Development and validation of a reduced mechanism for methane using a new integral algorithm in a premixed flame

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Abstract

A new algorithm based on Computational Singular Perturbation (CSP) is proposed to construct global reduced mechanism. The algorithm introduces species' concentrations, species' net production rates and heat release rates as integral weighting factors to integrate CSP-pointers, including radical pointers and fast reaction pointers, throughout the computational domain. A software package based on the algorithm was developed to make the reduction process more efficient. Input to the algorithm includes: i) the detailed mechanism, ii) the numerical solution of the problem for a specific set of operating conditions and iii) the number of quasi steady state (QSS) species. The proposed algorithm was applied to the reduction of GRI3.0 involving 53 species and 325 reactions leading to the development of a 15-species reduced mechanism with 10 lumped steps. Then the reduced mechanism was validated in a one-dimensional, unstretched, premixed, laminar steady flame over a wide range of equivalence ratio, and excellent agreements between results calculated with the detailed and the reduced mechanisms can be observed.

Keywords: mechanism reduction, CSP, integral-CSP algorithm, GRI3.0.

Simulation with chemical kinetic mechanisms plays an increasingly important role in both combustion design and scientific discoveries. 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 stiffness to the governing equations due to the dramatic differences in the time scales of the species. Consequently, it is necessary to develop reduced mechanisms with fewer variables and moderated stiffness from the detailed mechanisms, while maintaining the accuracy and comprehensiveness of the detailed mechanisms.

There have been various mechanism reduction methods developed to generate reduced mechanisms. Skeletal reduction techniques, including sensitivity analysis performed by multiplying the rate constant of a reaction by a factor of 2 (both forward and reverse rate constants) [1] or by solving the sensitivity equations, principal component analysis [2], path flux analysis (PFA) [3], directed related graph (DRG) [4–6], directed relation graph method with error propagation (DRGEP) [7], the DRG-aided sensitivity analysis (DRGASA) [8], and DRGEP with sensitivity analysis (DRGEPSA) [9] are used to develop skeletal mechanisms by eliminating unimportant species and reactions while introducing acceptable errors which can be controlled by self-defined threshold value. The PFA method analyses the formation and consumption fluxes of each species at 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 strongly connected components (SCC) group by group successively. 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 pick up all of the reaction path when more than one intermediate species exist and to identify the relation between the species that have both fast production and consumption rate, such as species having catalytic effect [3,10].

Skeletal mechanisms obtained only by removing redundant species and reactions are still stiff and contain some important radicals with short time scales which cannot be eliminated. The most acceptable approach to resolve the stiffness is further reducing the skeletal mechanisms by reasonable assumption, such as partial-equilibrium approximation and quasi-steady state approximation (QSSA) [11–17]. The partial-equilibrium approximation assumes that some reactions are partial-equilibrium and the forward and reverse reac-
tion rates are equal [18], and therefore the net production rates are approximate zero. The quasi-steady state approximation is based on the assumption that the species are in quasi-steady and their net production rates are zero. The partial-equilibrium approximation and the quasi-steady state approximation are effective ways in reducing the stiffness of reaction systems. However, they are based on the local (in time and space) conditions, which means the species may become non-QSS species in a different condition. Consequently the resulting reduced mechanisms got by the partial-equilibrium approximation and the quasi-steady state approximation do not always provide best accuracy. To resolve such problems, wide range of conditions (in time and space) in which the derived reduced mechanisms may be applied have to be taken into account, which will make the reduction process more complicated and limit the range of application of the reduced mechanisms. The computational singular perturbation (CSP) [19–24] method using a programmable computational algorithm generates time-resolved simplified models without the need of intuition and experiences. CSP data, such as radical pointer and fast reaction pointer, can be acquired by decoupling and analyzing the Jacobian matrix depending only on the state of a reaction system. The QSS species and fast reactions can be identified by analyzing the CSP data. Reduced mechanisms can be acquired by eliminating the QSS species whose concentrations are calculated by non-QSS species. A reduced mechanism can be called "global" if it is developed and based on global QSS species which do not vary according to time and space.

