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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

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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

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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

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 multigeneration 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

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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):

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

$$\rho \frac{D\mathbf{0}}{Dt} = -\nabla \bullet \mathbf{\sigma} \tag{2}$$

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

where ρ is the density of the mixture; *t* is time; **Y**_n, **V**_n and ω_n are the mass fraction, diffusion velocity and reaction rate of the *n*-th species, respectively; **U** is the flow velocity; **σ** 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)

system, and transport terms which include unsteady, convection and diffusion terms and described by a second order PDE system of an unreactive flow. In the first fractional step, only the ODE system governing chemical reactions are integrated. The thermodynamic state variables after solving chemical reaction terms are used as the initial conditions in the second fractional step to solve the transport terms.

The splitting method has been widely used in numerical simulations in the combustion community [21-26] and the details of the numerical errors of splitting method have been comprehensively studied and discussed [54,55]. It has been mathematically demonstrated that the splitting method works well when the time step is much smaller than the timescale of diffusion. In our calculation, the time step is limited by the chemical time scale as well as the restriction of the CFL number at the minimum grid size, so the minimal time step is below 10^{-8} s. This time step is much smaller than the diffusion timescale and the error caused by the splitting scheme is negligible.

The ODE system in the first fractional step is:

$$\frac{dY_n}{dt} = \frac{\omega_n}{\rho}, \quad (n = 1, \dots, N)$$
(4)

$$\frac{dT}{dt} = -\frac{1}{\rho C_p} \sum_{n=1}^{N} h_n \omega_n \tag{5}$$

Thus, the dimension of this ODE system is N + 1. The computation time to integrate this ODE system is strongly dependent on the total species number, N, and the methods to find the appropriate reduced mechanisms computationally efficiently. The goal of the CO-DAC method is to generate correlated reduced mechanisms on the fly to decrease the number of species, i.e. the dimension of the ODE system, and to increase the efficiency to generate the reduced mechanism.

2.1. Correlated dynamic adaptive chemistry method

As stated above, the computation time to integrate the ODE system depends on *N*. For different ODE solvers, if the total number of computation steps is N_t and the total grid number is N_g , the time of chemistry integration can be given as,

$$t_{int} \propto N^{\alpha} N_t N_g$$
 (6a)

where α is between 1 and 3. For a large reaction system, the number of species, *N*, can be a very large numbers. Therefore, it is critical to reduce the reaction system on the fly so that a smaller *N* can be generated at different time steps and grid points.

To generate a reduced kinetic mechanism on the fly, the reaction flux analysis (e.g. DRG and PFA) based DAC methods [33,34] are often used. In this method the total computation time to generate the DAC on the fly is proportional to

$$t_{DAC} \propto N_d^m I_d N_t N_g, \tag{6b}$$

where *m* is between 1 and 2. N_d and I_d are the total numbers of species and reactions of the starting mechanism and normally N_d is much greater than *N*. Therefore, for a large reaction system, it is possible that the time of DAC can be much greater than that of integration:

$$t_{DAC} > t_{\rm int},\tag{7}$$

especially when a high-order model reduction approach is employed. In this case, the DAC method will be very computationally inefficient to be used in numerical simulation.

It is well known that for a given fuel mixtures, the chemical kinetics of each grid depends on temperature, pressure, and equivalence ratio. In an unsteady, multi-dimensional reaction system, the similar thermodynamics conditions may occur or repeat at different time and space coordinates frequently. If a computationally efficient chemistry integrator (e.g. HMTS), in which α is close to unity, is used, it is not necessary to generate a reduced mechanism on the fly at every time step and every grid point. Instead, only a few correlated reduced mechanisms are needed to be generated at different thermodynamic conditions and these reduced mechanisms can be reused if the local thermodynamic parameters are correlated. As such, the total computation time required for CO-DAC will be reduced to,

$$t_{\text{CO-DAC}} \propto N_d^m I_d(\varepsilon_t N_t)(\varepsilon_g N_g) \tag{8}$$

where the ε_t and ε_g are small numbers. If this can be done, from the above equations Eqs. (6) and (8) the CO-DAC method will be more efficient for multi-dimensional direct numerical simulations for a large reaction system.

