Combustion and Flame 160 (2013) 225–231

Contents lists available at SciVerse ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

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

Xiaolong Gou [a,*], Zheng Chen [b], Wenting Sun [c], Yiguang Ju [c,*]

[a] School of Power Engineering, Chongqing University, Chongqing 400044, China
[b] SKLTCS, Department of Mechanics and Aerospace Engineering, College of Engineering, Peking University, Beijing 100871, China
[c] Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544, USA

ARTICLE INFO

Article history:
Received 22 May 2012
Received in revised form 29 July 2012
Accepted 18 October 2012
Available online 5 November 2012

Keywords:
Dynamic adaptive chemistry
Error control
Progress variable
n-Heptane
n-Decane

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

---

* Corresponding authors. Fax: +86 23 6510 2473 (X. Gou), Fax: +1 609 258 6233 (Y. Ju).

E-mail addresses: simgxl@cqu.edu.cn (X. Gou), yju@princeton.edu (Y. Ju).

0010-2180/$ - see front matter © 2012 The Combustion Institute. Published by Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.combustflame.2012.10.015

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.

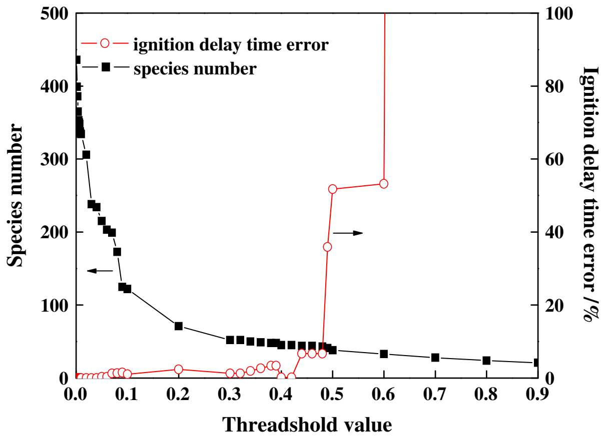


Fig. 1. Change of the number of species in the reduced mechanism and the relative error in ignition delay time prediction with the threshold for stoichiometric *n*-heptane/air mixture at initial condition of 1 atm pressure and 1200 K temperature.

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 *i*th reaction, ω_i is the net reaction rate of the *i*th 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 *i*th 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.

An iterative process is employed to find the path fluxes of each selected species. For example, given the species in set X which are known important, such as fuel and oxygen, the PFA algorithm identifies another set of species, say set Y which must be retained in the skeletal mechanism via the criterion in Eq. (7). Then the species in set X is updated by including the species in set Y and the PFA algorithm further repeats the process by identifying a new set Y. This iterative process will continue until no species can be updated in set X. Therefore, the skeletal mechanism can be constructed by the species contained in set X.

2.2. Reaction progress variable

According to Eq. (7) and the results shown in Fig. 1, the threshold determines the complexity and accuracy of the reduced mechanism. No quantitative rule has been reported in previous studies. Most of previous studies claimed to use a "small" threshold value, but it was not clear how small is small. This ambiguity becomes more problematic for a dynamic model reduction because with the progress of ignition and combustion in flames, both the critical threshold value and its correlation with the accuracy of the reduced model will change. In the present study, to obtain a dynamically reduced mechanism which satisfies a pre-specified error bound of a problem, a database that correlates the accuracy of the model with the thresholds at different stages of combustion by using a reaction progress variable is constructed. This threshold and accuracy database is created by using the PFA method with a detailed mechanism for different initial conditions of the mixtures and different combustion progress variables. Since the mass fraction of O_2 keeps monotonically decreasing in the ignition process, as shown in Fig. 2, a progress variable based on the oxygen mass fraction is used in this study [38,39]. The results of the comparison between using fuel and oxygen as the progress variable justify this choice.

Note that for homogeneous ignition and flame propagation (as shown below), the combustion progress is mainly controlled by chemical kinetics and the mixing by diffusion transport plays a minor role. As such, the progress of the reaction system can be described by a single parameter like the mass of oxygen. For laminar diffusion flames, a single parameter for fuel oxidation progress such as the mixture fraction may also be defined. However, for turbulent flames at high Reynolds number, the turbulent mixing may change the local fuel and oxidizer ratio significantly and a single parameter for a single progress variable may be difficult to be defined. Nevertheless, since the transport equations for all species (unsteady convection–diffusion equations) are solved and the fuel and oxidizer mixing is computed before the dynamic reduction, the progress variable at every grid and time step can be dynamically recalculated and updated at every time step. The focus of the present paper is to present the concept of the reaction progress variable in dynamic model reduction. The mixing effect will be addressed in our future research.