Lu [25] used the user specified error tolerance to distinguish the quasi steady state (QSS) species from non-QSS species for methane–air mixtures sampled from PSR and auto-ignition, and deduced a 15-steps reduced mechanism. Belcadi [26] derived a 10-steps reduced mechanism from a complex detailed chemical kinetics mechanism consisting of 279 reactions and 49 species. The PSR reactor used in Lu [25] is easy to handle, but provide no information about the changes of the state of reaction system (species concentrations, temperature, etc.) over time and space. Reduced mechanisms deduced in such reactor may not provide satisfied simulation results in transient or in spatial inhomogeneous reactors. Massiasa [19] applied the CSP method to a laminar premixed CH$_4$/air flame and derived a 7-step reduced mechanism from a complex detailed chemical kinetics mechanism consisting of 279 reactions and 49 species. The PSR reactor used in Lu [25] is easy to handle, but provide no information about the changes of the state of reaction system (species concentrations, temperature, etc.) over time and space. Reduced mechanisms deduced in such reactor may not provide satisfied simulation results in transient or in spatial inhomogeneous reactors. Massiasa [19] integrated the radical pointers with species' concentrations and species' production rates as weighting factors in reducing the stiffness of reaction systems. This is reasonable for species with small concentrations or large production rates which yield large radical pointers, and will be deemed as QSS species. The integrated radical pointers are better for choosing QSS species, but are prone to neglect some domains where species' concentrations are relatively too large or species' production rates are too small. Such domains make little contribution to the final integrated radical pointers, thus causing these domains being neglected. Such problem is called "neglecting" problem.

Heat release rate is a critical parameter in evaluating the intensity of a reaction system. Domains with higher heat release rate mean intensive chemical process and should be placed more emphasis on. Adding heat release rate to weighting factors in the process of integrating radical pointers and fast reaction pointers can reflect the importance of each computational domain and is a good way to relieve the "neglecting" problem. In this article, the emphasis is on changing the integrands and weighting factors in integrating process to get reasonable QSS species and fast reactions.

The structure of the manuscript is as follows. First, a brief outline of the CSP method shall be introduced. Then, the new integral CSP algorithm shall be presented and shall be applied over GRI3.0 to develop global reduced mechanism. Finally, the obtained global reduced mechanism shall be validated in a one-dimensional, unstretched, premixed, laminar steady flame over a wide range of equivalence ratio.

**METHODOLOGIES**

**Outline of the CSP method**

A thorough description of the CSP method may be found in [20,21,28]. Here, an overview of the CSP method will be given. A general chemical reaction system which contains $R$ elementary chemical reactions and $N$ species can be expressed as:

$$g(y) = \frac{dy}{dt} = SF(y)$$

(1)

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

$$\frac{dg}{dt} = Jg$$

(2)

where

$$J = \frac{dg}{dy}$$

(3)
is the time-dependent Jacobian matrix. J depends only on the state of reaction system at every time step. By undertaking eigendecomposition of the matrix J, J can be decomposed as:

\[ J = A A^T \]

(4)

where A is the matrix of basis vectors and B the inverse matrix of A. If ideal base vector A (eigenvectors) exists, then \( \Lambda \) reduces to a diagonal matrix and its diagonal elements are the eigenvalues of intersect. The biggest eigenvalue to directly integrate the radical pointers on a one-dimensional, unstretched, premixed, laminar steady CH₄/air flame, the \( I_r \) method produced poor results. The reactant CH₄ was identified as QSS species, which is obviously absurd.

A better integral algorithm is to involve species concentrations and species production rates [19]:

\[ I_r' = \frac{1}{A} \int_{L}^{L} D' dx \]

(9)

For transient reaction systems:

\[ I_r' = \frac{1}{T} \int_{0}^{T} D' dt \]

(10)

where \( D' \) is the \( i \)-th radical pointer in \( D \), \( X' \) the \( i \)-th species' production rate, \( q' \) the net production rate of \( i \)-th species, \( q_{max} \) the maximum production rate for \( i \)-th species throughout the computational domain \( D \), \( \epsilon_1 \) and \( \epsilon_2 \) are small positive numbers which are used to avoid numerical problems when \( X' \) and \( q_{max} \) equal zero. \( \epsilon_1 \) and \( \epsilon_2 \) must be chosen with care. Their order must be much lower than \( X' \) and \( q_{max} \) so that their influence to \( I_r' \) can be neglected. By adding species' concentrations and species' production rates as weighting factors in the integral algorithm, the resulting QSS species turn out to be more reasonable [19]. This is consistent with the fact that species with small concentrations and fast production rates, which result in larger \( I_r' \), are prone to be deemed as candidates for QSS species.