Therefore, the basic idea of the CO-DAC method is schematically shown in Fig. 1a. The local reaction systems are represented by using a set of phase parameters to define the correlations between different local grids in time and space. The reduced mechanism is firstly generated on the fly based on the local phase parameter on one grid. Correlation thresholds for the local phase parameters are defined to represent the similarity in chemistry. If the phase parameters of the current computation grid are correlated to a different grid at the same computational time step (i.e. space correlation) or to the same grid at the previous time-step (i.e. time correlation) at which a reduced kinetic mechanism has been generated, then the same reduced mechanism will be reused for time integration of the current grid. Otherwise, if neither time nor space correlation is found, a new reduced mechanism will be generated and the phase parameters and the associated active species will be stored. If the above process repeats, less and less on the fly model reduction is needed due to the increase of time and space correlations. As a result, the validity of Eq. (8) will be realized.

The success of CO-DAC depends on the definition of the phase parameters. In order to construct an appropriate phase space, we need to understand which species are important and govern the reaction processes in low, intermediate, and high temperature, respectively. First, due to the Arrhenius law, temperature is always a dominant factor in a chemical reaction system. Second, the radial pool is strongly affected by the fuel and oxygen concentrations or the equivalence ratio. Third, at the same temperature and equivalence ratio, the concentrations of a few key intermediate species and radicals govern the ignition transition from low temperature to intermediate temperature, and from intermediate temperature to high temperature. The typical reaction pathways of a



Fig. 1a. Schematic of time and space correlation. Black cells are time correlation and red, blue and green cells are space correlation groups. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

conventional hydrocarbon fuel with low temperature chemistry are shown in Fig. 1b. The reaction pathway clearly shows that CH_2O and HO_2 are the key species dominate the low temperature chemistry, and OH is an important radical in the entire temperature range. In fact, a recent study shows that the low temperature ignition of various jet fuel surrogate mixture can be correlated to OH and HO_2 concentrations [47]. Therefore, we choose temperature and the mass fractions of fuel, OH, CH_2O and HO_2 as the key phase parameters to construct the correlated reaction mechanisms.

The correlated kinetic mechanisms in time and space can be identified by using a set of user specified threshold values for the phase parameters, $\boldsymbol{\varepsilon} = (\varepsilon_T, \varepsilon_{Fuel}, \varepsilon_{OH}, \varepsilon_{CH_2O}, \varepsilon_{HO_2})^T$. In the phase parameters fall within the variation of the phase thresholds, the local kinetic mechanism will be correlated and the same reduced mechanism will be reused.

The time correlation will be examined and applied firstly: we compare the local thermodynamic conditions between time step n and time step n + 1 in each cells and define the variation between two steps as,

$$\Delta = \left(\frac{|T_{n+1} - T_n|}{\varepsilon_T}, \frac{|\ln Y_{\text{Fuel},n+1} - \ln Y_{\text{Fuel},n}|}{\varepsilon_{\text{Fuel}}}, \frac{|\ln Y_{\text{OH},n+1} - \ln Y_{\text{OH},n}|}{\varepsilon_{\text{OH}}}, \frac{|\ln Y_{\text{CH}_20,n+1} - \ln Y_{\text{CH}_20,n}|}{\varepsilon_{\text{CH}_20}}, \frac{|\ln Y_{\text{HO}_2,n+1} - \ln Y_{\text{HO}_2,n}|}{\varepsilon_{\text{HO}_2}}\right)$$
(9a)

If $||\Delta||_{\infty} < 1$, the local chemistry is correlated and we can simply pass the reduced mechanism at time step *n* to time step *n* + 1. For the rest of cells, we introduce the space correlation. The total number of correlated reaction groups in spatial coordinate, $\mathbf{M} = (M_T, M_{\text{Fuel}}, M_{\text{OH}}, M_{\text{CH}_20}, M_{\text{HO}_2})^T$, and the group index of the *i*-th cell, $\mathbf{m}^{i} = (m_T^{i}, m_{\text{Fuel}}^{i}, m_{\text{OH}}^{i}, m_{\text{CH}_20}^{i}, m_{\text{HO}_2}^{i})^T$, can be obtained as,

$$M_T = \frac{T^{\max} - T^{\min}}{\varepsilon_T} + 1, \quad M_j = \frac{\ln Y_j^{\max} - \ln Y_j^{\min}}{\varepsilon_j} + 1$$
(9b)

$$m_T^i = \frac{T^i - T^{\min}}{\varepsilon_T} + 1, \quad m_j^i = \frac{\ln Y_j^i - \ln Y_j^{\min}}{\varepsilon_j} + 1$$
(9c)

where j = Fuel, OH, CH₂O and HO₂, respectively.

