

Development of an Ethanol Reduced Kinetic Mechanism Based on the Quasi-Steady State Assumption and Feasibility Evaluation for Multi-Dimensional Flame Analysis*

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Abstract

A 20-step reduced kinetic mechanism of ethanol, a potential sustainable energy source as a biofuel, was developed based on the detailed reaction mechanism proposed by Saxena and Williams using the Computational Singular Perturbation (CSP) method based on the Quasi-steady State Assumption (QSSA). Feasibility evaluation of the reduced kinetic mechanism for multi-dimensional flame analysis, i.e., the difference in numerical results and convergence time between the detailed reaction mechanism and the reduced kinetic mechanism, was also performed to investigate the applicability of the ethanol reduced kinetic mechanism to the development of practical combustors. To consider further industrial applications, the reduced kinetic mechanism was incorporated into the commercial computational fluid dynamics (CFD) code FLUENT 6.3.26 using the User Defined Function (UDF) code developed in the present study. Numerical results calculated with the detailed reaction mechanism and the reduced kinetic mechanism, i.e., temperature profiles, chemical species profiles and laminar burning velocities, were in good agreement for both two-dimensional premixed and non-premixed flame calculations. Convergence time using the reduced kinetic mechanism was considerably reduced compared to that using the detailed reaction mechanism, indicating the applicability and advantage of a reduced kinetic mechanism based on QSSA for multi-dimensional flame analysis. An additional reduction of the computational time was achieved by using both the reduced kinetic mechanism and In Situ Adaptive Tabulation (ISAT) solver by Pope et al.

Key words: Reduced Kinetic Mechanism, Quasi-Steady State Assumption, Ethanol, Multi-Dimensional Flame Analysis, Computational Time

1. Introduction

Biomass ethanol, which is a potential sustainable energy source, is expected as an alternative fuel of practical combustors such as internal combustion engines due to its low CO₂ emissions from the viewpoint of "Carbon neutral". It is also expected as a hydrogen carrier for further applications. These facts have motivated experimental and numerical studies on the chemical kinetics of ethanol oxidation. In previous works, several detailed reaction mechanisms of ethanol oxidation have been proposed⁽¹⁾⁻⁽⁵⁾, e.g., a 383-step reaction

mechanism including 57 species by Marinov⁽³⁾ and a 235-step reaction mechanism including 46 species by Saxena and Williams⁽⁵⁾, the validity of which was also tested against the experimental data.

However, despite the availability of detailed ethanol reaction mechanisms, application of these mechanisms to multi-dimensional flame analysis for industrial purposes is difficult because the present performance of computers is limited. Namely, recently available detailed reaction mechanisms of ethanol oxidation consist of tens of chemical species and hundreds of elementary reactions, which require a large memory and convergence time, thus making it quite difficult to perform multi-dimensional numerical simulations with detailed reaction mechanisms. Hence, the overall reaction mechanism which consists of a single reaction or two reactions is currently used in many cases⁽⁶⁾; however, the accurate prediction of the flame temperature and gas emissions, which is essential for practical combustor design, is difficult when the overall reaction mechanism is used. Furthermore, the overall reaction mechanism is not capable of numerical simulations under a wide range of operating conditions⁽⁷⁾, i.e., ambient pressures, equivalence ratios and initial gas temperatures.

The reduced kinetic mechanism based on the Quasi-steady State Assumption (QSSA) has been a promising solution to this problem. The reduced kinetic mechanism decreases the calculation cost by reducing the number of chemical species which are considered and simultaneously presents better numerical results, i.e., the accurate flame temperature and major species mole fraction profiles, under a relatively wide range of conditions when the Quasi-steady State (QSS) species are selected appropriately for the target condition⁽⁷⁾⁻⁽⁹⁾. In previous studies, a large number of reduced kinetic mechanisms were proposed for methane and other major fuels⁽⁸⁾; however, to the best of our knowledge, little research on the reduced kinetic mechanism of ethanol combustion has been conducted.

Moreover, the feasibility of reduced kinetic mechanisms proposed in the previous research^(8,9) was mostly evaluated based on ignition delay calculations and one-dimensional laminar flame calculations, few of which were applied to the multi-dimensional practical numerical simulations. Saito et al.⁽⁷⁾ pointed out that numerical instability was caused by the molecular diffusion of the H radical into the cold area in the case of two-dimensional diffusion flame calculations using the 4-step CH₄/air reduced kinetic mechanism by Peters⁽⁸⁾. This indicates that the feasibility of the reduced kinetic mechanism for such things as the choice of QSS species should be tested on multi-dimensional numerical simulations before being applied to highly time-consuming industrial flame analysis. Although some reduced kinetic mechanisms have been successfully implemented into the Computational Fluid Dynamics (CFD) code^(10,11), the comparison of the total convergence time and numerical results between the detailed reaction mechanism and reduced kinetic mechanism has not been sufficient.