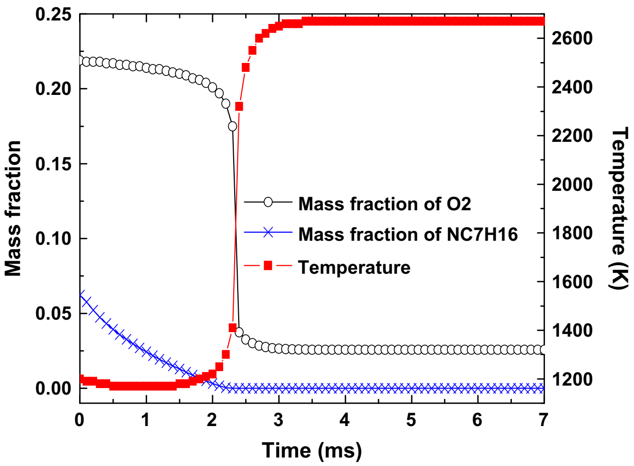


Fig. 2. Mass fraction profile of O_2, n-C_7H_{16} and temperature for stoichiometric n-heptane/air mixture at initial condition of 1 atm pressure and 1200 K temperature.

2.3. Tabulation of threshold value

The tabulation is conducted according to the following procedures.

a. First, the ranges for initial temperature, pressure, and equivalence ratio are specified.
b. Second, data of key parameters such as the mass fractions of major species (fuel, oxidizer, CO_2, H_2O and OH are used in this paper), temperature, and pressure should be calculated using a detailed mechanism.
c. Third, these key parameters are used to obtain the maximum threshold to achieve the defined accuracy, 1% local error for the key parameters compared with the results of the detailed mechanism. And the controlling error is the maximum value of the mass fraction errors of major species and temperature (or pressure in other cases). This process also needs an iteration to find the local maximum threshold which satisfies the defined accuracy. The threshold value sets are saved and combined with the data of progress variable to build a threshold table.

A threshold table consists of the thresholds, the values of the initial conditions (temperature, pressure, and equivalence ratio), and the value of the progress variable. For the ignition case in this work, a five-dimensional table is used. According to the initial conditions and the current value of progress variable, the new threshold can be obtained from the threshold table to construct a new reduced mechanism during the calculation process. If the specific initial condition cannot be found in the table, an interpolation method is used. At every time step and grid point, this new threshold is obtained and a skeletal mechanism is generated dynamically.

3. Results and discussion

In order to assess the performance of the present method for both detailed and reduced mechanisms, a large, detailed, n-heptane mechanism [33,34] with 1034 species and 4236 reactions and a comprehensively reduced high temperature n-decane mechanism [35] with 121 species and 866 reaction are used in the simulations, respectively. The homogeneous ignition processes of n-heptane/air and n-decane/air mixtures at different initial temperatures, pressures, and equivalent ratios are modeled with and without error controlled dynamically reduced mechanisms. The time step of one microsecond and 1% relative control error of mass fraction of fuel, products, and temperature are used in all simulations. Note that in shock tube experiments, the uncertainty of ignition delay time measurements with the same or different research groups is larger than 10% [40,41]. Therefore, even a validated detailed kinetic mechanism is not able to achieve 10% accuracy of prediction of ignition delay time. For flame speed measurements, the experimental uncertainty is around 5% [42–44].

Figure 3 shows the threshold as a function of mass fraction of O_2 for the stoichiometric n-heptane/air mixture initially at 1200 K and atmospheric pressure. It is seen that for a given 1% of accuracy bound, the threshold changes significantly in the whole ignition process, which indicates that it is difficult and not computationally

