A criterion based on computational singular perturbation for the construction of a reduced mechanism for dimethyl ether oxidation

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Abstract: A criterion based on the computational singular perturbation (CSP) method is proposed in order to determine the number of quasi-steady state (QSS) species. This criterion is employed for the reduction of a detailed chemical kinetics mechanism for the oxidation of dimethyl ether (DME), involving 55 species and 290 reactions, leading to a 20-step reduced mechanism that involves 26 species. A software package, named I-CSP, was developed to make the reduction process algorithmic. The input to the I-CSP includes: a) the detailed mechanism, b) the numerical solution of the problem for a specific set of operating conditions and c) the number of quasi steady state (QSS) species. The resulting reduced mechanism was validated both in homogenous reactor, including auto-ignition and a perfectly stirred reaction (PSR), over a wide range of pressures and equivalence ratios, and in a one-dimensional, unstretched, premixed, laminar steady DME/air flame. Comparison of the results calculated with the detailed and the reduced mechanisms shows excellent agreement in the case of a homogenous reactor, but discrepancies could be observed in the case of a premixed laminar flame.

Keyword: I-CSP; auto-ignition; perfectly stirred reaction; premixed flame; ignition delay; combustion.

INTRODUCTION

Dimethyl ether (DME) has drawn much attention because of its low emissions of nitrogen oxides (NO_x), reduction of engine noise, and high diesel thermal efficiency[1,2] and soot-free combustion.[3,4] However, making full use of its advantages or further improvement of these favorable results requires a thorough understanding of the underlying combustion chemistry. Simulations with detailed chemical kinetics are useful methods to explore combustion pro-

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cesses. However, even for the simplest fossil fuels, combustion simulation with detailed mechanisms still involves hundreds of species and thousands of reactions, which causes large amount of CPU times and low economic efficiency. The simulation is further complicated by the existence of highly reactive radicals, which induce significant rigidity to the governing equations due to the dramatic differences in the time scales of the species. Consequently, it is necessary to develop reduced mechanisms of a few detailed mechanisms.

Skeletal mechanisms are derived from detailed mechanisms by the removal of unimportant species and reactions. The methods that are used to develop skeletal mechanisms include sensitivity analysis performed by multiplying the rate constant of a reaction by a factor of 2 (both forward and reverse rate constants)[5] or by solving sensitivity equations, principal component analysis,[6] path flux analysis (PFA),[7] directed related graph (DRG),[8–10] and directed relation graph with error propagation (DRGEP)[11] methods, DRG-aided sensitivity analysis (DRGASA)[12] and DRGEP with sensitivity analysis (DRGEPSA).[13] The PFA method analyses the formation and consumption fluxes of each species for multiple reaction path generations and uses the fluxes to identify the important reaction pathways and the associated species. The DRG algorithm maps species to a graph and consequently identifies the species strongly coupled to the major species, thus solving successively strongly connected components (SCC) group by group. The DRG method uses absolute reaction rates, which makes the relation index not conservative (the interaction coefficient or relation index is the ratio of species flux). The DRGEP method which employs net reaction rates fails to identify all of the reaction paths when more than one intermediate species exist and to identify the relation between the species that have both fast production and consumption rates, such as species having catalytic effects.[7,14]

The skeletal mechanisms can be further reduced by time-scale reduction methods, which are based on the concept that fast time-scale species are in equilibrium state when related fast time-scale modes are exhausted and will result in algebraic relations of the species. Such methods include the partial-equilibrium approximation and the quasi-steady state approximation (QSSA),[15–21] intrinsic low-dimensional manifold (ILDM)[22,23], *in situ* adaptive tabulation (ISAT)[24,25] and computational singular perturbation (CSP).[26–31]

The CSP method using a programmable computational algorithm generates CSP data, such as radical pointer and fast reaction pointer, without the need of intuition and experience. The CSP data can then be used to identify quasi-steady state (QSS) species and fast reactions (using the fast reaction pointer) that are essential for the construction of reduced mechanisms. Valorani *et al.*[30] developed an automatic procedure based on CSP to generate skeletal mechanisms, which could replicate the dynamics of a user-specified set of species at sampling points. J. Prager *et al.*[32] used this method[30] to develop skeletal mechanisms for pre-

mixed *n*-heptane flames. A reduced mechanism can be called "global" if it is developed based on global QSS species that do not vary according to time and space.