The purpose of the present study, therefore, was to develop a reduced kinetic mechanism of ethanol oxidation based on QSSA and to evaluate the feasibility of that mechanism for multi-dimensional numerical simulations. Firstly, several possible ethanol-reduced kinetic mechanisms were developed and each of them was tested on one-dimensional premixed flame calculation, which is more suitable for the evaluation of mechanism validity and computational cost because the sensitivity to the reaction kinetics is significant. Then the fastest and stable one was applied to two-dimensional premixed Bunsen flame calculations and diffusion flame calculations to elucidate the applicability of the reduced kinetic mechanism based on QSSA to multi-dimensional numerical simulations.

2. Numerical methods

2.1 Development of an ethanol reduced kinetic mechanism

In this study, a reduced kinetic mechanism was developed by using the method of

Computational Singular Perturbation (CSP) by Lu et al.⁽¹²⁾ based on the QSSA. In this method, to specify the QSS species, reaction time scale analysis was conducted on the result of the zero-dimensional calculation using the Perfect Stirred Reactor (PSR)⁽¹³⁾ model. This was performed over a wide range of equivalence ratio, ϕ , of 0.5 to 1.6 and ambient pressure, P , of 0.1 to 5.0 MPa. Then the QSS species was specified when its time scale is less than the critical time scale based on the extinction residence time and the threshold factor⁽¹²⁾. As a starting mechanism, the detailed reaction mechanism of ethanol oxidation proposed by Saxena and Williams⁽⁵⁾, which consists of 46 chemical species and 235 reactions, was chosen. In this strategy, various reduced mechanisms, i.e., 19- to 26-step reduced kinetic mechanisms, were generated. The procedure of generation and evaluation of reduced kinetic mechanisms are described in the results and discussion section. The global reactions, considered species and QSS species of the 20-step ethanol reduced kinetic mechanism developed in the present study are shown in Table 1. Here the considered species are the chemical species used in the calculation with the reduced kinetic mechanism. The 20-step reduced kinetic mechanism of the present study includes important species for the combustion analysis, e.g., CO, H₂ and OH, this analysis being expected to calculate the flame structure properly under a wide range of conditions.

Table 1. Global reactions of 20-step reduced kinetic mechanism developed in the present study.

Considered species			
C ₂ H ₅ OH, O ₂ , H ₂ O, CO ₂ , CO, H ₂ , H, OH, O, HO ₂ , H ₂ O ₂ , CH ₂ O, CH ₄ , CH ₃ , C ₂ H ₄ , C ₂ H ₆ , C ₂ H ₂ , CH ₂ CO, HCCO, CH ₃ OH, CH ₃ CHO, C ₃ H ₃ , C ₃ H ₆ , Ar, He, N ₂			
QSS species			
C ₂ H ₄ O, C ₂ H ₃ , C ₃ H ₈ , C ₃ H ₄ , CH ₂ OH, C ₃ H ₅ , CH ₃ CHOH, CH, T-CH ₂ , C ₂ H, I-C ₃ H ₇ , C ₂ H ₅ , HCO, N-C ₃ H ₇ , CH ₃ O, CH ₃ CH ₂ O, CH ₂ CHO, S-CH ₂ , CH ₃ CO, CH ₂ CH ₂ OH			
No	Global reactions		
R1	H + O ₂	⇌	OH + O
R2	O + H ₂	⇌	H + OH
R3	OH + H ₂	⇌	H + H ₂ O
R4	2H	⇌	H ₂
R5	OH + O	⇌	HO ₂
R6	2OH	⇌	H ₂ O ₂
R7	OH + CO	⇌	H + CO ₂
R8	H + CH ₃	⇌	CH ₄
R9	2H + CO	⇌	CH ₂ O
R10	O + CH ₃	⇌	H + CH ₂ O
R11	O + C ₂ H ₄	⇌	2H + CH ₂ CO
R12	OH + 2CH ₃	⇌	H + H ₂ O + C ₂ H ₄
R13	2CH ₃	⇌	C ₂ H ₆
R14	2OH + 2CH ₃	⇌	2H + 2H ₂ O + C ₂ H ₂
R15	O + C ₂ H ₂	⇌	H + HCCO
R16	H + CH ₃ OH	⇌	H ₂ O + CH ₃
R17	H + HO ₂ + CH ₂ CO	⇌	O ₂ + CH ₃ CHO
R18	H + C ₂ H ₅ OH	⇌	OH + 2CH ₃
R19	H + O + C ₃ H ₃	⇌	CO + C ₂ H ₄
R20	O + C ₃ H ₆	⇌	2H + CO + C ₂ H ₄