The threshold values used in this paper are: 20 K for ε_T and 0.05 for ε_j . Based on the sensitivity tests, the most sensitive threshold value is ε_T . When the threshold values located in the reasonable range, i.e. $\varepsilon_T < 50$ and $\varepsilon_j < 0.2$, the change of computational accuracy



Fig. 1b. The typical reaction pathways of a conventional hydrocarbon fuel at different temperature range [46].

is negligible. After the grid points are agglomerated to correlated groups in the phase space, the multi-generation path flux analysis (PFA) method [19] is applied to conduct the chemical reduction for each group.

Comparing with the cell clustering methods [21–26], which map the computation cells from physical domain into phase space with a few thermodynamic variables, the differences and advantages of the proposed CO-DAC method are: (1) in the CO-DAC method, we identify cells which have correlated similarity in chemistry pathways in phase space to obtain reduced chemical mechanisms instead of doing numerical extrapolation of the chemistry solution like that in the cell clustering method. The following ODE integrations in CO-DAC method are conducted accurately at each cells in physical space based on the local reduced mechanism. The species number in the reduced mechanism is much larger than the parameters in phase space and all the important reaction pathways related to the phase species are included and integrated by HMTS method accurately. Therefore, the CO-DAC method avoids the backward mapping errors in cell clustering methods and guarantees the conservation of mass and energy. (2) In the CO-DAC method, the phase parameters (T, Fuel, CH₂O, HO₂ and OH) cover the low temperature chemistry by the intermediate species and radicals of CH₂O, HO₂ and OH. While in the cell clustering methods, their phase parameters do not involve the key radicals and intermediate species at low temperature region [23]. The cell clustering method may work reasonably for high temperature flames of simple fuels. However, it will become problematic when low temperature chemistry is involved because the solution can be non-monotonic and multi-valued, and thus cannot be simply extrapolated linearly or nonlinearly. So the proposed CO-DAC method can avoid the difficulty of nonlinear extrapolation by directly solving the reduced chemistry using a faster HMTS solver. Therefore, the results are accurate and the method is much more comprehensive

Comparing with the ISAT method [14], which does the storage and retrieval during the calculation and gets the integration solutions by looking up a table and conducting linear interpolation, the CO-DAC method just simply passes the on the fly reduced mechanism in phase space to the physical domain and the rest of the ODE integrations are locally and independently conducted by the HMTS method. Therefore, the advantages of the CO-DAC method are: (1) more accurate and no CPU time required to create the store, (2) no memory required for the store, (3) no interpolation error in the retrieval mapping, and (4) no CPU time required retrieving the mapping.

The differences between the cell agglomeration methods, the ISAT method and the proposed CO-DAC method are summarized as Fig. 1c. Moreover, the main purpose of the CO-DAC method is



Fig. 1c. Schematic of the differences between cell clustering method, ISAT method and the proposed CO-DAC method.

to provide an efficient, flexible, and robust way to do the chemical reduction on the fly and to generate local reduced mechanisms. It can be integrated with any fast ODE solvers such as HMTS method.

2.2. Multi-generation path flux analysis method

The multi-generation PFA method can identify important species and reaction pathways based on multi-generation production and consumption fluxes, and remove trivial species and reactions below the flux threshold. For example, for species A, the overall production and consumption fluxes, P_A and C_A can be expressed as [19]:

$$P_{A} = \sum_{i=1,l} \max(v_{A,i}\omega_{i}, \mathbf{0})$$

$$C_{A} = \sum_{i=1,l} \max(-v_{A,i}\omega_{i}, \mathbf{0})$$
(10a)

where $v_{A,i}$ is the stoichiometric coefficient of species *A* in the *i*-th reaction, ω_i is the net reaction rate of reaction *i*. *I* is the total number of reactions. The first generation production and consumption fluxes between species *A* and *B*, P_{AB} , C_{AB} , are:

$$P_{AB} = \sum_{i=1,l} \max(v_{A,i}\omega_i\delta_B^i, \mathbf{0})$$

$$C_{AB} = \sum_{i=1,l} \max(-v_{A,i}\omega_i\delta_B^i, \mathbf{0})$$
(10b)

where δ_{i}^{b} is unity if species *B* is involved in *i*-th reaction and 0 otherwise.