Massias *et al.*[26] used a concentration-weighted CSP pointer to derive a 7-step reduced mechanism for CH_4/air that accounted for both thermal and prompt NO_x production. Lu *et al.*[33] extended the CSP method to complex eigensystems and employed a complex CSP to generate a 4-step and a 10-step reduced mechanism for the high-temperature oxidation of H_2/air and CH_4/air, respectively.

DME oxidation process contains both low and high temperature oxidation. Curran *et al.*[34] studied the low temperature oxidation of DME over the temperature range 550–850 K and formic acid was observed as the major intermediate. It was found that dimethyl ether exhibits a negative temperature coefficient (NTC) behavior. The high temperature oxidation of DME was studied by Fischer et al.[35.] It was found that the most important initiation reaction for the oxidation of dimethyl ether was its unimolecular decomposition to form methoxy and methyl radicals. Much emphasis has been placed on the development of a reduced mechanism for DME. Yamada *et al.*[36] developed a reduced mechanism consisting of 23 species and 23 reactions by extracting essential elementary reactions from the detailed mechanism of DME. Chin *et al.*[37] constructed a 28-species reduced mechanism for DME combustion using the QSSA method based on the detailed mechanism given by Zhao *et al.*[38] Ryu *et al.*[39] deduced a 44-species and 166-reaction reduced mechanism for DME from a detailed 79-species and 351-reaction mechanism using sensitivity analysis.

In this manuscript, a criterion based on computational singular perturbation is presented and applied to the detailed mechanism for DME oxidation given by Zhao *et al.*[38] for the construction of a 20-step reduced mechanism.

METHODOLOGIES

A thorough description of the CSP method may be found in the literature.[27,28,40] Herein, an overview of the CSP method is given. A general chemical reaction system that contains *R* elementary chemical reactions and *N* species can be expressed as:

$$g(y) \equiv \frac{dy}{dt} = \mathbf{S}F(y) \tag{1}$$

where *y* is the $N \times 1$ concentration vector of all the species, **S** the $N \times R$ stoichiometric coefficients matrix and $F(y)$ is the $R \times 1$ species production rates vector of the elementary reactions. By taking the time derivative of Eq. (1), one obtains:

$$\frac{dg}{dt} = \mathbf{J}g \tag{2}$$

where:

$$\mathbf{J} = \frac{\partial g}{\partial y} \tag{3}$$

is the time-dependent Jacobian matrix. $\mathbf{J}$ depends only on the state of reaction system at every time step. By undertaking eigen-decomposition of the matrix $\mathbf{J}$, $\mathbf{J}$ can be decomposed as:

$$\mathbf{J} = \mathbf{A}\boldsymbol{\Lambda}\mathbf{B} \tag{4}$$

where $\mathbf{A}$ is the matrix of the basis vectors and $\mathbf{B}$ is the inverse matrix of $\mathbf{A}$. If an ideal base vector $\mathbf{A}$ (eigenvectors) exists, then $\boldsymbol{\Lambda}$ reduces to a diagonal matrix and its diagonal elements are the eigenvalues of $\mathbf{J}$. Supposing there are M fast modes and that $\mathbf{A}_m$ and $\mathbf{B}^m$ correspond to the $N{\times}M$ and the $M{\times}N$ fast base matrix, respectively, then the matrix:

$$\mathbf{Q}_m \equiv \mathbf{A}_m\mathbf{B}^m \tag{5}$$

is called the fast projection matrix. The diagonal elements of $\mathbf{Q}_m$:

$$D = \mathrm{diag}\big[\mathbf{Q}_m\big] \tag{6}$$

are radical pointers that identify the locally optimal QSS species, where D is an N-dimensional vector. A larger diagonal element suggests a better CSP radical candidate, namely a QSS specie.

