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Multi-timescale and correlated dynamic adaptive chemistry modeling of ignition and flame propagation using a real jet fuel surrogate model

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ABSTRACT

A new correlated dynamic adaptive chemistry (CO-DAC) method is developed and integrated with the hybrid multi-timescale (HMTS) method for computationally efficient modeling of ignition and unsteady flame propagation of real jet fuel surrogate mixtures with a detailed and comprehensively reduced kinetic mechanism. A concept of correlated dynamic adaptive chemistry (CO-DAC) method in both time and space coordinates is proposed by using a few key phase parameters which govern the low, intermediate, and high temperature chemistry, respectively. Correlated reduced mechanisms in time and space are generated dynamically on the fly from the detailed kinetic mechanism by specifying thresholds of phase parameters of correlation and using the multi-generation path flux analysis (PFA) method. The advantages of the CO-DAC methods are that it not only provides the flexibility and accuracy of kinetic model and chemistry integration but also avoids redundant model reduction in time and space when the chemistry is frequently correlated in phase space. To further increase the computational efficiency in chemistry integration, the hybrid multi-timescale (HMTS) method is integrated with the CO-DAC method to solve the stiff ordinary differential equations (ODEs) of the reduced chemistry generated on the fly by CO-DAC. The present algorithm is compared and validated against the conventional VODE solver, DAC and HMTS/DAC methods for simulating ignition and unsteady flame propagation of real jet fuel surrogate mixtures consisting of four component fuels, n-dodecane, iso-octane, n-propyl benzene, and 1,3,5-trimethyl benzene. The results show the present HMTS/CO-DAC algorithm is not only computationally efficient but also robust and accurate. Moreover, it is shown that compared to the DAC and HMTS/DAC methods, the computation time of model reduction in CO-DAC is almost negligible even for a large kinetic mechanism involving hundreds of species. In addition, the results show that computation efficiency of CO-DAC increases from homogeneous ignition to one-dimensional flame propagation for both the first and second generation PFA reduction. Therefore, the present HMTS/CO-DAC method can enable high-order model reduction and achieve higher computation efficiency for multi-dimensional numerical modeling.

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1. Introduction

More than 60% of energy is lost either from the exhaust gas and heat loss in the current gasoline engines. The concerns of energy sustainability and global warming require drastic increase of energy conversion efficiency and reduction of emissions of internal combustion engines. Recently, tremendous efforts have been devoted to develop more efficient and lower emission internal combustion engines working at lower temperature combustion and higher pressure. These advanced engines include the homogeneous charge compression ignition (HCCI), the partially premixed compression ignition (PPCI), the reactivity controlled compression ignition (RCCI) engines, and the next generation TAPS engine [1–3]. However, control of fuel injection time, ignition timing, and heat release rates at different engine loads requires advanced understanding of turbulence-chemistry coupling, especially from low temperature (700 K) to intermediate temperature range (1100 K). Unfortunately, modeling of turbulence-chemistry interaction in this temperature range of real transportation fuels need a large kinetic mechanism including low temperature chemistry, which involves hundreds of species and thousands of reactions. For

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example, a detailed n-heptane mechanism can have 1034 species and 4236 reactions [4] and a recent semi-detailed kinetic model for real jet fuel surrogate mixture has more than two thousand species and eight thousand species [5].

However, the large number of species and the stiffness of the combustion kinetics result in a great challenge in combustion modeling [6]. Even with the availability of supercomputing capability at petascale and beyond, numerical simulations using such large kinetic mechanisms remain to be difficult.