Then, we use the maximal production or consumption flux to normalize P_{AB} and C_{AB} and obtain the first generation flux ratios for production and consumption of species *A* via species *B*:

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

$$r_{AB}^{con-1st} = \frac{C_{AB}}{\max(P_A, C_A)}$$
(11a)

Similarly, the second generation flux ratios between A and B via a intermediate species M_i are:

$$r_{AB}^{pro-2nd} = \sum_{i=1,l} \left[\frac{P_{AM_i}}{\max(P_A, C_A)} \times \frac{P_{M_iB}}{\max(P_{M_i}, C_{M_i})} \right]$$

$$r_{AB}^{con-2nd} = \sum_{i=1,l} \left[\frac{C_{AM_i}}{\max(P_A, C_A)} \times \frac{C_{M_iB}}{\max(P_{M_i}, C_{M_i})} \right]$$
(11b)

The PFA calculation starts from a preselect list of important species and flags all the species related to the preselect species. If the summations of their flux ratios $r_{AB}^{pro-1st}$, r_{AB}^{on-1st} , $r_{AB}^{pro-2nd}$ and $r_{Con-2nd}^{con-2nd}$ are greater than a user specified threshold value, ε_r , they will be add to the selected list. Then, the PFA program will start from the selected list and do the subsequent iterations, until there is no new species added into the selected list. Finally, the local reduced mechanism can be constructed by the species contained in the selected list. Unless specified, the threshold value ε_r used in this paper for PFA reduction is 0.005.

2.3. Hybrid multi-timescale method

The hybrid multi-timescale (HMTS) method is used to integrate the ODE system based on the local reduced mechanisms from CO-DAC method. In the conventional Euler method, ODE equations are integrated explicitly by using a single time step smaller than the minimum characteristic time of all species. However, the multitimescale nature of chemical reactions introduces a strong stiffness to the ODE system. The computation efficiency of the conventional Euler method is very low due to the strong constraint in time step. In the HMTS method, unlike the conventional Euler method, the species equations are integrated with their own characteristic times. The timescale of *n*-th species, τ_n , is estimated as [13]:

$$\tau_n = -\left[\frac{\partial}{\partial Y_n} \left(\frac{dY_n}{dt}\right)\right]^{-1} = \left(\frac{\partial D_n}{\partial Y_n}\right)^{-1}$$
(12)

where Y_n and D_n are the mass fraction and the destruction rate of *n*th species, respectively. In the HMTS calculation, all the species are grouped into integration groups based on their own timescales. By defining each neighboring group has a difference of timescale in one-order, the group index of the *n*-th species, G_n can be obtained as:

$$G_n = \left\lfloor \log_{10} \left(\frac{t_{base}}{\tau_n} \right) \right\rfloor + 1 \tag{13}$$

where t_{base} is the base time step in DNS calculations.

With the definitions of the timescale and group index, all the groups are integrated separately based on their own timescale. Moreover, if we are not interested in the detailed history of the fast modes, we can apply implicit Euler method to further increase the integration efficiency. This HMTS method has been demonstrated to be more efficient than the VODE solver [13].

2.4. Kinetic model and fuel mixtures

The goal of this paper is to develop a CO-DAC method integrated with HMTS to achieve improved computational efficiency and rigorous combustion modeling with large chemical kinetics. The Real Fuel 2 mechanism developed at Princeton by Won et al. [5], which is a kinetic model for a real jet fuel surrogate consisting of four component fuels (40% n-dodecane, 30% iso-octane, 23% n-propyl benzene, and 7% 1,3,5-trimethyl by mole fraction), is used to validate the integrated HMTS/CO-DAC method. Both the detailed Real Fuel 2 mechanism [5] (2051 species and 8428 reactions) and the comprehensively reduced one (425 species and 2275 reactions) are employed in the calculation to test the performance of HMTS/CO-DAC method when the sizes of mechanisms are in different orders of magnitudes. Numerical simulations of homogeneous ignition and unsteady outwardly propagating spherical flames of jet surrogate mixtures are carried out to demonstrate the accuracy and robustness of the proposed algorithm.