By defining the participation and importance index as:[30]

$$P_r^i \equiv \frac{b^i s_r F^r}{\displaystyle\sum_{r=1}^{R}\big|b^i s_r F^r\big|}, \quad i = 1,\ 2,\ ...,\ M,\ \ r = 1,\ 2,\ ...,\ R \tag{7}$$

$$I_r^i \equiv \frac{s_r^i F^r}{\displaystyle\sum_{r=1}^{R}\big|s_r^i F^r\big|}, \quad i = 1,\ 2,\ ...,\ M,\ \ r = 1,\ 2,\ ...,\ R \tag{8}$$

where P_r^i and I_r^i are the participation index and importance index, b^i is the i-th row vector in B^m, s_r (column vector) is the stoichiometric vector of the r-th reaction, F^r the reaction rate of the r-th reaction and s_r^i is the i-th element of the stoichiometric vector of the r-th reaction, one can estimate: a) where the major cancellations occur and b) the contribution of each step in the production of the i-th species. The fast reactions for each QSS species can be identified by the importance index. The largest I_r^i in the i-th row means the r-th reaction is the fast reaction for the i-th specie.

Massias $et\ al.$[26] used the following algorithm to integrate the radical pointers through the computational domain:

$$I^i \equiv \frac{1}{L}\int_0^L D^i \frac{1}{X^i + \varepsilon_1} \frac{q^i}{q_{\max}^i + \varepsilon_2}\,\mathrm{d}x. \tag{9}$$

where D^i is the i-th radical pointer in D, X^i the i-th species concentration, q^i the net production rate of the i-th species, $q_{\max}^i$ is the maximum production rate for the i-th species throughout the computational domain D, ε_1 and ε_2 are small positive numbers that are used to avoid numerical problems when X^i and $q_{\max}^i$ equal zero. The values of ε_1 and ε_2 must be chosen with care. Their order must be much lower than X^i and $q_{\max}^i$ so that their influence to I^i can be neglected.

For transient reaction systems:

$$I^i \equiv \frac{1}{T}\int_0^L D^i \frac{1}{X^i + \varepsilon_1} \frac{q^i}{q_{\max}^i + \varepsilon_2}\,\mathrm{d}t \tag{10}$$

To apply the CSP method, a prior *M* needs to be determined. A possible way to realize this is to calculate the errors between the detailed and the reduced mechanisms and then choose *M* with the specified error. Considering the importance of ignition delay in a closed homogenous reaction system, it is chosen as the target variable of which the errors are calculated.

The following discussion is based in the context of developing a reduced mechanism for DME, which consists of 55 species and 290 reactions.[38] The results of the ignition delay with respect to M in a closed homogeneous transient reactor (constant pressure and variable volume), is shown in Fig. 1. As can be seen, the errors become larger with increasing *M*. Numerical difficulties occur when *M* increases to a certain number. In this manuscript, the specified error for ignition delay will be chosen as 5 %. Consequently, the number of QSS species *M* will be 29 and non-QSS species will be 26. The steps of the reduced mechanism will be 20 as there are 6 elements.[26]
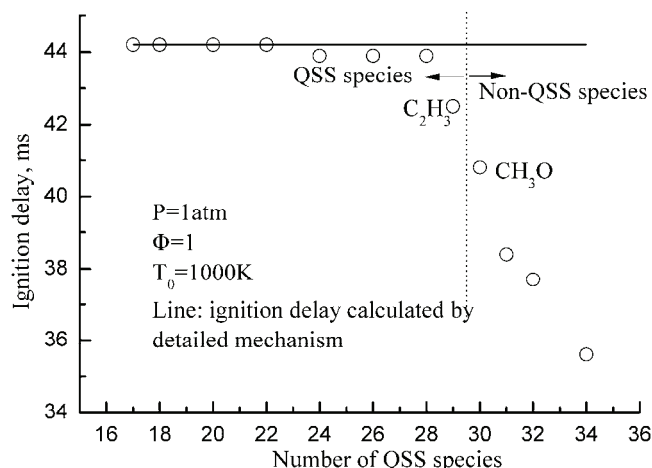