2.2 One-dimensional premixed flame analysis

The reduced kinetic mechanisms were firstly applied to the one-dimensional premixed flame calculations using the PREMIX⁽¹⁴⁾ code, and their performance were evaluated preliminary to the two-dimensional flame simulations. The continuity, momentum, energy and species equations for a steady laminar flow were solved with the damped Newton method⁽¹⁴⁾. Coefficients for viscosity, thermal conductivity and mass diffusion were

calculated using the thermodynamic and transport database by Saxena and Williams⁽⁵⁾ and transport model by CHEMKIN-II⁽¹⁵⁾. To enable the numerical simulation with the reduced mechanism, the subroutine CKWYP in the PREMIX code, which calculates the rate of each elementary reaction, was replaced by a subroutine developed by the authors. Numerical simulations were conducted under various conditions, i.e., equivalence ratios, ϕ , of 0.5 to 1.5 and ambient pressures, P , of 0.1 to 3.0 MPa. The temperature of the premixed gas, T , was constant at 298 K. The length of the calculation domain was $X = 100$ cm in this study. Zero-gradient boundary condition for all physical quantities was specified at the end of calculation domain. CPU time was measured to evaluate the convergence time using a typical personal computer (CPU: Pentium4-3.00 GHz, memory: 2.00 GB).

2.3 Two-dimensional premixed and non-premixed flame analysis

A reduced kinetic mechanism was applied to the 2-D premixed Bunsen flame calculations and 2-D diffusion flame calculations using the commercial code FLUENT 6.3.26⁽¹⁶⁾ for further practical calculations. The continuity, momentum, energy and species equations for a laminar steady flow were solved with the SIMPLE algorithm. Effects of buoyancy and radiation were not considered in this study. Coefficients for viscosity, thermal conductivity and mass diffusion were calculated using the thermodynamic and transport database by Saxena and Williams⁽⁵⁾ and the transport model by FLUENT.

Figure 1 shows the computational domains of the 2-D numerical simulations in this study. The domain sizes were 2 mm x 4 mm and 5 mm x 10 mm for 2-D Bunsen flame calculations and 2-D diffusion flame calculations, respectively. A structured grid was employed for both calculation domains. The grid interval was 50 μ m and 100 μ m for each calculation, and the total numbers of grid points were 3200 and 5000, respectively. The left-hand sides of both domains were symmetric planes. The constant velocities, temperature, chemical species mole fractions were given at the burner inlet for both calculations. As for 2-D Bunsen flame calculations, the velocity profile of the laminar plug flow was employed at the flow inlet boundary. As for 2-D diffusion flame calculations, the gas phase C_2H_5OH jet normal to the boundary with a uniform velocity of 1.0 m/s flowed into the air co-flow with a uniform velocity of 0.2 m/s. The gauge pressure was set to zero, and the zero-gradient condition normal to the boundary was adopted for other variables at the burner outlet. The right-hand sides of both calculation domains and the burner lip were considered as adiabatic walls. The initial temperature of the fuel and the oxidizer, T , was constant at 298 K.

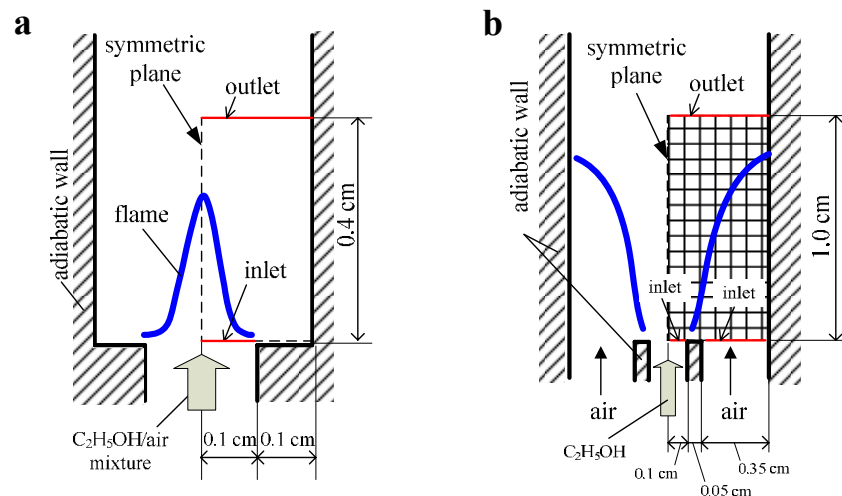


Figure 1. Computational domains of the two-dimensional flame calculations of the present study: (a) two-dimensional Bunsen flame calculations; (b) two-dimensional diffusion flame calculations.

To enable calculation with the reduced kinetic mechanism, the subroutine developed by the authors was implemented as a User Defined Function (UDF) to the solver of FLUENT. The UDF subroutine is called just once per iteration at each grid point, and it creates a reference table of reaction rates for all global reactions of the reduced kinetic mechanism in the computer memory. The convergence of the calculation was judged when residuals of the above-mentioned equations became steady. Two-dimensional numerical simulations were performed using the Altix3700 supercomputer system of the Institute of Fluid Science, Tohoku University (CPU: 256 CPU x 4, performance: 1.64 TFLOPS x 4, memory: 3 TB x 4). To evaluate the convergence time, the CPU time was measured.