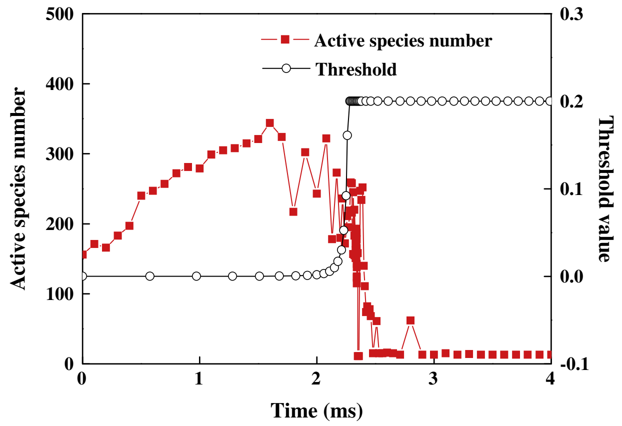
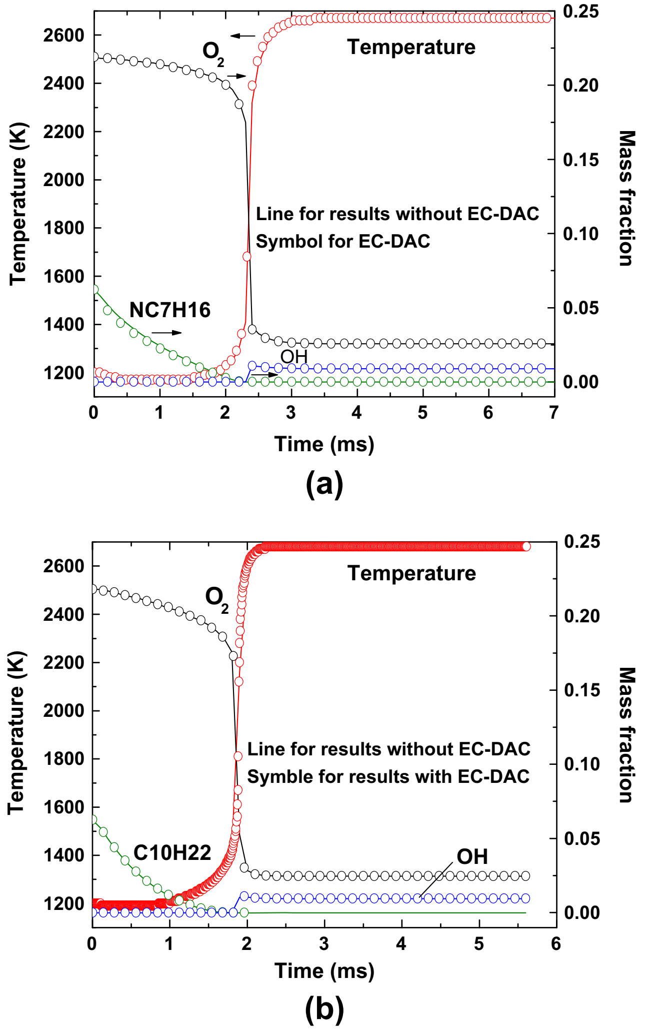


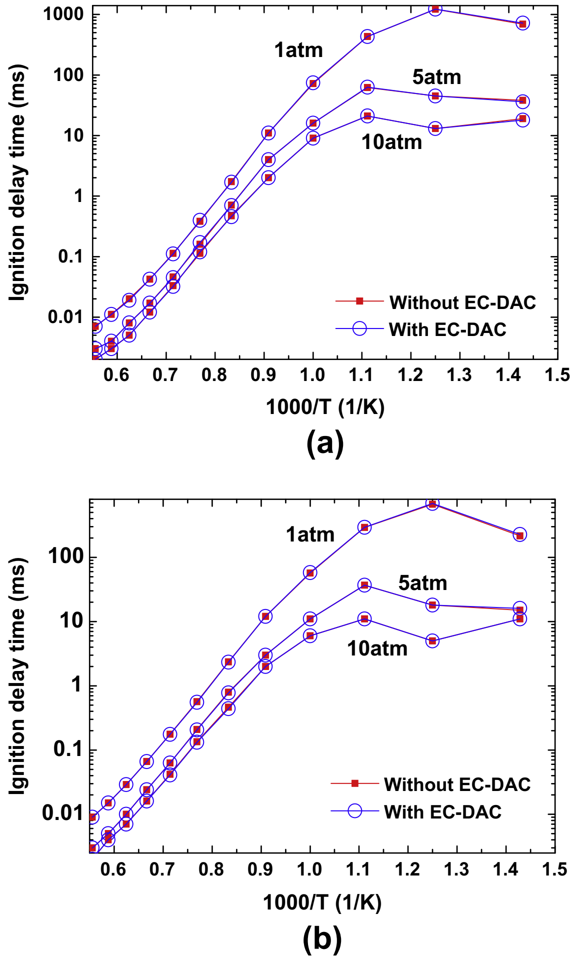
Fig. 3. Active species number and threshold profile for stoichiometric *n*-heptane/air mixture ignition at 1 atm initial pressure and 1200 K initial temperature.