Fig. 1. Errors in the calculation of the ignition delay as a function of number of QSS species.

Radical pointers were calculated with Eq. (10). The 29 species with largest integrated radical pointers are considered as QSS species and the remaining 26 species are non-QSS species (in the same order as appearing in the detailed mechanism): H_2, CH_2, $CH_2(S)$, CH_3, CH_4, OH, H_2O, CH_2O, C_2H_6, CH_3O, O_2, CH_3OH, HO_2, H_2O_2, CH_2HCO, CO_2, $OCHO$, $HCOOH$, CH_3OCH_3, CH_3OCHO, H, O, CO, N_2, Ar and He.

The fast reactions can be determined by Eqs. (7) and (8). These two equations reflect the contribution of each reaction to the production of QSS species:

$$\frac{d[C_2H_5]}{dt} = s_{94}^{13}F^{94} + s_{105}^{13}F^{105} + s_{117}^{13}F^{117} + s_{238}^{13}F^{238} + s_{109}^{13}F^{109} + s_{111}^{13}F^{111} + s_{103}^{13}F^{103} +$$
$$+ s_{115}^{13}F^{112} = -0.268204 + 0.19623 + 0.15421 - 0.141398 - 0.052505 - \qquad (11)$$
$$-0.047145 + 0.044899 - -0.028644 - 0.018679 + 0.016272$$

$$\frac{d[HCCO]}{dt} = s_{143}^{22}F^{143} + s_{149}^{22}F^{149} + s_{145}^{22}F^{145} + s_{135}^{22}F^{135} + s_{144}^{22}F^{144} + s_{146}^{22}F^{146} = \qquad (12)$$
$$= -0.327922 - 0.195474 - 0.152123 + 0.14655 - 0.114665 - 0.027255$$

$$\frac{\mathrm{d}[CH_3HCO]}{\mathrm{d}t} = s_{174}^{28}F^{174} + s_{115}^{28}F^{115} + s_{220}^{28}F^{220} + s_{176}^{28}F^{176} + s_{181}^{28}F^{181} + s_{180}^{28}F^{180} = \tag{13}$$
$$= -0.642532 + 0.122233 + 0.080127 - 0.077731 - 0.032477 - 0.015273$$

where d[C]/dt is the derivative of the concentration of species C over time, s_k^i is the stoichiometric coefficient of i-th specie in the k-th reaction, F^k the reaction rate of the k-th reaction. The first item on the right side of equal mark in Eq. (11) refers to the contribution of the 94-th reaction to the consumption of C_2H_5. The number below is the specific value that is calculated by Eqs. (7) and (8). Sufficient terms are kept so that the total error of the omitted terms is below a user-defined error criterion. It can be seen from Eq. (13) that the 174th reaction contributes the most to the destruction of CH_3HCO, it is therefore deemed a fast reaction for CH_3HCO. By the same method, the fast reactions for the 29 QSS species could be calculated, as shown in Table I.