3. Results and Discussion

3.1 Development and selection of an ethanol reduced kinetic mechanism based on 1-D laminar flame analysis

Figure 2 shows the relationship between the convergence time and the number of species considered in the reduced kinetic mechanisms developed in the present study, including 25 to 32 species. The convergence time using the detailed reaction mechanism is also plotted in Fig. 2. Overall, the convergence time was reduced linearly as the number of tracked species decreased, indicating that the number of considered species was dominant in the calculation cost of one-dimensional numerical simulations of the present study. Adaptive mesh refinement was performed several times during the calculation; however, the computational time for the mesh refinement was negligibly small compared with the total CPU time. The fastest tested mechanisms is already shown in Table 1, i.e., the 20-step reduced kinetic mechanism including 26 chemical species (Table 1) that converged 4 times faster than the detailed mechanism, indicating the advantage of the ethanol reduced kinetic mechanism in the present study. Locally, the convergence time using the 19-step reduced kinetic mechanism, in which C_2H_6 was eliminated as the QSS species from the 20-step reduced kinetic mechanism, was slightly larger than that using the 20-step reduced kinetic mechanism. It was presumed that the decrease of the number of the considered species does not always contribute to the reduction of the convergence time, indicating that the choice of steady-state species in the reduced kinetic mechanism, e.g., C_2H_6 mentioned above, affects the calculation stability even if the total number of considered species and reaction steps are the same.

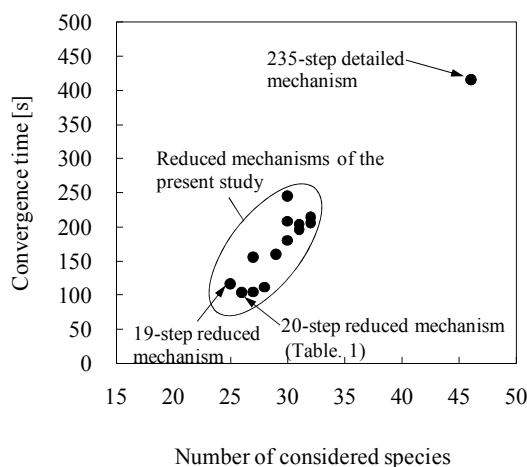


Figure 2. Relationship between number of species and convergence time (C_2H_5OH/air 1-D flame calculation, $\phi = 1.0$, $P = 0.1$ MPa, $T = 298$ K).

Figure 3 shows the species mole fraction profiles and temperature profiles in the flame zone calculated with the detailed reaction mechanism and the 20-step reduced mechanism under the condition of $\phi = 1.0$ and $P = 0.1$ MPa. Both results, including the intermediate species mole fraction, were in good agreement. The application range of the 20-step reduced kinetic mechanism was subsequently tested at various equivalence ratios and ambient pressures, as shown in Fig. 4. Experimental data by Gülder⁽¹⁷⁾ and Egolfopoulos⁽¹⁸⁾ et al. at atmospheric pressure are also plotted in Fig. 4. Generally, the laminar burning velocities calculated using the detailed reaction mechanism and the 20-step reduced kinetic mechanism showed good agreement at various ambient pressures up to 3.0 MPa. They also agreed well with the experimental data. Although Schwer et al.⁽¹⁹⁾ pointed out the problem of limited application range of the reduced kinetic mechanism, the 20-step reduced kinetic mechanism developed in the present study (Table 1) includes a sufficient numbers of chemical species and reactions to perform industrial flame analysis under a certain range of conditions. Thus, the 20-step reduced kinetic mechanism of the ethanol combustion was chosen and applied in the two-dimensional numerical simulations detailed in the next section.

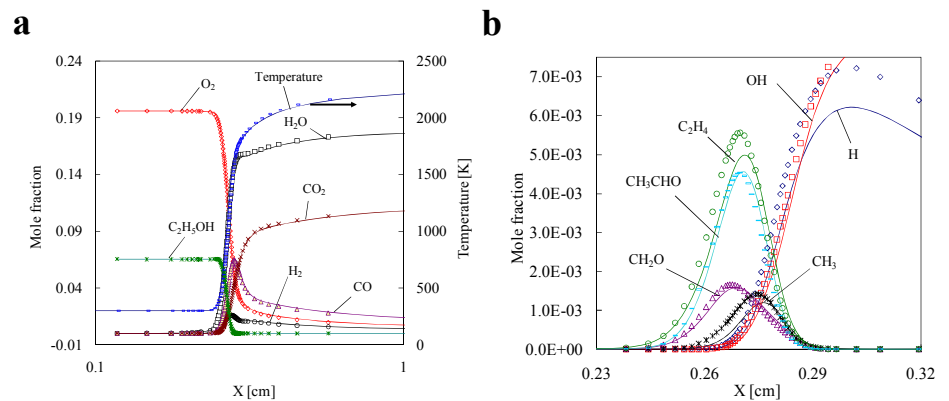


Figure 3. Profiles of species mole fraction and temperature with the detailed reaction mechanism (Lines) and the 20-step reduced kinetic mechanism (Symbols): (a) major species; (b) intermediate species (C₂H₅OH/air 1-D flame calculation, $\phi = 1.0$, $P = 0.1$ MPa, $T = 298$ K).