The present CO-DAC method with the HMTS solver is implemented into the adaptive simulation of unsteady reactive flow (ASURF+) code [37,38,51] to simulate compressible, unsteady reactive flow. ASURF+ is an updated version ASURF [37] with a higher-order numerical scheme, and is fully compatible with CHEMKIN [39] for transport and elementary reactions and conducts multi-level local grid adaption to resolve the reaction zone and flame front. In this the simulation of propagating flames, the base grid size is chosen as 0.5 mm and maximal grid level is 5, which results in the minimum grid size of 15 µm. Briefly, at first, the CO-DAC method is used to generate correlated reduced kinetic mechanisms on each computation grid. Secondly, the HMTS or VODE solver is used to solve the stiff ODE system based on the local reduced mechanism generated from the CO-DAC method. Finally, the third-order weighted essentially non-oscillatory (WENO) scheme [40–44] and the finite volume central difference methods are applied to discretize and integrate the PDE system involving convection and diffusion, respectively. The ASURF and ASURF+ code have been validated extensively in our previous studies and in collaborations with other researchers [48–51].

3. Results and discussion

In order to validate the algorithm and test its performance, the present HMTS/CO-DAC method will be compared to VODE, VODE/

DAC, HMTS, and HMTS/DAC methods to examine the computation accuracy and efficiency for both detailed and comprehensively reduced mechanisms. The homogeneous ignition of Real Fuel 2 at different initial temperatures is modeled by the HMTS and VODE solvers with and without CO-DAC method. To further test the effect of computation dimension on the algorithm efficiency, calculations of an outwardly propagating premixed spherical flame of stoichiometric Real Fuel 2/air mixture with and without CO-DAC are also carried out to validate the CO-DAC method in an unsteady flame propagation process.

Figure 2 shows the time histories of active species number as well as the accumulated mechanism reduction time calculated by both CO-DAC method and DAC method during an auto ignition process of the stoichiometric Real Fuel 2/air mixture using the comprehensively reduced mechanism. The initial pressure is 10 atm and temperature is 800 K. This figure clearly shows that the number of active species varies significantly at different ignition stages. Initially, only about half of the total species are involved in the reactions. However, when the first stage ignition occurs at 1 ms, the number of active species increases rapidly due to the low temperature chemistry. After the second stage ignition, the system approaches near equilibrium state and only a few species is active. This result demonstrates clearly that a large number of species is required to capture the detailed reaction process of low temperature ignition. Therefore, the comprehensively prereduced kinetic mechanism is not efficient because it requires a large set of species and reactions in order to guarantee the accuracy of the reduced mechanism at different conditions for different fuel mixtures. Moreover, compared with DAC method, our CO-DAC method is more than two-orders faster in terms of the on the fly model reduction time. Due to the time correlation, our CO-DAC method simply passes the reduced mechanisms to correlated following time-steps, while the DAC method needs to do mechanism reduction at every time steps even when the chemical equilibrium is achieved. Therefore, the CO-DAC method is much more efficient than the DAC method without correlation, especially in the equilibrium or near equilibrium region. As such, a combination of CO-DAC method with the comprehensively reduced mechanism is a computationally efficient way for direct numerical simulations.

3.1. CO-DAC with the first generation PFA reduction

In this section, the CO-DAC method only includes the first generation PFA reduction, i.e. only the first generation flux shown in



Fig. 2. Comparison of number of active species and the accumulated on-the-fly mechanism reduction time by using CO-DAC and DAC methods in a homogeneous ignition process with a stoichiometric Real Fuel 2/air mixture at 10 atm. The solid line is calculated by CO-DAC method and the dash line is calculated by DAC method.

Eq. (11a) was used in the model reduction. The comparison between the first and second generation PFA reduction will be discussed later. Figure 3(a) and (b) shows the comparison of ignition delay time of the jet fuel surrogate mixture at 10 atm and stoichiometric condition as a function of initial temperature calculated by using HMTS and VODE methods, respectively, with and without DAC or CO-DAC for both reduced and detailed kinetic mechanisms. It is seen that the CO-DAC method can predict the ignition time in both low and high temperatures and for both reduced and detailed mechanisms very well. The maximum discrepancy of the predicted ignition delay time in all computation conditions between CO-DAC and the VODE methods is 2%. The small discrepancy at both low and high pressures compared with the large thresholds in phase space for the determination of mechanism correlation suggests that the proposed parametric space using OH, HO₂, and CH₂O as the key intermediate species to distinguish low and high temperature kinetics is very effective.