TABLE I. 29 QSS species and the corresponding fast reactions

QSS species	Fast reactions	QSS species	Fast reactions	QSS species	Fast reactions
CH_3OCH_2OH	267	$CH_3OCH_2O_2$	264	C_2H	152
HO_2CH_2OCHO	274	CH_3OCO	261	CH_3HCO	174
$O_2CH_2OCH_2O_2H$	273	$HCCOH$	139	HCO	31
$CH_3OCH_2O_2H$	268	$HOCH_2O$	280	C_2H_4	117
OCH_2OCHO	276	C_2H_5OH	203	C_2H_2	126
CH_3OCH_2O	251	CH_3OCH_2	240	CH_2OH	64
$HOC_2H_4O_2$	235	CH_3CO	176	C_2H_5	94
$CH_2OCH_2O_2H$	272	C_2H_4OH	237	$HCCO$	143
CH_3CHOH	227	CH_3CH_2O	238	C_2H_3	131
$HOCH_2OCO$	277	CH_2CO	127		

The reduced mechanism could be constructed after the QSS species and fast reactions had been determined. In order to make the process more efficient, a software package called Integral CSP (I-CSP) was developed. The I-CSP is written in C++ language and uses the interface functions provided by CHEMKIN-PRO[43] to read the reaction solutions generated in Chemkin. The I-CSP first reads temperatures, heat release rates and species concentrations and then calculates the Jacobian matrix and generates radical pointers and fast reaction pointers automatically. The outputs of the program contain three files. The first is the copied file with file extension asc. The second is a .inp file containing all elements, species and reduced mechanism. The third is a .dat file containing a (N–M–E)×(R–M) dimension matrix, which indicates the reaction rate of each step. Finally, the I-CSP uses the method developed by Goussis[42] to construct a reduced mechanism compatible with Chemkin and is convenient for validation, which is the content of next part of this manuscript.

RESULTS AND VALIDATION

A reduced mechanism that consists of 26 species and 20 steps was constructed with the help of I-CSP. The 20-step reduced mechanism was first validated over a closed homogeneous transient reactor with the same conditions as the reduced mechanisms being conducted. The results of the ignition delay over a wide range of equivalence ratios and with three different pressures, calculated with the detailed and the 20-step reduced mechanisms are shown in Fig. 2.

Excellent agreements can be observed, which demonstrate the high accuracy of the reduced mechanism in predicting ignition delay. Results calculated with the detailed and the reduced mechanisms under various initial temperatures, pressures, and equivalence ratios in auto-ignition are shown in Fig. 3. It can be seen that the results calculated with the reduced mechanism are quite consistent with those calculated with the detailed mechanism.
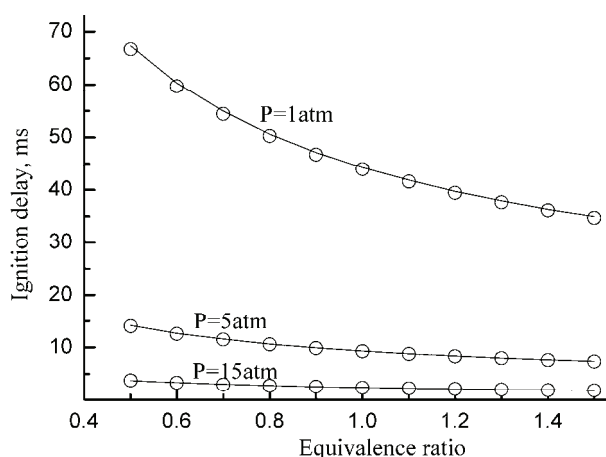

Fig. 2. Ignition delay as a function of equivalence ratio, in a constant pressure auto-ignition process, calculated for both the detailed and the reduced mechanisms.

To demonstrate further the ability of the reduced mechanism in predicting species concentrations, the results of calculation in a constant pressure auto-ignition reactor are displayed in Fig. 4 and no discrepancy could be found. The results of the calculation of temperature in a perfectly stirred reactor (PSR) over a wide range of equivalence ratios and pressures are shown in Fig. 5 and excellent agreements were found. The results of the variations of the mole fractions of H_2, O_2, H_2O in a PSR, calculated with the detailed and the 20-step reduced mechanisms, are presented in Fig. 6. Good agreements were observed therefore demonstrating the ability of the 20-step reduced mechanism in predicting the species concentrations in a PSR.