(a)

(b)

Fig. 4. Comparison of temperature profiles and mass fractions of selected species between modeling without and with EC-DAC for stoichiometric (a) *n*-heptane/air and (b) *n*-decane/air mixture ignition process at 1 atm initial pressure and 1200 K initial temperature.



(a)

(b)

Fig. 5. Ignition delay time comparison between modeling without and with EC-DAC for *n*-heptane/air mixture ignition at (a) $\varphi = 0.5$, (b) $\varphi = 1.0$.

efficient to use a single threshold value to generate a dynamic mechanism which can satisfy a given error bound. It is also seen that the active species number does not change monotonically during the ignition process. Therefore, an error controlled dynamic mechanism reduction with a varying threshold value with the progress of fuel oxidation will dramatically improve the computation efficiency. Moreover, it is seen that the use of a constant threshold for dynamic model reduction will either have an unbound error in the reduced mechanism or lead to a large reduced mechanism when a very conservative small threshold is used.

Figure 4 shows the comparisons of the temperature, major species, and radical concentrations calculated with and without the EC-DAC algorithm (with detailed mechanism in the whole process) for homogeneous ignition of stoichiometric *n*-heptane/air and *n*-decane/air mixtures at 1 atm and 1200 K. It is seen that EC-DAC method reproduces well the results of the ODE solver for the large detailed kinetic mechanism in all predictions. The results further confirmed that the predicted error satisfied the condition of less than 1% relative error of mass fraction and temperature.

To demonstrate the robustness of the EC-DAC for both large detailed and comprehensively reduced mechanisms, the ignition processes of *n*-heptane/air and *n*-decane/air mixtures at different initial pressures, temperatures, and equivalence ratios are computed with and without EC-DAC. Figures 5 and 6 show the comparison of the dependence of ignition delay time on the initial temperature for *n*-heptane/air and *n*-decane/air mixtures at 1, 5 and 10 atmospheric pressures, 0.5 and 1.0 equivalence ratios, respectively. The maximum error is 5.5% in Fig. 5a, 6.2% in Fig. 5b, 7.7% in Fig. 6a and 7.4% in Fig. 6b. The excellent agreement of EC-DAC with the results calculated by the detailed mechanisms

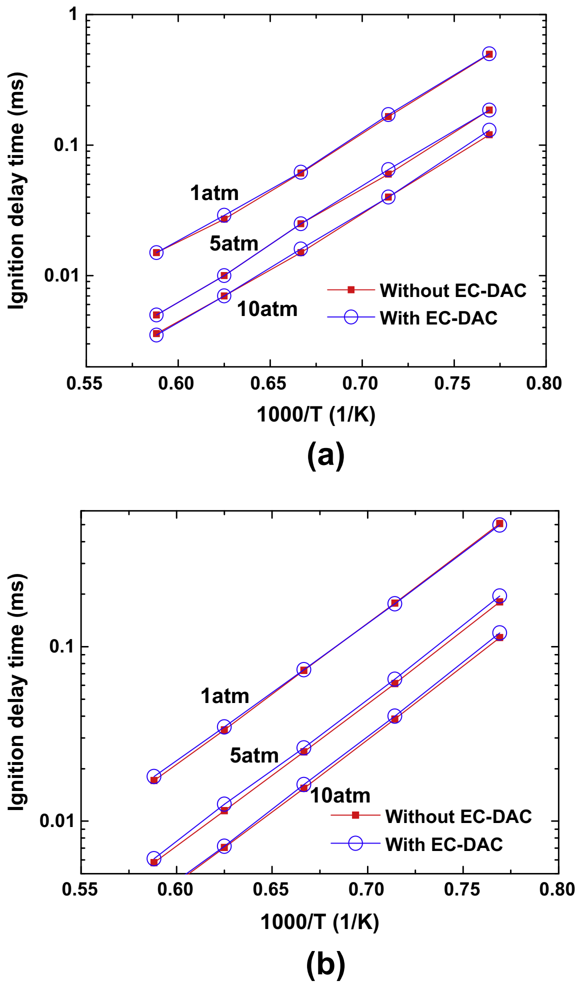


Fig. 6. Ignition delay time comparison between modeling without and with EC-DAC for *n*-decane/air mixture ignition at (a) $\varphi = 0.5$, (b) $\varphi = 1.0$.

demonstrates that EC-DAC is accurate enough to reproduce the ignition delay time in a broad temperature, pressure and equivalence ratio range.