The method expressed by Eqs. (11) and (12) can give reasonable results. However, to relieve the “neglecting” problem, a better algorithm shall be presented next.

Let \( R_n^i \) denote integrand for the \( i \)-th species in the \( n \)-th computational domain (representing \( n \)-th physical space domain in spatial inhomogeneous reactors or \( n \)-th time step in transient reactors):
where $D_i^r$ is the original radical pointer, $X_i^r$ and $q_i^r$ the specie concentration and the net production rate of $i$-th specie in the $n$-th computational domain, respectively. Equation (13) has similar form as Eq. (11) and (12). The percentage of $i$-th specie of the summation of all radical pointers in the $n$-th computational domain define as:

$$W_{i, n} = \frac{R_{i, n}}{R_{i, \text{sum}, n}}$$

(14)

where $R_{i, \text{sum}, n}$ is the summation of all radical pointers in the $n$-th computational domain. With the definition of $W_{i, n}$, we can define a new algorithm:

$$I_3 = \frac{1}{L} \int_0^L W_i^r \, dx$$

(15)

For transient reaction systems:

$$I_3 = \frac{1}{T} \int_0^T W_i^r \, dt$$

(16)

By adding heat release rates to Eq. (14), we get:

$$H_i^n = \frac{R_{i, n}}{R_{i, \text{sum}, n}} - h_n$$

(17)

where $h_n$ is the heat release rate in the $n$-th computational domain. By integrating Eq. (17), we obtain:

$$I_4 = \frac{1}{L} \int_0^L H_i^n \, dx$$

(18)

For transient reaction systems:

$$I_4 = \frac{1}{T} \int_0^T H_i^n \, dt$$

(19)

In this section, two new radical integral algorithms, $I_3$ and $I_4$, have been proposed. The global QSS species can be identified once the global radical pointers have been determined. Fast reactions corresponding to each QSS species can be determined using Eq. (8). The global reduced mechanisms can be constructed after the QSS species and fast reactions being found out [13, 18–20]. The global reduced mechanisms can be further reduced by using participation index and importance index with user-defined error criterion, which is called “simplification” or “truncation”.

To construct a global reduced mechanism, the number of QSS species $M$ which used to determine the steps of global reduced mechanism (N–M–E), the M QSS species and M fast reactions need to be known. The above method for producing these data will be discussed next in the context of a laminar premixed CH$_4$/air flame.

**Identification of QSS species and fast reactions**

To construct global reduced mechanism over a specific problem, the number of QSS species $M$ need to be determined in advance. However no algorithmic method exists for obtaining a prior $M$. A possible way is to sort the magnitude of integral radical pointers in descending order and then choose the first $M$ species as QSS species, and the remaining N–M species as non-QSS species. Verify the $M$ QSS species until the results is satisfied. If not, change $M$ and iterate the above process. A good human intuition and experience would be helpful for this choosing procedure.

In the following discussion, we shall begin with GRI3.0 which contains 325 reactions, 53 species and 5 elements to develop a global reduced mechanism. A one-dimensional, unstretched, premixed, laminar steady CH$_4$/air flame shall be the problem under study. The equivalence ratio is 1.0 and the pressure is 1 atm. It is presumed that there are 15 non-QSS species, which means the number of QSS species is 38 and 10-steps reduced mechanism. Table 1 shows the twenty species with the smallest integral radical pointer in descending order, calculated with $I_3$ and $I_4$, respectively. The $I_3$ method which excludes Ar (inert specie) as non-QSS species leads to unrealistic results. The $I_4$ and $I_4$ method produce almost the same results except for the order of the non-QSS species. The $I_4$ method contains two different non-QSS species (including CH$_3$CO and C$_2$H$_3$) compared with the $I_3$ and $I_4$ method (including HO$_2$ and CH$_3$O). In this manuscript, the $I_4$ method will be adopted to identify the global non-QSS species.

**Table 1**

By analyzing with the $I_4$, the following 15 species are deemed as non-QSS species: HO$_2$, CH$_3$O, H, NO, O, OH, CH$_4$, CO, H$_2$, CO$_2$, H$_2$O, N$_2$O, O$_2$, N$_2$, Ar and the remaining 38 species will be identified as QSS species.