In order to demonstrate the validity of the reduced mechanism in predicting the profiles of the species in a premixed flame, the mole fractions of five species calculated in a steady, one-dimensional, burner-stabilized freely propagating premixed laminar flame are presented in Fig, 7. Obvious discrepancies could be observed for O_2 and H. Small discrepancies could be found for H_2 and CO. From Fig. 7, it could be learnt that the 20-step reduced mechanism shows limited accuracy in the prediction of species profiles in a freely propagating premixed laminar flame.

In this section, the reduced mechanism was validated over several reactors. Excellent agreements could be found in a homogenous reactor, such as auto-

ignition and PSR. However, in an inhomogeneous reactor, the reduced mechanism exhibited limited accuracy.
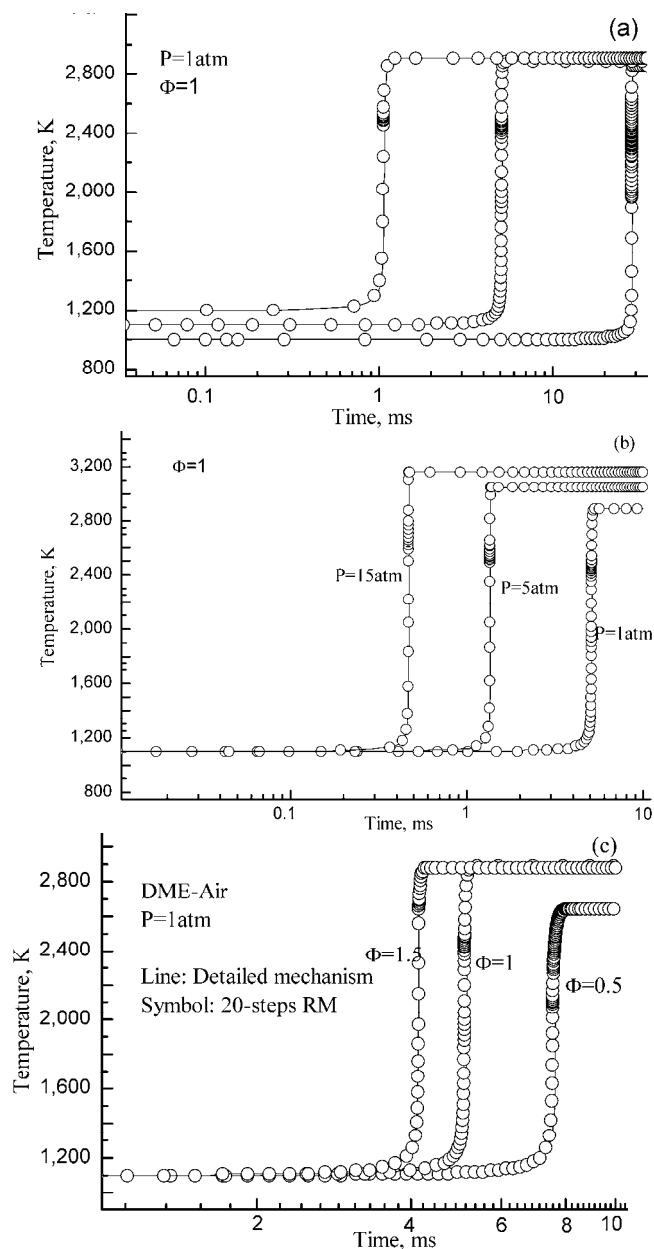