Figures 7 and 8 show the comparison of the dependence of CPU time on temperature for the *n*-heptane/air and *n*-decane/air mixtures at 1, 5 and 10 atmospheric pressures, 0.5 and 1.0 equivalence ratios, respectively. It is seen that EC-DAC is much faster than the method without EC-DAC in a broad temperature, pressure and equivalence ratio range. Moreover, the results show that the efficiency of EC-DAC increases with the increase of the size of initial mechanism. For the cases in Figs. 7 and 8, the time step of 10^{-6} s is used. It is clear that the smaller computation time step, the more CPU time can be saved.

In order to apply the EC-DAC method to model unsteady flame propagation which involves diffusion, we integrated the EC-DAC method with the adaptive simulation of unsteady reactive flow (A-SURF) code [45,46]. A-SURF can simulate unsteady flame propagation with adaptive grids and detailed chemistry and has been successfully used in our previous studies on spherical flame initiation and propagation [2,22,45–47]. The details on the governing equations, numerical schemes, and code validation of A-SURF can be found in [45,46] and thus only a brief description will be given below.

The unsteady compressible Navier–Stokes equations for multi-component reactive flow are solved in A-SURF [45,46]. Multi-level grid refinement is used to resolve the reaction zone. The finite volume method is used to discretize the conservation governing equations in the spherical coordinate. The splitting fractional-step procedure is utilized to separate the integration of convection and diffusion transport from that of chemical reaction. In the first fractional step, the non-reactive flow is solved. The Runge–Kutta, MUSCL-Hancock, and central difference schemes, all of second-order accuracy, are employed for the temporal integration of convective flux, and diffusive flux, respectively. The chemical reaction is solved in the second fractional step using the EC-DAC method. The mass fractions of all species via convection and diffusion transport are updated in the first fraction step. However, in the section fraction step only the mass fractions of active species are updated and inactive species are not solved and their mass fractions remain unchanged. The activity of each species is determined by EC-DAC and the threshold for dynamic model reduction is determined by the reaction progress variable. Since most of the CPU time (above 90%) is spent on the second fractional step solving the dynamically reduced chemistry, the computation time can be greatly reduced using the dynamic adaptive chemistry method developed in this work.

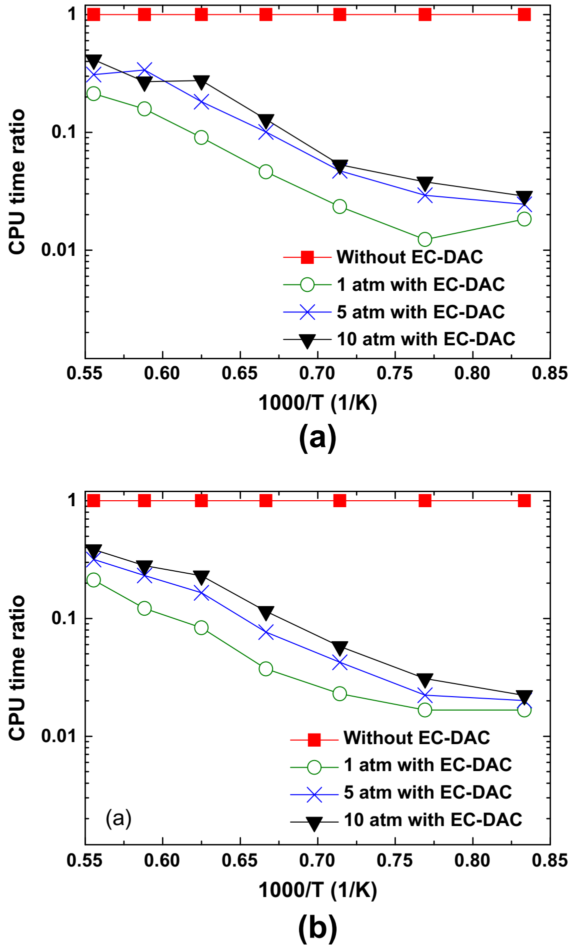


Fig. 7. CPU time comparison between modeling without and with EC-DAC for *n*-heptane/air mixture ignition at (a) $\varphi = 0.5$, (b) $\varphi = 1.0$.