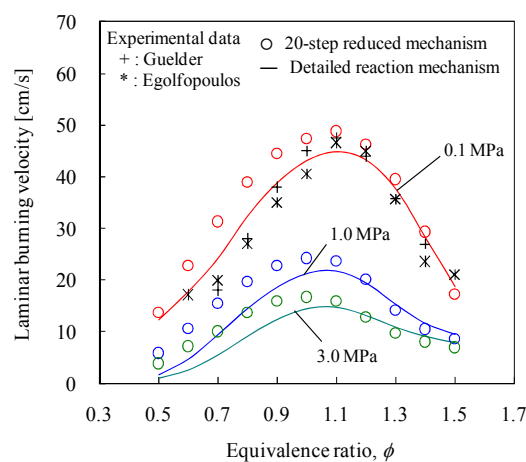


Figure 4. Laminar burning velocities calculated with the detailed reaction mechanism (Lines) and the 20-step reduced kinetic mechanism (Symbols) (C₂H₅OH/air 1-D flame calculation, $T = 298$ K).

3.2 Application of the ethanol reduced mechanism for two-dimensional flame analysis

Convergence of the two-dimensional flame analysis with the 20-step ethanol reduced kinetic mechanism (Table 1) was achieved after the following improvements. In the reduced kinetic mechanism based on QSSA, the mole fractions of QSS species were calculated internally using an algebraic division equation derived from the steady-state relation⁽⁸⁾ in the UDF code developed in the present study. For example, the mole fraction of the CH radical, which is one of the QSS species, is calculated as follows:

$$[\text{CH}] = \frac{\text{ABV}}{\text{DEN}}$$

$$\begin{aligned} \text{ABV} &= R_f(59) \times [\text{T-CH}_2] \times [\text{H}] + R_f(61) \times [\text{T-CH}_2] \times [\text{OH}] \\ &\quad + R_b(67) \times [\text{CO}] \times [\text{H}] + R_b(68) \times [\text{HCO}] \times [\text{O}] \\ &\quad + R_b(69) \times [\text{CH}_2\text{O}] \times [\text{H}] + R_b(70) \times [\text{HCO}] \times [\text{CO}] \\ &\quad + R_f(118) \times [\text{C}_2\text{H}] \times [\text{O}] + R_f(120) \times [\text{C}_2\text{H}] \times [\text{O}_2] \\ \text{DEN} &= R_b(59) \times [\text{H}_2] + R_b(61) \times [\text{H}_2\text{O}] \\ &\quad + R_f(67) \times [\text{O}] + R_f(68) \times [\text{O}_2] \\ &\quad + R_f(69) \times [\text{H}_2\text{O}] + R_f(70) \times [\text{CO}_2] \\ &\quad + R_b(118) \times [\text{CO}] + R_b(120) \times [\text{CO}_2], \end{aligned} \quad (1)$$

where R_f and R_b are the forward and backward rate constants of elementary reactions in the detailed reaction mechanism by Saxena and Williams. The number in parenthesis is the number of the elementary reaction in the detailed reaction mechanism by Saxena and Williams. It is considered that this expression tends to cause numerical instability because species mole fractions in the equation are near zero at the initial step of the calculation even when the under-relaxation factors are sufficiently small. In the present study, therefore, the initial temperature and species profile were used to avoid this problem. The initial solution was calculated using the following overall one-step reaction of the FLUENT database⁽¹⁶⁾:



$$\omega_{\text{C}_2\text{H}_5\text{OH}} = -A \exp\left(-\frac{E}{RT}\right) [\text{C}_2\text{H}_5\text{OH}]^{0.15} [\text{O}_2]^{1.6}. \quad (3)$$

Here the pre-exponential factor, A , is $8.435 \times 10^9 \text{ m}^{2.25}/\text{mol}^{0.75}\text{s}$ and the activation energy, E , is $1.256 \times 10^8 \text{ J/kmol}$. It is considered that the chemical species included in Eq. (2) prevented the calculation instability caused by the above mentioned algebraic equations. This method could also lead to the reduction of the total convergence time.