Fig. 3. Comparison of the temperature profiles in auto-ignition, calculated with the detailed and the reduced mechanisms under various a) initial temperatures, b) pressures and c) equivalence ratios.
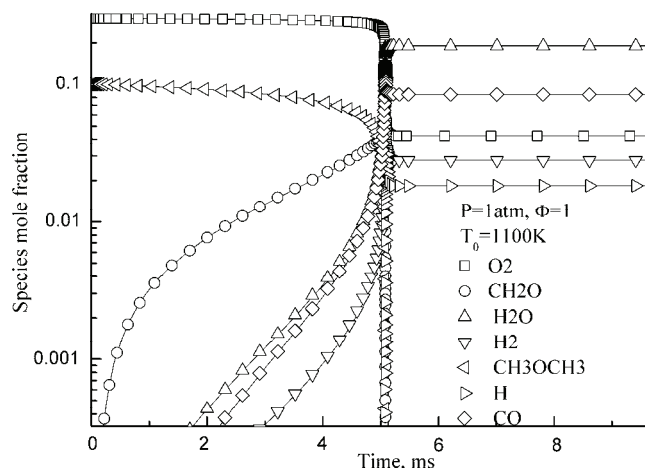
Fig. 4. Comparison of the mass fractions of the species in a constant pressure auto-ignition process, calculated with the detailed (lines) and the reduced (symbols) mechanisms.
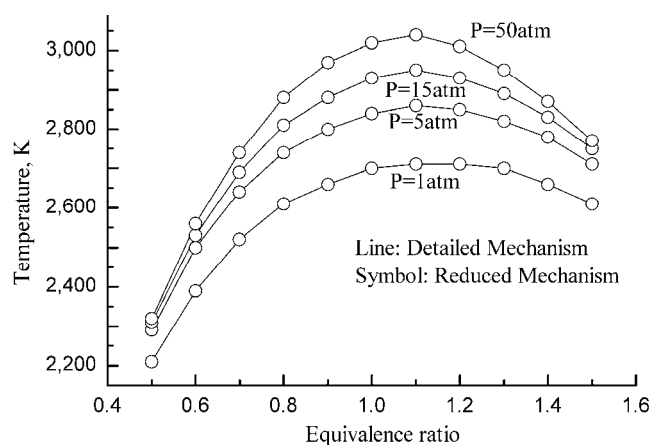

Fig. 5. Comparison of the temperature in a PSR, at 4 different pressures, calculated with the detailed and the reduced mechanisms.

CONCLUSIONS

In the present study, a criterion for determining the number of QSS species *M* was presented. A software package named Integral CSP (I-CSP) was developed to construct the reduced mechanism. The input to I-CSP includes the detailed mechanism, the numerical solution of the problem on a specific set of operating conditions, under which the reduced mechanism is expected to be valid, and the number of QSS species. The I-CSP can be obtained by mailing to: zuozhuwu@gmail.com. The output of I-CSP is three files that describe the reduced mechanism and the numerical relations between the QSS species and

non-QSS species. These files are compatible with Chemkin, which makes the validation of the reduced mechanism easier.
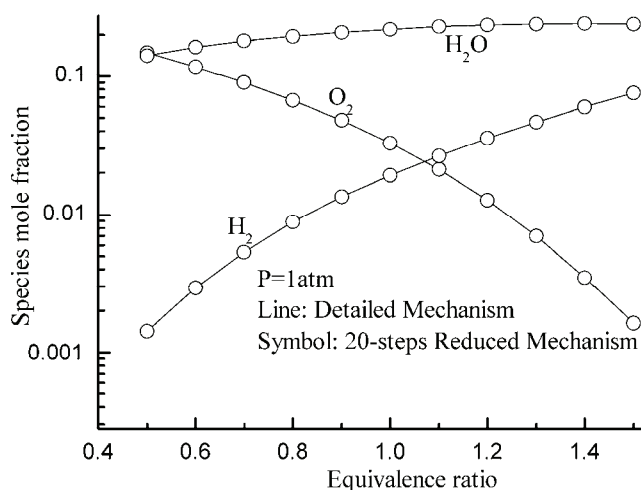