The outwardly propagating spherical flames of static premixed *n*-heptane/air initially at 500 K and 1 atm are initiated at the center by a hot kernel of 1800 K with a radius of 1.5 mm. Figures 9 and 10 show the transient flame trajectories (the location of maximum heat release rate) and the distribution of selected parameters of stoichiometric *n*-heptane/air mixtures predicted by VODE solver with and without error-controlled dynamically adaptive method.

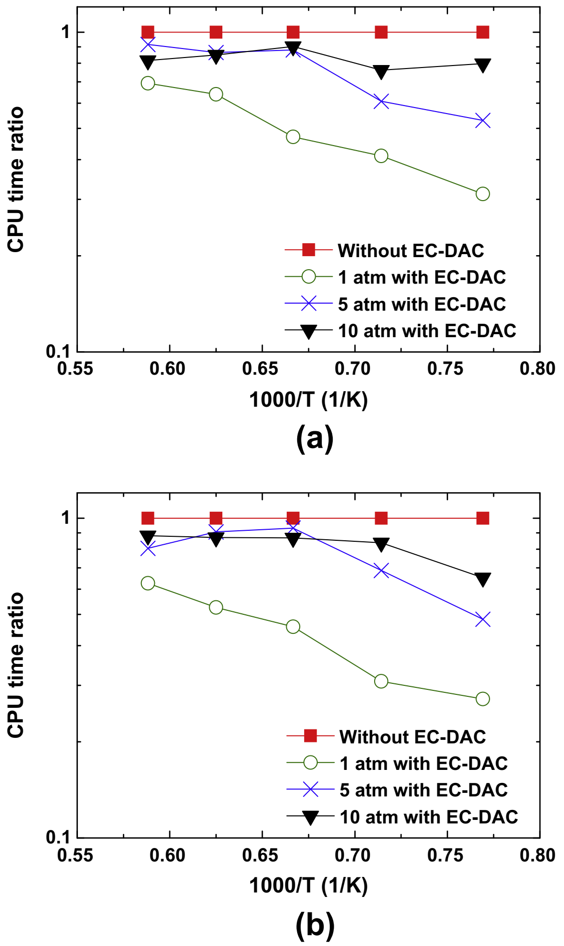


Fig. 8. CPU time comparison between modeling without and with EC-DAC for *n*-decane/air mixture ignition at (a) $\varphi = 0.5$, (b) $\varphi = 1.0$.

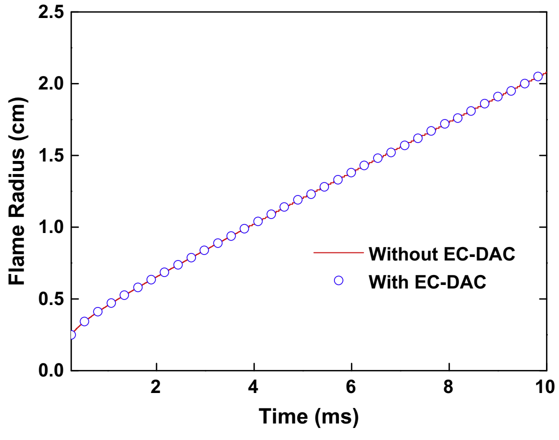


Fig. 9. Transient flame front location as a function of time for propagating spherical flames of stoichiometric *n*-heptane/air mixture.

The errors are below 5% (Fig. 9). The detailed mechanism [33,34] of 1034 species and 4236 reactions had been reduced by the PFA [22] method, and the obtained reduced mechanism of 128 species and 565 reactions was used in these calculations with and without the EC-DAC scheme. It is seen that the flame trajectories are almost the same, demonstrating that the accuracy can be maintained by using the EC-DAC method. Regarding to the computational efficiency, it is found that compared with the simulation with detailed mechanism, EC-DAC can save the CPU time considerably. Thus, a great computational efficiency is achieved for modeling transient flame propagation with the implementation of EC-DAC. This result implies that the EC-DAC method can be used directly in direct numerical simulation of reactive flow with detailed and reduced mechanism.