Figure 5 shows the numerical results of the 2-D premixed Bunsen flame calculated with the 20-step reduced kinetic mechanism (Table 1) and the detailed reaction mechanism at $\phi = 1.0$ and $P = 0.1 \text{ MPa}$. As for the result using 20-step reduced kinetic mechanism, the numerical instability of the reduced kinetic mechanism caused by the intermediate species diffusion reported by Saito et al.⁽⁷⁾ was successfully avoided, indicating that QSS species were appropriately selected in the 20-step reduced kinetic mechanism of the present study. The calculation results with the detailed reaction mechanism shown in Fig. 5 were obtained using the In Situ Adaptive Tabulation (ISAT)⁽²⁰⁾ solver module of FLUENT based on the in-situ generation of look-up tables because those without ISAT could not converge as mentioned later. The profiles of temperature, major chemical species, e.g., H_2O and CO , and intermediate species, e.g., C_2H_4 , were in good agreement, meaning that the 20-step reduced kinetic mechanism based on QSSA is applicable to two-dimensional premixed flame calculations.

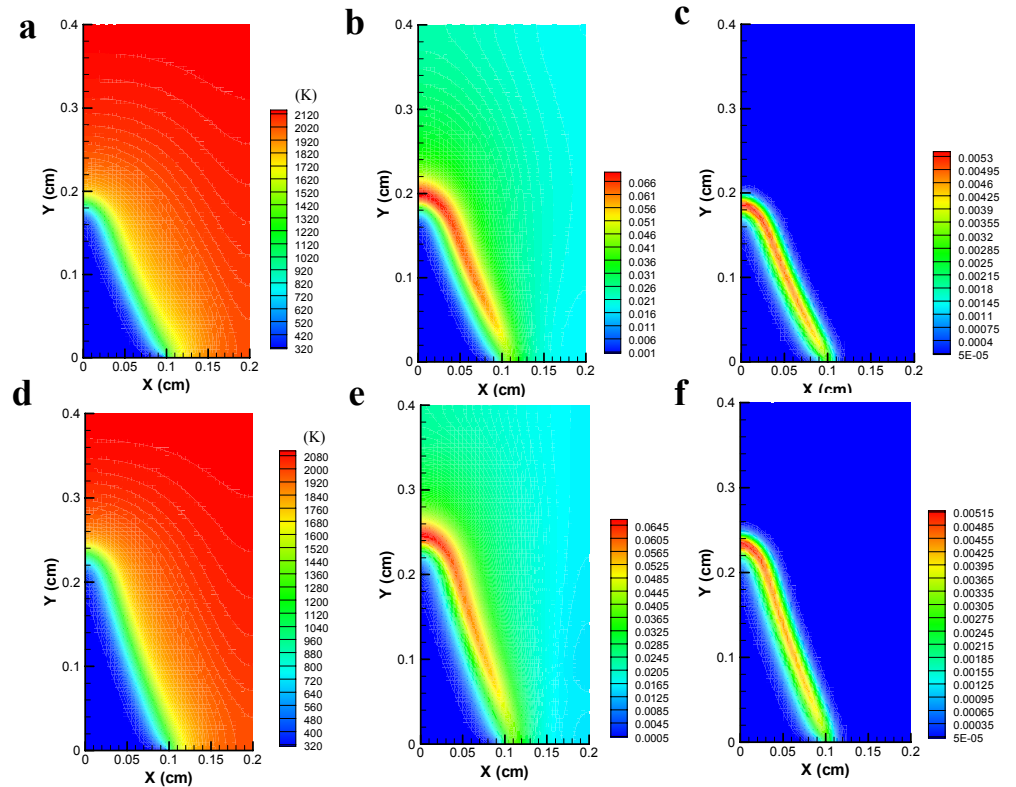


Figure 5. Temperature and species mole fraction profiles calculated with the 20-step reduced kinetic mechanism: (a) Temperature; (b) CO mole fractions; (c) C₂H₄ mole fractions, and those with the detailed reaction mechanism: (d) Temperature; (e) CO mole fractions; (f) C₂H₄ mole fractions (C₂H₅OH/air 2-D premixed flame calculation, $\phi = 1.0$, $P = 0.1$ MPa, $T = 298$ K).

