Path Flux Analysis (PFA) method. The method leads to an error-controlled kinetic model reduction according to the local mixture reactivity and improves the computation efficiency. Numerical simulations of the homogeneous ignition of n-heptane/air and *n*-decane/air mixtures at different initial conditions are conducted with one detailed and one comprehensively reduced mechanism involving 1034 and 121 species, respectively. The results show that the present algorithm of error-controlled adaptive chemistry scheme is accurate. The computation efficiency is improved by more than one-order for both mechanisms. Moreover, unsteady simulations of outwardly propagating spherical *n*-heptane/air premixed flames demonstrate that the method is rigorous even when transport is included. The successful validation in both ignition and unsteady flame propagation for both detailed and reduced mechanisms demonstrates that this method can be efficiently used in the direct numerical simulation of reactive flow for large kinetic mechanisms.

1. Introduction

In order to develop efficient and low emission engines working at low temperature combustion regime, recently there have been a lot of efforts to incorporate detailed kinetic mechanisms of large hydrocarbon fuels in combustion modeling [1,2]. However, a detailed combustion mechanism of a large hydrocarbon fuel usually consists of hundreds of species and thousands of reactions. Numerical simulations with a detailed mechanism require a computational resource which is not available in a foreseeable future. As such, to enable direct numerical simulations with a detailed chemical kinetics, the mechanism has to be reduced either dynamically or before simulation with an appropriate error control.

There are different reduction methods to generate a reduced kinetic mechanism [3,4]. A typical way is to reduce the number of species and reactions in the mechanism, while maintaining a certain accuracy required for a given application [5]. In these reduction methods, the sensitivity reduction method [6–8] is the most popular one, which has been used in some commercial software. Chen and Tham [9] developed a more efficient method to solve for quasi steady-state (QSS) species in reduced chemical kinetic mechanisms. They identified that QSS species are strongly coupled and solved separately using a fixed point iteration and matrix inversion method. Besides that, the reaction Jacobian analysis methods which include the computational singular perturbation (CSP) method [10–13] and the intrinsic low dimensional manifold (ILDM) [14,15] are also popularly used. In order to achieve efficient calculations of fast mode species, different parameterization methods have been proposed [16–19]. Recently, the Direct Relation Graph (DRG) [20], DRG with Error Propagation (DRGEP) [21] and multi-generation Path Flux Analysis (PFA) [22] have been developed using a reaction flux threshold [23]. However, one of the main difficulties in these methods is that there is no direct relation between the model reduction threshold and the error of the reduced mechanism. Thus, it is difficult to determine the error of reduced mechanism and to decide what threshold needs to be chosen. Moreover, for the off-line comprehensively pre-reduced mechanism approach, in order to make the comprehensively reduced mechanism applicable to different combustion conditions, the size

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of pre-reduced mechanism is normally very large and the improvement of the computation efficiency is low.

Alternatively, the adaptive chemistry scheme [24–27] can generate a more compact reduced mechanism locally than the comprehensively pre-reduced model to achieve better efficiency. Liang et al. [24] developed a on-the-fly mechanism reduction scheme, termed dynamic adaptive chemistry (DAC) based on the DRGEP method. Their results showed that adaptively reduced mechanisms worked well for their local and instantaneous conditions. However, in DAC method, the choice of the single threshold value in DRG or DRGEP for the dynamic reduction remains arbitrary and heavily relies on user's experience [28,29]. Therefore, in order to guarantee the accuracy of the dynamically reduced model, a very conservative and small threshold is often used in model reduction. In fact, in a reduction method such as the sensitivity method, DRG, DRGEP, PFA, and DAC, different threshold values result in different skeletal mechanisms with different accuracies. Figure 1 shows the number of species in the reduced mechanism and the error in ignition delay prediction as a function of the threshold value for stoichiometric *n*-heptane/air mixture. It is seen that the size of the reduced mechanism and the relative error in ignition delay time depend strongly on the threshold value. As a result, when a fixed threshold value is specified, not only the error of the dynamically reduced mechanism is not known but also the reduced mechanism size is not minimized. Therefore, it is necessary to develop a method which is able to not only generate a minimized reduced mechanism locally but also satisfy the required accuracy. Recently, Blurock et al. [30] presented an adaptive chemistry for engine simulations based on fuzzy logic optimization. Oluwole et al. [31] developed an exact-steady-state adaptive chemistry method. Nagy and Turanyi [32] presented a reduction method of very large reaction mechanisms using methods based on simulation error minimization. However, this method needs to save a set of reduced mechanisms.