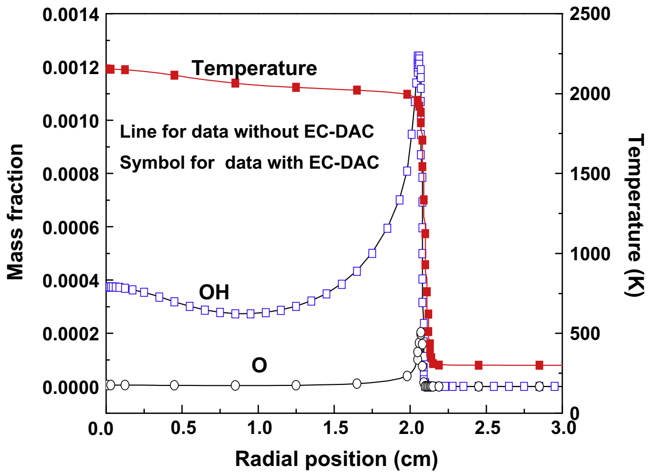


Fig. 10. Distributions of the temperature and mass fractions of OH and O for a propagating spherical flame of stoichiometric *n*-heptane/air mixture.

4. Conclusion

An error-controlled dynamic adaptive chemistry (EC-DAC) method is developed based on the path flux analysis model reduction method and a fuel oxidation progress index. The results show that the oxygen mass fraction is a good fuel oxidation progress variable to create a database which correlates the threshold value for the local mechanism reduction to the accuracy of the model at various combustion stages. Compared to the previous model reduction methods reported in the literature, one of the main advantages of the EC-DAC method is that the threshold is constrained by the pre-described error control parameter and thus is not arbitrarily specified. The results demonstrate that the EC-DAC method is accurate and can greatly improve the computational efficiency for both detailed and reduced kinetic mechanisms. Simulations of homogeneous ignition processes of *n*-heptane/air and *n*-decane/air mixtures at different initial conditions using the EC-DAC method demonstrated that the present algorithm of error-controlled dynamic adaptive chemistry scheme can improve computation efficiency by more than one-order for both mechanisms. Moreover, unsteady simulations of outwardly propagating spherical flames also demonstrate that the method is rigorous even when transport is included. Therefore, this method has a great potential to be used in the direct numerical simulation of reactive flow with detailed and reduced mechanisms.

Acknowledgments

X.L. Gou and Z. Chen were supported by National Natural Science Foundation of China (Grant Nos. 50976003 and 51276206) and Y. Ju would like to acknowledge the support of the research grant on multiscale modeling from the Army Research Office and the support of US Department of Energy, Office of Basic Energy Sciences as part of an Energy Frontier Research Center on Combustion with Grant No. DE-SC0001198.