Fast reactions for each QSS species can be found by integrating importance index in Eq. (8):

$$F_i^r = \frac{1}{T} \int_0^T I_i^r h_n \, dt$$

(20)

For transient reaction systems:

$$F_i^r = \frac{1}{T} \int_0^T I_i^r h_n \, dt$$

(21)

where $I_i^r$ is the importance index in Eq. (8), $h_n$ the heat release rate in the $n$-th computational domain. The fast reactions indexes for the 38 QSS species, CN, H$_2$CN, HCNN, C, NH$_2$, NH$_3$, NNH, C$_2$N, NCO, NH, HCN, CH, HCNO, N, C$_2$H$_7$, HNO, HCCO, HOCN, CH$_3$OH, C$_2$H$_5$, CH$_3$S, HCCO, CH$_3$, CH$_3$CHO, HCO, C$_3$H$_6$, C$_2$H$_5$, HNCO,
CH₃O, NO₂, CH₃CHO, C₂H₂, CH₃OH, C₂H₂O, CH₃CO, C₃H₄, CH₄ and H₂O₂ are 220, 237, 241, 49, 201, 278, 204, 171, 224, 192, 250, 125, 274, 180, 319, 212, 82, 273, 169, 173, 97, 176, 148, 304, 168, 312, 286, 249, 119, 187, 301, 295, 95, 158, 114, 25, 10 and 85. The reaction rates of the global reduced mechanism are calculated by those of the detailed mechanism. However, the reaction rates of the 38 fast reactions will not be included.

Once the global QSS species and fast reactions have been identified, the global reduced mechanisms can be constructed. This is the content of next part.

The Integral CSP (I-CSP) software package and global reduced mechanism

A software package called Integral CSP (I-CSP) was developed to construct the global reduced mechanism. The I-CSP is written in C++ language and uses the interface functions provided by CHEMKIN-PRO to read the reaction solutions generated in Chemkin. The source code can be delivered by corresponding author on request. In this manuscript, first, a one-dimensional, unstretched, premixed, laminar steady CH₄/air flame is run in Chemkin. Then, the I-CSP reads the necessary information, such as species’ concentrations, temperatures, heat release rates, etc. Next, the I-CSP calculates the radical pointers and fast reaction pointers in each domain and integrates these pointers to get integral radical pointers and integral fast reaction pointers which are used in identifying global QSS species and related fast reactions. Finally, once these 15 species: H₂, H, O, OH, HO₂, CH₄, CO₂, CH₂O, NO, N₂O, CO, O₂, H₂O, N₂ and Ar (the same order as they appear in the detailed mechanism) are identified as non-QSS species, the following 10-steps global reduced mechanism can be constructed with the help of I-CSP:

\[ \text{H}_2\text{O} = H_2 + 0.5\text{O}_2 \]
\[ 0.5\text{H}_2\text{O} = \text{H} + 0.25\text{O}_2 \]
\[ 0.5\text{O}_2 = \text{O} \]
\[ 0.25\text{O}_2 + 0.5\text{H}_2\text{O} = \text{OH} \]
\[ 0.75\text{O}_2 + 0.5\text{H}_2\text{O} = \text{HO}_2 \]
\[ \text{CO} + 2\text{H}_2\text{O} = \text{CH}_4 + 1.5\text{O}_2 \]
\[ \text{CO} + 0.5\text{O}_2 = \text{CO}_2 \]
\[ \text{H}_2\text{O} + \text{CO} = \text{CH}_2\text{O} + 0.5\text{O}_2 \]
\[ 0.5\text{O}_2 + 0.5\text{N}_2 = \text{NO} \]
\[ 0.5\text{O}_2 + \text{N}_2 = \text{N}_2\text{O} \]
in which Ar is not included for it is an inert specie.