Fig. 6. Comparison of mole fraction of the species H_2, O_2, H_2O in a PSR, calculated with the detailed and the reduced mechanisms.
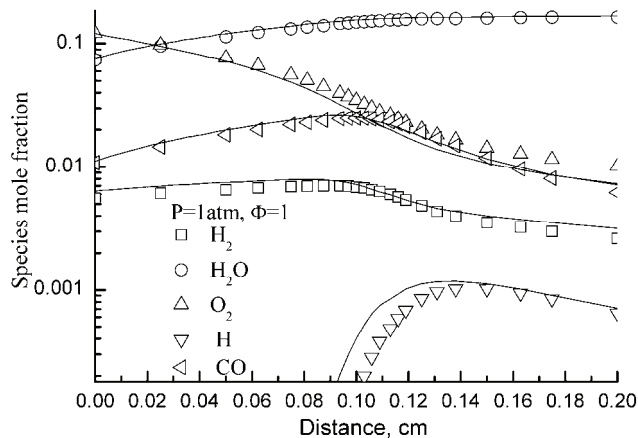

Fig. 7. Comparison of the mole fractions of species in a freely propagating premixed laminar flame, calculated with the detailed (lines) and the reduced (symbols) mechanisms.

To construct global reduced mechanism, the following four steps need to be performed. First, the QSS species require to be identified with the help of the CSP-pointer. These species will not appear in the reduced mechanism and their concentrations are calculated by the non-QSS species. Second, fast elementary reactions need to be determined. Reactions consuming most QSS species are deemed as "fast". The fast reactions must be unique which means that one reac-

tion cannot be chosen twice as a fast reaction. The third step is the construction of global reduced mechanism. The purpose of the final step, which is called "simplification" or "truncation", is to enable faster computation of the solution to problems where the reduced mechanism is implemented. The "simplification" or "truncation" is realized with the help of an importance index and a participation index.

The I-CSP was implemented over auto-ignition calculation with DME and conducted using a 20-step reduced mechanism. The reduced mechanism was validated first in a homogenous reactor including auto-ignition and PSR over a wide range of equivalence ratios and pressures, and then in a steady, one-dimensional, burner-stabilized freely propagating premixed laminar flame. Good agreements were observed therefore demonstrating the validity of the reduced mechanism, especially in homogenous reactors.

ИЗВОД

КРИТЕРИЈУМ ЗАСНОВАН НА РАЧУНСКОЈ СИНГУЛАРНОЈ ПЕРТУБАЦИЈИ ЗА ОДРЕЂИВАЊЕ РЕДУКОВАНОГ МЕХАНИЗМА ОКСИДАЦИЈЕ ДИМЕТИЛ-ЕТРА

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Предложен је критеријум заснован на методу рачунске сингуларне пертурбације за одређивање броја квази-равнотежних врста. Овај критеријум је коришћен за редукцију детаљног кинетичког механизма за оксидацију диметил-етра (ДМЕ), који укључује 55 врста и 290 реакција, а који доводи до редукованог механизма од 20 корака који укључује 26 врста. Софтверски пакет I-CSP је развијен да би редукциони процес постао алгоритмичан. Улазни подаци за I-CSP укључују: 1) детаљни механизам, 2) нумеричко решење проблема за одређени скуп радних услова и 3) број квази равнотежних врста. Добијени редуковани механизам је проверен у хомогеном реактору са аутоматским паљењем и савршеним мешањем у широком опсегу притисака и еквивалентних односа, и такође у једнодимензионалном, неиздуженом, помешаном, ламинарном, равнотежном DME/ваздух пламену. Поређење резултата добијених са детаљним и редукованим механизмом показује одлично слагање у случају хомогеног реактора док се одступања примећују у случају помешаног ламинарног пламена.

(Примљено 22. новембра 2012, ревидирано 9. фебруара 2013)

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