References

[1] UDOE. 2007 Basic Energy Sciences Workshop, Basic Energy Needs for Clean and Efficient Combustion of 21st Century Transportation Fuels, 2007.
[2] X.L. Gou, W.T. Sun, Z. Chen, Y.G. Ju, Combust. Flame 157 (6) (2010) 1111–1121.
[3] M.S. Okino, M.L. Mavrovouniotis, Chem. Rev. 98 (2) (1998) 391–408.
[4] D.A. Goussis, Model reduction for combustion chemistry, in: T. Echekki, E. Mastorakos (Eds.), Turbulent Combustion Modeling, Springer, 2011.
[5] W.J. Pitz, C.J. Mueller, Prog. Energy Combust. Sci. 37 (3) (2011) 330–350.
[6] N. Peters, R.J. Kee, Combust. Flame 68 (1) (1987) 17–29.
[7] J.Y. Chen, Combust. Sci. Technol. 57 (1–3) (1988) 89–94.
[8] Y. Ju, T. Niioka, Combust. Flame 97 (3–4) (1994) 423–428.
[9] J.Y. Chen, Y.F. Tham, Combust. Flame 153 (4) (2008) 634–646.
[10] S.H. Lam, Combust. Sci. Technol. 89 (5–6) (1993) 375–404.
[11] A. Massias, D. Diamantis, E. Mastorakos, D.A. Goussis, Combust. Flame 117 (4) (1999) 685–708.
[12] T.F. Lu, Y.G. Ju, C.K. Law, Combust. Flame 126 (1–2) (2001) 445–1455.
[13] J. Prager, H.N. Najm, M. Valorani, D.A. Goussis, Proc. Combust. Inst. 32 (2009) 509–517.
[14] U. Maas, S.B. Pope, Combust. Flame 88 (3–4) (1992) 239–264.
[15] K. Konig, U. Maas, Proc. Combust. Inst. 32 (2009) 553–560.
[16] S.B. Pope, Combust. Theor. Model. 1 (1) (1997) 41–63.
[17] S.R. Tonse, N.W. Moriarty, M. Frenklach, N.J. Brown, Int. J. Chem. Kinet. 35 (9) (2003) 438–452.
[18] G.Y. Li, H. Rabitz, J.S. Hu, Z. Chen, Y.G. Ju, J. Math. Chem. 43 (3) (2008) 1207–1232.
[19] T. Turanyi, Comput. Chem. 18 (1) (1994) 45–54.
[20] T.F. Lu, C.K. Law, Proc. Combust. Inst. 30 (2005) 1333–1341.
[21] P. Pepiot-Desjardins, H. Pitsch, Combust. Flame 154 (1–2) (2008) 67–81.
[22] W.T. Sun, Z. Chen, X.L. Gou, Y.G. Ju, Combust. Flame 157 (7) (2010) 1298–1307.
[23] A.B. Bendtsen, P. Glarborg, K. Dam-Johansen, Comput. Chem. 25 (2) (2001) 161–170.
[24] L. Liang, J.G. Stevens, J.T. Farrell, Proc. Combust. Inst. 32 (2009) 527–534.
[25] L. Liang, J.G. Stevens, S. Raman, J.T. Farrell, Combust. Flame 156 (7) (2009) 1493–1502.
[26] I. Banerjee, M.G. Ierapetritou, Combust. Flame 144 (3) (2006) 619–633.
[27] O.O. Oluwole, B. Bhattacharjee, J.E. Tolsma, P.I. Barton, W.H. Green, Combust. Flame 146 (1–2) (2006) 348–365.
[28] X.L. Zheng, T.F. Lu, C.K. Law, Proc. Combust. Inst. 31 (2007) 367–375.
[29] K.E. Niemeyer, C.J. Sung, M.P. Raju, Combust. Flame 157 (9) (2010) 1760–1770.
[30] E.S. Blurock, M. Tuner, F. Mauss, Combust. Theor. Model. 14 (3) (2010) 295–313.
[31] O.O. Oluwole, Y. Shi, H.W. Wong, W.H. Green, Combust. Flame 159 (7) (2012) 2352–2362.
[32] T. Nagy, T. Turanyi, Combust. Flame 156 (2) (2009) 417–428.
[33] http://www-cms.llnl.gov/combustion/combustion_home.html.
[34] H.J. Curran, P. Gaffuri, W.J. Pitz, C.K. Westbrook, Combust. Flame 129 (3) (2002) 253–280.
[35] M. Chaos, A. Kazakov, Z.W. Zhao, F.L. Dryer, Int. J. Chem. Kinet. 39 (7) (2007) 399–414.
[36] P.N. Brown, G.D. Byrne, A.C. Hindmarsh, SIAM J. Sci. Stat. Comput 10 (5) (1989) 1038–1051.
[37] W. Sun, Z. Chen, X.L. Gou, Y.G. Ju, The 6th US National Combustion Meeting, Ann Arbor, Michigan, USA, 2009; paper 22FA.
[38] J.A. Van Oijen, F.A. Lammers, L.P.H. De Goey, Combust. Flame 127 (3) (2001) 2124–2134.
[39] J.A. Van Oijen, L.P.H. de Goey, Combust. Theor. Model. 8 (1) (2004) 141–163.
[40] R.K. Hanson, Proc. Combust. Inst. 33 (2011) 1–40.
[41] E.L. Petersen, D.F. Davidson, R.K. Hanson, Combust. Flame 117 (1–2) (1999) 272–290.
[42] M.P. Burke, M. Chaos, F.L. Dryer, Y.G. Ju, Combust. Flame 157 (4) (2010) 618–631.
[43] Z. Chen, Combust. Flame 158 (2) (2011) 291–300.
[44] A.P. Kelley, A.J. Smallbone, D.L. Zhu, C.K. Law, Proc. Combust. Inst. 33 (2011) 963–970.
[45] Z. Chen, M.P. Burke, Y.G. Ju, Proc. Combust. Inst. 32 (2009) 1253–1260.
[46] Z. Chen, Combust. Flame 157 (12) (2010) 2267–2276.
[47] H. Zhang, Z. Chen, Combust. Flame 158 (2011) 1520–1531.