The goal of this paper is to develop an error controlled dynamic model reduction method to achieve computationally efficient modeling of combustion with a large detailed mechanism. The approach is validated for *n*-heptane and *n*-decane/air mixtures for different large mechanisms, a detailed *n*-heptane mechanism [33,34] with 1034 species and 4236 reactions and a comprehensively reduced *n*-decane mechanism [35] with 121 species and 866 reactions. First, the error-controlled dynamic adaptive chemistry (EC-DAC) scheme is described in Section 2. Then, the integrated EC-DAC scheme is evaluated by simulating homogeneous ignition of *n*-heptane/air and *n*-decane/air mixtures under various concentrations, temperatures, and pressure conditions, and the accuracy and efficiency of the EC-DAC scheme are examined. The method is further validated in simulating unsteady spherical flame propagation. Finally, the main conclusions are drawn.

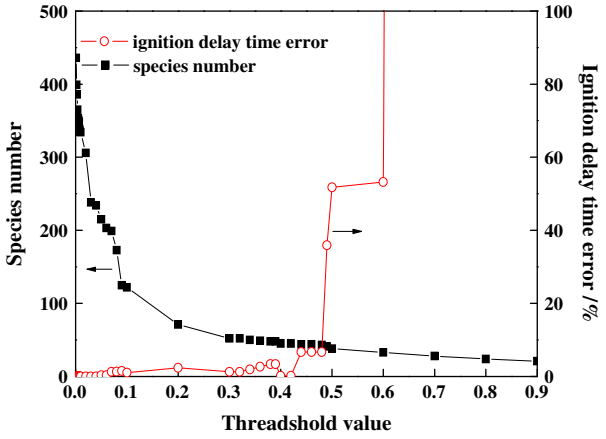

Fig. 1. Change of the number of species in the reduced mechanism and the relative error in ignition delay time prediction with the threshold for stoichiometric *n*-heptane/air mixture at initial condition of 1 atm pressure and 1200 K temperature.

2. Methodologies

The stiff ODEs of detailed chemistry are solved using the VODE solver [36]. The adaptive sub-mechanism at each grid point and each time step is obtained using the on-the-fly PFA reduction method [22].

2.1. Mechanism reduction using PFA

In the PFA method [22], the production and consumption fluxes are used to identify the important reaction pathways. The first generation production and consumption fluxes of species A, P_A and C_A, are evaluated according to

$$P_A = \sum_{i=1,I} \max(\nu_{A,i}\omega_i, 0) \tag{1}$$

$$C_A = \sum_{i=1,I} \max(-\nu_{A,i}\omega_i, 0) \tag{2}$$

where $\nu_{A,i}$ is the stoichiometric coefficient of species A in the ith reaction, ω_i is the net reaction rate of the ith reaction. I is the number of reaction order. The production and consumption fluxes of species A via species B, P_{AB} and C_{AB}, are calculated, respectively, by

$$P_{AB} = \sum_{i=1,I} \max\left(\nu_{A,i}\omega_i\delta_B^i, 0\right) \tag{3}$$

$$C_{AB} = \sum_{i=1,I} \max\left(-\nu_{A,i}\omega_i\delta_B^i, 0\right) \tag{4}$$

δ_B^i is unity if species B is involved in ith reaction and 0 otherwise.

In order to consider the conservative flux information, a flux ratio is introduced to represent the flux ratio of a particular production and consumption path via species B to the total production and consumption flux of species A [22]. The first generation flux ratios for production and consumption of species A via species B are defined as:

$$r_{AB}^{pro\text{-}1st} = \frac{P_{AB}}{\max(P_A, C_A)} \tag{5}$$

$$r_{AB}^{con\text{-}1st} = \frac{C_{AB}}{\max(P_A, C_A)} \tag{6}$$

Although the scheme can include multi-generation reaction fluxes [22,37] to achieve more accurate model reduction, in order to reduce the overhead time of dynamic reduction for a large detailed mechanism with more than one-thousand species, in this study, only the first generation flux is used to generate a locally reduced mechanism.

At each time step, production and consumption flux ratios of $r_{AB}^{pro\text{-}1st}$ and $r_{AB}^{con\text{-}1st}$ are calculated. This process is very efficient because it only involves the calculation of the reaction rates and the time is linearly proportional to the number of species. The reduction starts from a few selected species such as the fuel and oxidizer, and then identifies whether to retain species B in the reduced model by evaluating whether the flux ratios of species A via species B satisfies the following equation.

$$r_{AB} > \varepsilon \tag{7}$$

where r_{AB} is the flux ratio of species A via species B, $r_{AB} = \max\left(r_{AB}^{pro\text{-}1st}, r_{AB}^{con\text{-}1st}\right)$, it can be $r_{AB}^{pro\text{-}1st}$ or $r_{AB}^{con\text{-}1st}$, and ε is the threshold value.