Figure 4(a) and (b) shows the comparisons of time histories of species mass fraction profiles of CH_2O , HO_2 and OH radicals calculated by different methods at pressure of 10 atm, stoichiometric condition and initial temperature of 800 K, using reduced and detailed Real Fuel 2 mechanisms, respectively. There is a horizontal time shift of the profiles in the high temperature ignition region. For the calculations using the reduced mechanism, the maximal shift happened between HMTS and HMTS/CO-DAC methods and the value of the maximal shift is 0.021 ms. Compare with the



Fig. 3. Comparison of ignition delay times predicted by HMTS and VODE solvers with DAC and CO-DAC at 10 atm and stoichiometric condition. (a) Reduced Real Fuel 2/air and (b) detailed Real Fuel 2/air.





Fig. 4. Species mass fraction profiles calculated by different methods at 10 atm, stoichiometric condition and initiated at 800 K. (a) Reduced Real Fuel 2/air and (b) detailed Real Fuel 2/air.

average ignition delay time of all these five methods, 3.17 ms, the relative error in time is 0.67%. Similarly, the maximal shift of the detailed mechanism is 0.032 ms and it also happened between HMTS and HMTS/CO-DAC method. Considering the average ignition delay time, 5.46 ms, the maximal relative error in time is 0.59%. Besides the time shift, other properties calculated by different methods are identical. The excellent agreement for both stable species and radicals demonstrates that the accuracy of CO-DAC method is good enough to provide correlated reduced mechanism in a large range of temperature. Also the agreement in the two-stage ignition profile demonstrates the CO-DAC method has the capability to capture low temperature chemistry accurately.

In order to further demonstrate the accuracy of the CO-DAC method, the profiles of peroxides $(C_{12}H_{25}O_2)$ and H_2O_2 radicals at 10 atmosphere pressure, stoichiometric condition and initial temperature of 800 K are plotted in Fig. 5(a) (reduced mechanism) and Fig. 5(b) (detailed mechanism). They show that besides the phase parameters CH₂O, HO₂ and OH, other radicals can also be predicted accurately by the CO-DAC method. Therefore, the local reduced mechanisms generated in the 5-dimensional phase space (*T*, Fuel, CH₂O, HO₂ and OH) can capture the important reaction pathways and predict the ignition properties accurately.

Figure 6 show the CPU time comparison for the homogeneous ignition between the VODE and HMTS methods with and without DAC or CO-DAC. Again (6a) is the result of the comprehensively reduced mechanism for the real fuel surrogate mixture and (6b)

Fig. 5. Mass fraction profiles of O, H and H_2O_2 calculated by different methods at 10 atm, stoichiometric condition and initialed at 800 K. (a) Reduced Real Fuel 2/air and (b) detailed Real Fuel 2/air.

is the result of detailed mechanism. To demonstrate the increase of computation efficiency compared to the VODE method, the CPU time is normalized by that of VODE without DAC for different initial temperatures at 10 atm and stoichiometric condition. It is seen that the integration of DAC with the VODE can improve computation efficiency by 40-90%. However, the DAC method is not computationally efficient when it is integrated with HMTS. Figure 6 shows that DAC method even increases the computation time if integrated with HMTS. The cause of the computation time increase with DAC was discussed in Eqs. (6a), (6b) and (7). The reason is that HMTS is much more computationally efficient than the VODE solver, so the computation time for DAC method to do chemical reduction on-the-fly becomes comparable to or even longer than the chemistry integration time by the HMTS, thus offsetting the benefit of the generation of locally reduced kinetic mechanism. Fig. 6 also demonstrate that by using the CO-DAC method in the HMTS method, the PFA model reduction time is dramatically reduced and the resulting HMTS/CO-DAC method can increase computational efficiency by an additional factor of 2 in a broad temperature range.

Since the parameters chosen for the determination of mechanism correlation is a strong function of temperature, intermediate species, and radical pool. Different from ignition, flames have much different species distributions, radial pool, and reaction pathways. To prove the applicability of the CO-DAC method in a broad ignition and flame regimes, it needs to be tested in both unsteady and steady flame propagation. The unsteady, outwardly



Fig. 6. CPU time comparison between HMTS and VODE solvers with and without DAC or CO-DAC at 10 atm and stoichiometric condition. (a) Reduced Real Fuel 2/air and (b) detailed Real Fuel 2/air.