In last two decades, many kinetic model reduction methods have been developed. These methods can be divided into six categories (to the knowledge of the authors): (1) Sensitivity and reaction rate analysis (SA) methods [7–9] in which the important reactions and species are identified by perturbing each reaction rate and unimportant reactions and species are then removed to generate skeletal mechanisms. This method is computationally intensive when the number of reactions is large. (2) Timescale based dimension reduction methods such as the quasi-steady-state approximation (QSSA) method [10], the computational singular perturbation (CSP) method [11], the simple CSP method [45], the intrinsic low-dimensional manifold (ILDM) method [12], and the multi-timescale (MTS)/hybrid multi-timescale (HMTS) method [13]. These methods can remove the stiffness in the ordinary differential equation system governing chemical reactions by using either QSSA, timescale splitting, or low dimensional manifold. However, the QSSA method often depends on human experience and is not robust and valid for all temperature and pressure conditions. Moreover, CSP and ILDM methods are computationally expensive due to the Jacobin matrix decomposition. (3) Tabulation methods including the in-situ adaptive tabulation (ISAT) method [14] and the piecewise reusable implementation of solution mapping (PRISM) method [15]. In these methods the chemistry integration is tabulated by using multi-dimensional look-up tables instead of solving the large stiff ODE system. Although this method is very efficient for small reaction systems, for large kinetic models on-the-fly construction of tables and high dimensional table looking will significantly reduce the computation efficiency. (4) Reaction flux based reduction methods such as the visualization method developed by Bendsten et al. [16], the Direct Relation Graph (DRG) method [17], the DRG with error propagation (DRGEP) method [18], and the multi-generation path flux analysis (PFA) method with and without error control [19,20]. In these methods, species reductions are all based on the direct or multi-generation reaction fluxes. Thus, these methods have the advantage in generating reduced mechanisms on the fly. However, for a large kinetic mechanism of real fuels, as shown in this paper the computation time required for flux analysis can be a big challenge. (5) Cell clustering methods which include the dynamic multi-zone (DMZ) method [21,22], the chemistry coordinate mapping (CCM) method [23,24], the cell agglomeration (CA) method [25], and unsupervised high-dimensional clustering (UHDC) method [26]. Recently, FLUENT [53] also combined cell agglomeration method and DRG method to do the DRG reduction on top of cell agglomeration. In these methods, instead of reducing the chemical kinetics, the integration of chemistry is reduced by computationally mapping the cells with similar conditions. However, due to the nonlinear dependence of the intermediate species on parametric space, especially at low temperature, the uncertainty of backward cell mapping can be very large and sometimes is difficult to predict. (6) Adaptive chemistry (AC) methods developed by Green et al. [27], Peter et al. [28], Najm et al. [29] and Banerjee and Ierapetritou [30]. In these adaptive chemistry methods, the reduced sub-mechanisms valid for different thermochemical conditions that may be encountered in a reacting flow simulation are pre-generated and stored in a library. During the calculation, the algorithm will search for the library and select the appropriate sub-mechanism based on the local conditions. A difficulty of these AC methods is that it is hard to guarantee the sub-mechanisms contained in the pre-generated library can cover all the possible conditions in a complex reacting flow. Recently, to further increase the efficiency of model reduction, algorithms using a few combinations of the above methods to reduce chemical reactions on the fly and obtain the dynamic adaptive chemistry (DAC) are developed by Liang et al. [31,32], Lu et al. [33] and Gou et al. [34] with HMTS and the ordinary differential equation solver VODE [35].

Unfortunately, when a kinetic mechanism is very large, the DRG or PFA based DAC method becomes computationally expensive. Moreover, due to the increase of computation time of DAC for a large mechanism, the current DAC method makes it difficult to implement a higher-order path flux based model reduction method and may lead to larger reduced mechanisms for a given accuracy threshold [20]. On the other hand, the VODE method, which contains Jacobin matrix decomposition to solve the chemical reactions in the DAC methods, is also computationally expensive. The computation time by the VODE method is proportional to the cubic of number of species.

The goal of this paper is to develop and validate a correlated dynamic adaptive chemistry (CO-DAC) method integrated with the multi-timescale algorithm to take advantages of the similarity of kinetic mechanisms in both time and space domains in a large reaction system to dramatically increase the efficiency of model reduction and to retain the high accuracy of chemistry integration. At first, a concept of correlated kinetic mechanism is proposed by using temperature, equivalence ratio, and a few key intermediate species and radicals for both low and high temperature fuel oxidation. A correlated model reduction in time and space coordinates is conducted on the fly by using the multi-generation PFA method, which enables both first and second order accuracy of species fluxes. To further increase the computation efficiency, the mechanism generated by CO-DAC is integrated by using the hybrid multi-timescale (HMTS) method [13]. The present HMTS/CO-DAC method is validated and compared to VODE, VODE/DAC, HMTS, and HMTS/DAC methods in computations of ignition and unsteady flame propagation of a real jet fuel surrogate mixture with a comprehensively reduced large kinetic mechanism. Finally, the computation accuracy and efficiency are examined and conclusions are drawn.

2. Numerical methods

The motion and evolution of an unsteady, compressible, and reactive flow with N species and I reactions is described by a partial differential equation (PDE) system including mass, momentum and energy conservations (neglect body forces):

$$\rho\frac{DY_n}{Dt} = -\nabla\bullet(\rho Y_n\mathbf{V_n}) + \omega_n, \quad (n = 1,\ldots,N) \tag{1}$$

$$\rho\frac{D\mathbf{U}}{Dt} = -\nabla\bullet\boldsymbol{\sigma} \tag{2}$$

$$\rho C_p\frac{DT}{Dt} = \frac{DP}{Dt} + \nabla\bullet(\lambda\nabla T) - \rho\nabla T\bullet\sum_{n=1}^{N}C_{p,n}Y_n\mathbf{V_n} - \sum_{n=1}^{N}h_n\omega_n \tag{3}$$

where ρ is the density of the mixture; t is time; Y_n, $\mathbf{V_n}$ and ω_n are the mass fraction, diffusion velocity and reaction rate of the n-th species, respectively; $\mathbf{U}$ is the flow velocity; $\boldsymbol{\sigma}$ is the second order stress tensor; C_p is the specific heat at constant pressure; T is the temperature; P is the thermodynamic pressure; λ is the thermal conductivity; $C_{p,n}$ and h_n are the specific heat at constant pressure and specific enthalpy of the n-th species.

By using the splitting fractional-step procedure [36], the PDE system is decoupled to chemical reaction source terms which are described by a first-order ordinary differential equation (ODE)