The global reaction rates of the ten steps could be further simplified by using importance index with a user-defined error criterion. Samples of some of the ten non-QSS species are displayed below:

\[ \frac{d[H]}{dt} = s^{40\text{F}}_{38} + s^{40\text{F}}_{35} + s^{40\text{F}}_{34} + s^{40\text{F}}_{36} + s^{40\text{F}}_{33} + s^{40\text{F}}_{31} \]
\[ + s^{40\text{F}}_{23} + s^{40\text{F}}_{27} = 0.8246 - 0.0872 - 0.0309 - 0.0194 - 0.0180 - 0.0099 - 0.0088 \]

Table 1. The 20 species with smallest integral radical pointers calculated with \( I_i^2, I_i^3, I_i^4 \) and \( I_i^4 \)

<table>
<thead>
<tr>
<th>No.</th>
<th>( I_i^1 )</th>
<th>( I_i^2 )</th>
<th>( I_i^3 )</th>
<th>( I_i^4 )</th>
</tr>
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<tbody>
<tr>
<td>20</td>
<td>NO</td>
<td>C₂H₆</td>
<td>C₂H₄</td>
<td>C₂H₆</td>
</tr>
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<td>19</td>
<td>CH₂CO</td>
<td>C₂H₄</td>
<td>C₂H₆</td>
<td>CH₂CO</td>
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<td>CH₂CO</td>
<td>C₂H₄</td>
</tr>
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<td>C₂H₄</td>
<td>CH₃</td>
</tr>
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<td>CH₃</td>
<td>CH₃</td>
<td>H₂O₂</td>
</tr>
<tr>
<td>15</td>
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</tr>
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<td>NO</td>
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<tr>
<td>1</td>
<td>O₂</td>
<td>Ar</td>
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</tr>
</tbody>
</table>
\[
\frac{d[OH]}{dt} = s^{42}_{98}F^{85} + s^{42}_{35}F^{38} + s^{42}_{96}F^{86} + s^{42}_{43}F^{43} + 0.4781 + 0.3545 + 0.1536 + 0.0079 - 0.0043 + 0.0007
\]

\[
\frac{d[CH_4]}{dt} = s^{44}_{52}F^{52} + s^{118}_{118}F^{118} + s^{44}_{98}F^{98} + 0.9761 + 0.0146 - 0.0051 - 0.0029 + 0.0013
\]

where \(\frac{d[C]}{dt}\) is the derivative of the concentration of specie C over time, \(s_k\) the stoichiometric coefficient of \(i\)-th specie in \(k\)-th reaction, \(F_k\) the reaction rate of the \(k\)-th reaction. The number below is the integral important index ordered in descending magnitude. Sufficient terms are kept so that the total error of the omitted term is below a user-defined error criterion.

**Validation of the global reduced mechanism**

The 10-steps global reduced mechanism was validated over a one-dimensional, unstretched, premixed, laminar steady CH\(_4\)/air flame, which is the same circumstance as the 10-steps reduced mechanisms being conducted. Figures 1–3 show the results of mole fraction of three major species CH\(_4\), CO\(_2\) and CO, and four minor species H, O, OH and NO, and temperature calculated with GRI3.0 and the 10-steps reduced mechanism at equivalence ratio being 0.6, 1.0 and 1.5 and pressure being 1 atm, respectively. In Fig. 1a, the temperatures calculated by GRI3.0 and the 10-steps reduced mechanism agree well. Same agreement can be found in the comparison of mole fraction of CH\(_4\), CO\(_2\) and CO calculated by GRI3.0 and the 10-steps reduced mechanism. However, the 10-steps reduced mecha-
nism over predicts the mole fraction of CO when the distance is less than 0.4 cm. Figure 1b displays the changes of mole fraction of H, O, OH and NO against distance. Small discrepancies between results calculated by GRI3.0 and the 10-steps reduced mechanism can be found in the region of distance being less than 0.4 cm, where the mole fraction of H, O and OH grows rapidly. In the area of distance from 0.4 to 0.7 cm, the mole fraction of the three species decreases. In the following area of distance from 0.7 to 2.0 cm, the mole fraction increases with almost the same slope. Different from the aforementioned three species, NO increases once it is created and excellent agreement between results calculated by GRI3.0 and the 10-steps reduced mechanism can be observed.

Figure 2 shows the results calculated at equivalence ratio being 1.0 where the reduced mechanism is conducted. Good agreement between results calculated by GRI3.0 and the 10-steps reduced mechanism can be observed. Figure 3 displays reasonable agreement between results calculated by GRI3.0 and the 10-steps reduced mechanism in the region of distance being over 0.4 cm. However, in the region of distance being less than 0.4 cm, the 10-steps reduced mechanism over predicts mole fraction of CO2, CO, H, O and OH, and underestimates mole fraction of CH4. Good agreement can be observed for temperature and NO by comparing results calculated by GRI3.0 and the 10-steps reduced mechanism.