Fig. 7. Flame trajectories of stoichiometric reduced Real Fuel 2/air mixture at 1 atm and 400 K.

propagating spherical flames serve for both validation purpose of unsteady and quasi-steady flame structures and propagation speed. Figure 7 shows the time-dependent outwardly propagating spherical flame trajectories calculated by HMTS and VODE with and without DAC or CO-DAC. Here, only the comprehensively reduced kinetic mechanism of the real fuel surrogate mixture with



Fig. 8. Flame structure of stoichiometric reduced Real Fuel 2/air mixture at 1 atm and 400 K.

425 species is used. Stoichiometric fuel/air mixture at 1 atm and 400 K is considered. The mixture is ignited at the center by a hot spot with uniform temperature of 1600 K in a spherical region of 2 mm in radius. Again, it is seen from Fig. 7 that the present CO-DAC method shows excellent agreement compared with other methods even when the transport terms are involved. The largest relative error in flame trajectory is less than 2%, which is far below the experimental accuracy of flame speed measurements [52].

Figure 8 shows the predicted flame structure of the spherical flame. The distributions of temperature and selected species calculated by different methods are compared. It is seen that even for the detailed structures of the flame, the CO-DAC method is still accurate and robust for both unsteady and quasi-steady flame propagation.

Figure 9 is the comparison of the CPU times of the premixed spherical flame propagation calculated by HMTS and VODE with and without DAC or CO-DAC. Only 1st generation PFA reduction is involved to generate local reduced mechanisms. The black section represents the CPU time used for transport properties, diffusion, and convection. The summation of the red¹ and blue sections is the total computation time to solve the chemical reaction, including the PFA reduction time (red) and chemistry integration (blue). This figure clearly shows that compared to DAC method, the CO-DAC method can dramatically decrease the on the fly model reduction time and makes it almost negligible even for a large kinetic mechanism involving several hundreds of species. It is interesting to note that by using the CO-DAC method integrated with HMTS solver, the integration of chemical reactions for a large mechanism is no longer the most time consuming part in computation. Instead, the computation of the transport and convection is now the major cost of the computation time. It should be noted that as discussed in Eq. (8), the CO-DAC method will be more effective when multi-dimensional CFD computation is implemented because the time required for CO-DAC for the multi-dimensional CFD is similar to one-dimensional due to the increase of mechanism similarity in multi-dimensional computation domain. This advantage may allow us to use higher-order model reduction method such as the multi-generation PFA method [19]. As such, the CO-DAC method coupled with HMTS solver can significantly increase computational efficiency.

3.2. CO-DAC with the second generation PFA reduction

The above first generation PFA reduction results show that the CPU time for PFA reduction in the CO-DAC method is negligible.

 $^{^{1}\,}$ For interpretation of color in Fig. 9, the reader is referred to the web version of this article.



Fig. 9. CPU time comparison between HMTS and VODE method with and without DAC or CO-DAC of the 1D flame propagation case with stoichiometric reduced Real Fuel 2/air mixture at 1 atm and 400 K.

So the CO-DAC method may have capability to enable higher-order PFA model reduction. In this section, the second generation PFA reduction is utilized and examined with CO-DAC method, i.e. the second generation flux in Eq. (11b) is included. Compared with the first generation reduction shown in Eq. (11b) which calculate the path flux between species A and B directly, the second generation reduction needs to search all the species in the mechanism as the intermediate species to get the path flux between A and B. Therefore, the second generation reduction should be N times slower than the first generation reduction, where N is the number of species in a mechanism.

In order to test the performance of the CO-DAC method with the second generation reduction, the same reduced Real Fuel 2 mechanism [5] with 425 species and 2275 reactions is applied in the computation. The comparison between CO-DAC method with 1st and 2nd generation reduction are conducted in both homogeneous auto-ignition and unsteady flame propagation calculations.

The dash lines in Figs. 3(a) and 7 are the ignition delay time and flame trajectory, respectively, calculated by CO-DAC method with the 2nd generation PFA reduction. The difference between 1st and 2nd generation reduction is too small to be noticed. The reason for such a trivial discrepancy is that the threshold value which was used for the PFA reduction is very small (0.005). With such a small threshold value, both 1st and 2nd generation PFA reduction methods are equally accurate.



Fig. 10. Comparison of ignition delay time and PFA reduction time between CO-DAC method with 1st and 2nd generation PFA reduction for different threshold values calculated at 10 atm, stoichiometric condition, and initiated at 800 K.