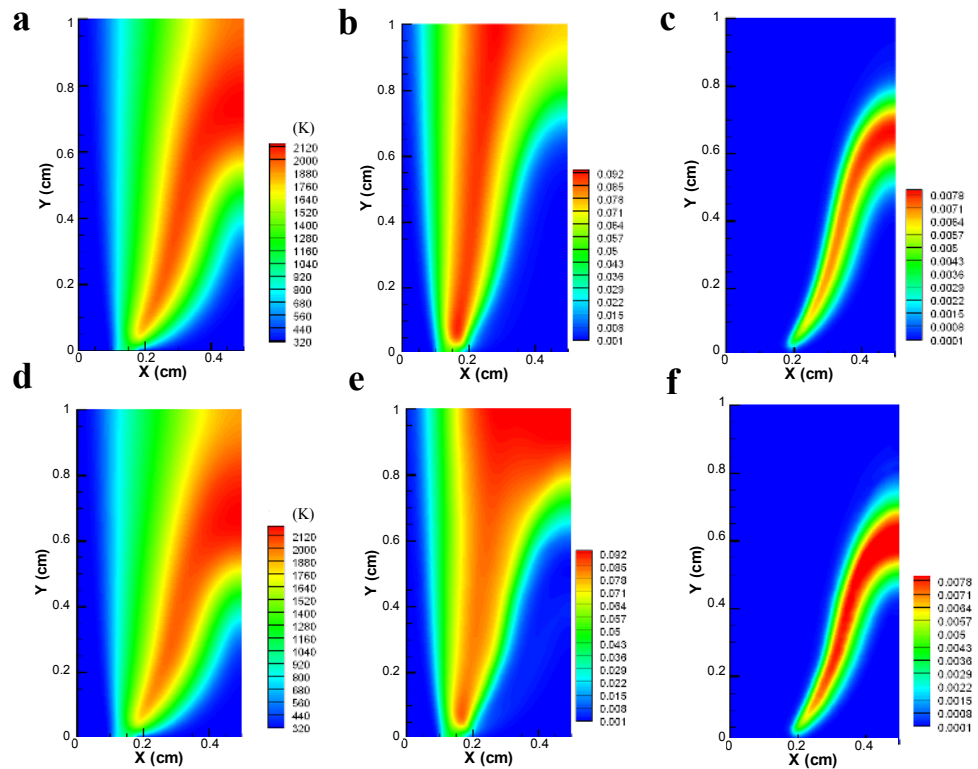


Figure 6. Temperature and species mole fraction profiles calculated with the 20-step reduced kinetic mechanism: (a) Temperature; (b) CO mole fractions; (c) OH mole fractions, and those with the detailed reaction mechanism: (d) Temperature; (e) CO mole fractions; (f) OH mole fractions (C₂H₅OH/air 2-D diffusion flame calculation, $P = 0.1$ MPa, $T = 298$ K).

Note that the effect of mesh refinement on these calculation results was small in the present study. It should also be noted that the temperature and species distribution normal to the flame front in Fig. 5 calculated with FLUENT agreed well with those calculated with the PREMIX code. The temperature and species mole fraction profiles of the 2-D diffusion flame calculated using the 20-step reduced kinetic mechanism and the detailed reaction mechanism are also shown in Fig. 6. Numerical results using the 20-step reduced kinetic mechanism were in good agreement with the results using the detailed reaction mechanism with the ISAT solver, meaning that the reduced kinetic mechanism developed in the present study is also applicable to 2-D non-premixed flame calculations.

Figure 7 shows the relationship between the number of iterations and CPU time for 2-D Bunsen flame and diffusion flame calculations. These calculations were all conducted under conditions of same ambient pressure, equivalence ratio, under-relaxation factor for every variable and the initial profiles of temperature and chemical species for the comparison of the computational time. As for the 2-D Bunsen flame calculation, the calculation with the detailed mechanism and the normal SIMPLE solver module of FLUENT were unable to converge within 350 hours, and the CPU time per iteration was more than 6 times longer than that with the 20-step reduced mechanism, showing the advantage of the multi-dimensional analysis using the reduced mechanism. It can also be considered that the computational time of the algebraic calculation for QSS species is sufficiently small compared with the total calculation cost. The calculation time with the detailed reaction mechanism using the ISAT solver was also plotted. The calculation with detailed reaction mechanism with ISAT could iterate 50 times faster than that without ISAT, i.e., ISAT speed-up factor⁽¹⁹⁾ of 50, showing that the ISAT is also effective for 2-D calculations in this study. The CPU time per iteration with the 20-step reduced mechanism without ISAT was 5 times longer than that using the detailed reaction mechanism using the ISAT solver; however, as for the total computational time, the calculation with the 20-step reduced mechanism converged 1.5 times faster than that using detailed reaction mechanism and ISAT solver. It can be concluded that the effect of the decrease of the calculation time by reducing the considered species is relatively larger than the speed-up effect by using ISAT in this case. As for the 2-D diffusion flame calculation, on the other hand, the calculation using the detailed reaction mechanism with the ISAT solver could converge faster than that with the 20-step reduced kinetic mechanism without ISAT, which indicates that the speed-up effect of ISAT is relatively larger in the case of diffusion flame calculations than the case of premixed flame calculations.