Figure 4 displays the final (x→∞) mass fraction of NO and CO2 over a wide range of equivalence ratio (0.4–1.6). Good agreements can be obtained over all
Figure 3. Comparison of mole fraction of (a) three major species CH$_4$, CO$_2$ and CO and temperature and (b) four minor species H, O, OH and NO, calculated with GRI3.0 and the 10-steps reduced mechanism at equivalence ratio being 1.5.

Figure 4. The final mass fraction of NO and CO$_2$ as a function of equivalence ratio, in a one-dimensional, unstretched, premixed, laminar steady CH$_4$/air flame, calculated with GRI3.0 and 10-steps reduced mechanism.
equivalence ratios except for the NO while the equivalence ratio is over 1.5. Figure 5 shows the final temperature with the equivalence ratio from 0.6 to 1.6. Satisfied agreements are obtained with the discrepancy less than 1.5%. The temperatures calculated with the 10-steps reduced mechanism are lower than those calculated with GRI3.0 while the equivalence ratio is below 1.5. However, the results are opposite while the equivalence ratio is upon 1.5.

It is clear from above validation that the 10-steps reduced mechanism produces high degree of accuracy in predicting concentration profiles of species and temperature on premixed flame. Although the global reduced mechanism is deduced on the condition of the equivalence ratio being 1.0, it is can be used over wide range of equivalence ratio and produces good results.

CONCLUSIONS

A software package named Integral CSP (I-CSP) was developed to construct the global reduced mechanism. I-CSP introduces heat release rates, species’ concentrations and specie net production rates as weighting factors to integrate radical pointers and fast reaction pointers throughout the computational domain. The input to I-CSP includes the detailed mechanism and the numerical solution of the problem on a specific set of operating conditions where the reduced mechanism is expected to be valid. The number of QSS species $M$ need to be determined in advance. The output of I-CSP is three files which describe the reduced mechanism and the numerical relations between QSS species and non-QSS species. These files are compatible with Chemkin, which makes the validation of the reduced mechanism easier.

The I-CSP method was implemented over a one-dimensional, unstretched, premixed, laminar steady $\text{CH}_4/\text{air}$ flame and conducted a 10-steps global reduced mechanism. The reduced mechanism was validated over a one-dimensional, unstretched, premixed laminar flame with equivalence ratio being 0.6, 1.0 and 1.5. Good agreements can be observed and therefore demonstrate the validity of the reduced mechanism.

One challenge step is determining the number of QSS species $M$ or the number of steps of global reduced mechanism. A feasible way to resolve the problem is first choosing $M$ approximately, then ordering the species with the help of CSP-pointers and checking out whether the species which should appear in the global reduced mechanism are in the $N-M$ non-QSS species, next changing the value of $M$ until reasonable non-QSS species are found, finally validating the resulting reduced mechanism until the error is less than user specified error tolerance. The procedure may iterate several times until the satisfied $M$ is obtained. Experiences and good human intuition will be helpful in the $M$ choosing procedure.

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(Naučni rad)

Predložen je novi algoritam baziran na kompjuterskoj singularnoj perturbaciji (KSP) u cilju konstruiranja globalnog redukovanog mehanizma. Algoritam predstavlja koncentracije vrsta, iznose neto proizvodnje vrsta i iznose oslobađanja toplote kao integralne faktore merenja radi integriranja KSP pokazatelja, uključujući radikalne pokazatelje i pokazatelje brze reakcija, putem kompjuterskog domena. Razvijen je softverski paket baziran na algoritmu u cilju efikasnijeg procesa redukcije. Input za algoritam uključuje: i) detaljni mahenizam, ii) numeričko rešenje problema za specifični set radnih uslova i iii) broj kvazi-stabilnih stanja vrsta (KSS). Predloženi algoritam je apliciran na redukciju GRI3.0 uključujući 53 vrste i 325 reakcija koje su vodile ka razvoju 15 vrsta sa redukovanim mehanizmom i 10 spojenih koraka. Tada je redukovani mehanizam potvrđen u jednodimenzionalnom, produženom, laminarnom plamenu shodno širokom spektaru ekvivalentnih odnosa i odličnih spojeva između pažljivo izračunatih rezultata i redukovanih mehanizama koji su posmatrani.

Ključne reči: Mehanizam redukcije • KSP • integralni KSP algoritam • GRI3.0