Figure 10 shows the ignition delay time as well as the PFA reduction time as the function of threshold value calculated at 800 K. 10 atm and stoichiometric condition. Both ignition delay time and PFA reduction time are plotted in logarithm coordinate. It is seen that both the 1st and 2nd generation PFA reduction are accurate when the threshold value is small. When the threshold value increases, the ignition times of the PFA reduced mechanisms deviate from the exact value, but the error of the 2nd generation PFA reduction is always smaller than that of the 1st generation PFA reduction. On the other hand, the computation time ratio of the 2nd generation reduction to the 1st generation reduction only slightly decreases with the increase of threshold value. The increase of the computation time by the 2nd generation of PFA is close to the number of species (425). This figure demonstrates that the 2nd generation reduction is more accurate than the 1st generation reduction, especially when the threshold value is large. However, the 2nd generation PFA is N times slower than the 1st generation PFA reduction, as mentioned earlier. Therefore, for a large reaction system and low dimensional simulation, the 1st generation PFA reduction with a small threshold value is more computationally efficient.

Figure 11 is the computation time comparison between CO-DAC method with 1st and 2nd generation PFA reduction in a spherical flame propagation calculation initiated by a hot spot with uniform temperature of 1600 K in a spherical region of 2 mm in radius. It is seen that the HMTS times in two calculations are comparable due to the similar active species. However, the PFA time of the 2nd generation reduction is 462 times more than the 1st generation reduction. Again this number is close to the number of species (425) in the mechanism. This result further demonstrate that the 2nd generation reduction is *N* times slower than the 1st generation reduction.

However, even if the 2nd generation PFA reduction is much slower than the 1st generation one, it may be able to be utilized in higher dimensional simulation by taking the advantage of the space correlation. Table 1 shows the HMTS time and 2nd generation PFA time as well as the ratio of PFA/HMTS of the 0D auto-ignition and 1D spherical flame propagation calculations. The ratio of PFA reduction time to HMTS time decreases by factor of 4 when the calculation goes from 0D to 1D. The reason of the decrease of the PFA/HMTS ratio in a higher dimensional calculation is that in 0D calculation, only time correlation is effective, but in 1D calculation, not only time correlation but also space correlation are utilized to reduce the number of chemical reduction. In higher dimensional calculations, the space correlation will be more effi-



Fig. 11. CPU time comparison between CO-DAC method with 1st and 2nd generation PFA reduction in a spherical flame propagation calculation of stoichiometric reduced Real Fuel 2/air mixture at 1 atm and 400 K.

Table 1

Computation time comparison of HMTS, 2nd generation PFA and PFA/HMTS between 0D and 1D calculation.

	0D	1D
HMTS time	13.1 min	11.7 h
2nd generation PFA time	274.0 min	61.8 h
PFA/HMTS	20.9	5.3

cient and the PFA/HMTS ratio will further decreases. Therefore, the 2nd generation has the capability to be applied in higher dimensional simulation.

4. Conclusion

A correlated dynamic adaptive chemistry (CO-DAC) method integrated with the HMTS solver is developed by using the similarity of chemistry in phase space. The results show that the CO-DAC method can significantly increase the computational efficiency while keeping excellent accuracy. The simulations of homogeneous ignition of Real Fuel 2/air mixtures with different initial temperatures and equivalence ratios show that the chemical reduction time in CO-DAC method is two-order faster than that in DAC method. In addition, the results show that in a large reaction system DAC will increase the computation time when coupled with an efficient HMTS solver. However, the present HMTS/CO-DAC method can improve the efficiency of the total chemical integration by a factor of 2. Moreover, the results of unsteady flame propagation demonstrate that the computation efficiency of the CO-DAC method is further increased for a higher dimensional computation problem. The actual computation time for the model reduction by CO-DAC becomes almost negligible. Moreover, the HMTS/ CO-DAC method is also more efficient and can accurately predict the flame speeds, structure, and distributions of radicals in flames. Furthermore, comparison between the 1st and the 2nd generation PFA reduction shows the 2nd generation PFA has a better accuracy but is much more computationally expensive than the 1st generation PFA. However, the increase of PFA reduction time compared to the chemistry solver decreases rapidly from zero-dimension ignition calculation to one-dimensional unsteady flame propagation due to the space correlation. The promising results in the present study indicate that with the proposed CO-DAC method, a large kinetic mechanism can be efficiently handled in a multi-dimensional numerical simulation and the remaining challenge is how to accelerate calculations of transport terms. This will be addressed in our future research.

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