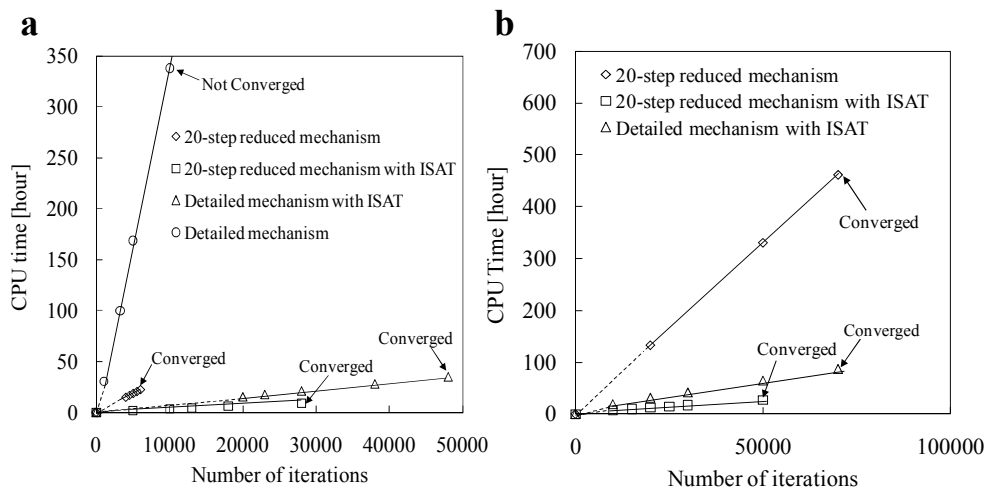


Figure 7. Relationship between the number of iterations and the CPU time: (a) 2-D Bunsen flame calculations, $\phi = 1.0$, $P = 0.1$ MPa; (b) 2-D diffusion flame calculations, $P = 0.1$ MPa.

Furthermore, as in the study by Montgomery et al.⁽¹¹⁾ the computational time when both the 20-step reduced kinetic mechanism and ISAT solver were simultaneously used was considerably less than that using only the detailed reaction mechanism for 2-D premixed and non-premixed flame calculations. It should be noted here that the accuracy of the final solution and the total computational time strongly depend on the error tolerance parameter when the ISAT solver is used^(11, 16, 21). At the same time, unrealistic profiles of some intermediate species such as C_3H_3 with split peaks could be seen depending on the error tolerance⁽¹⁶⁾, as shown in Fig. 8, in the present 2-D diffusion flame calculations using the ISAT solver of FLUENT, showing the advantage of the reduced kinetic mechanism based on QSSA over the ISAT solver in terms of the prediction of the chemical species profiles including intermediate species with low calculation cost.

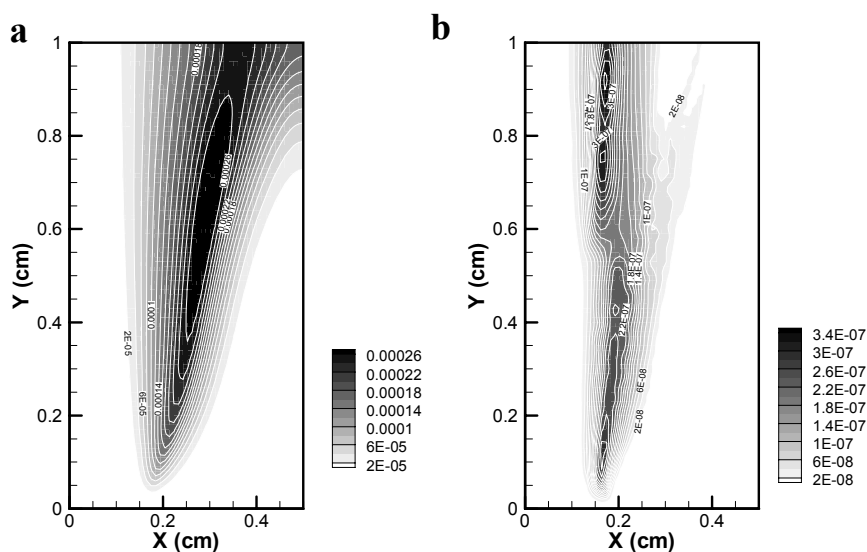


Figure 8. C_3H_3 mole fraction profiles: (a) numerical result calculated with the 20-step reduced kinetic mechanism of the present study; (b) numerical result calculated with the detailed reaction mechanism and ISAT solver of FLUENT (2-D diffusion flame calculation, $P = 0.1$ MPa).

4. Conclusions

A 20-step reduced kinetic mechanism for ethanol combustion based on QSSA was developed in this study and the feasibility of that mechanism for multi-dimensional numerical simulation was evaluated. The validity of the ethanol reduced kinetic mechanism was firstly tested on 1-D premixed flame calculations, and it was confirmed that the numerical results with a reduced kinetic mechanism and a detailed reaction mechanism showed better agreement at various equivalence ratios and ambient pressures. The developed ethanol reduced mechanism was then applied to two-dimensional premixed and non-premixed flame calculations. The 2-D flame calculations using the ethanol reduced kinetic mechanism successfully converged after improvement of initial temperature and species profiles. The numerical results agreed well with those with the detailed reaction mechanism, and the convergence time was sufficiently reduced by using the reduced kinetic mechanism for 2-D numerical simulations, indicating that the reduced kinetic mechanism based on QSSA can be applied to the multi-dimensional industrial flame analysis with excellent results. Moreover, computational time was considerably decreased when the reduced kinetic mechanism was used with ISAT, although depending on its error tolerance parameter, some problems were seen on the prediction of intermediate species profiles when the ISAT solver of FLUENT was used.

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