Numerical Simulation of Ignition Process on Boundary Layer Combustion with Chemical Reaction Model

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Abstract

In order to simulate ignition of boundary layer combustion, unsteady and non-equilibrium chemical reaction model and compressible fluid dynamics code is necessary because the time scale of chemical reactions are similar to those of fluid dynamics in this condition. However, direct integration of this model is unstable and too time consuming. Authors' modified methods reduce the calculation cost of chemical reactions to 1/50 of the original, but even with proper selection of time integration method, the wall time necessary for a simulation of ignition is still unrealistic.

1. Introduction

The interest in hybrid propulsion is now growing in application to spacecraft propulsion and space transpotation. One of the attractive features of this technology is safety, which is important in space tourism industry.

In usual hybrid rocket engines, solid fuel is contained in combustion chamber into which liquid oxidizer is injected. The mixture of gasified fuel and oxidizer combust in the boundary layer over the fuel surface (Fig.1). Polypropylene and liquid oxygen, for example, are used as solid fuel and liquid oxydizer respectively.[3]

In order to realize a practical hybrid rocket, high rate fuel gas generation has to be achieved. Various studies have been performed such as low-melting point fuels and innovative oxidzer injection. To understand these methods closely, modeling and understanding of the mechanism, including fuel gasification, mixing of fuel and oxidizer, and turblent combusting flow, is necessary.

Although there are lots of studies performed on these themes, most of them consider the rate of reaction as infinity. However, because of the boundary layer combustion, the time scale of chemical reaction can be comparable to that of flow during ignition and extinction. Therfore ignoring unsteadiness of chemical reaction can result in the failure of modeling ignition and extinction of hybrid rocket engine. Although "KUCRS[7]" can generates a list of elementary reactions and necessary various coefficients from a set of reactants, when this detailed reactions are included into fluid dynamics computation directly, the necessary wall clock time will be too large for a practical use.

In this paper, in order to reduce the wall clock time necessary for the simulation of ignition, two themes are discussed: one of them is chemical reaction reduction, and the other is cost reduction of numerical simulation of boundary layer combustion, which imitates a hybrid rocket engine chamber.

2. Chemical Models and Reduction Method

2.1 Description of Model

In this paper, three chemical model are used: the flame sheet model, the chemical equilibrium model, and the unsteady chemical reaction model.

Flame Sheet Model The flame sheet model is used at the boundary layer combustion calculations of CH_4/Air, that is

$$CH_4 + 2O_2 + 7.3N_2 \rightarrow CO_2 + 2H_2O + 7.3N_2$$

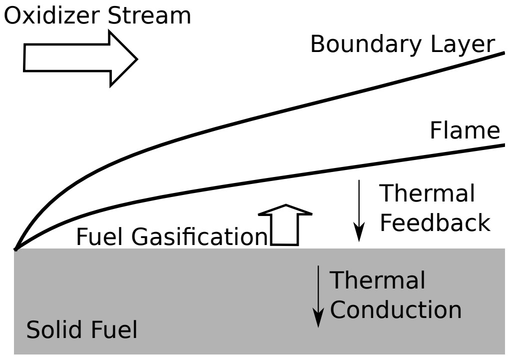

Figure 1: Schematic of combustion at hybrid rocket engine

when this model is used, either methane or air can exist at the same cell. Both of them cannot exist at the same cell because this reaction is one direction so products generates as much as can. In particular, at stoichiometric mixture ratio, all species are of the right hand side. Therefore the composition of species are calculated only from the mass fraction, and the other thermodynamic properties such as temperature and heat ratio are calculated from this composition and the internal energy because the internal energy is conserved quantity at compressible flow. For more descriptions, see [5].

Chemical Equilibrium Model Chemcal equilibrium calculation is conducted in the condition of constant volume and energy because these values are the conserved quantities of compressible flow. Governing equations are those of NASA-CEA[6]. Also for thermodynamical and transportal database, NASA-CEA is used.

Unsteady Chemical Reaction Model In this model, chemical reactions mechanism are originally generated by KUCRS[7]. This mechanism is consist of elementary reactions. The rates of reactions are represented as follows.

$$q_{f,k} = k_{f,k}[M_k]\prod_{j=1}^{ns}[X_j]^{\nu'_{jk}}, \quad q_{r,k} = k_{r,k}[M_k]\prod_{j=1}^{ns}[X_j]^{\nu''_{jk}} \tag{1}$$

where $q_{f,k}, q_{r,k}$ are kth forward / backward elementary reaction rates each other($k = 1...nr$). nr is the number of elementary reactions. $k_{f,k}$ and $k_{r,k}$ are the rate constants of the kth reaction, and $[X_j]$ is the molar concentration of jth species, and ν'_{jk}, ν''_{jk} is stoichiometric coefficients for the reactants and the products of the kth elementary reaction each other. M_k is third body and calculated by the equation below.

$$[M_k] = \sum_{j=1} \alpha_{jk}[X_j] \tag{2}$$

where α_{jk} is the enhancement factor for species j of the kth elementary reaction. $k_{f,k}$ and $k_{r,k}$ are calculated by Arrhenius forms separately, by equilibrium factor, by using reduced pressure or by troe forms. For closer description, see [9]. Overall reaction rate of kth elementary reaction q_k is

$$q_k = q_{f,k} - q_{r,k} \tag{3}$$

and the production rate of molar concentration of species j is

$$\dot{\omega}_j = \sum_{k=1}^{nr}(\nu''_{jk} - \nu'_{jk})q_k \tag{4}$$

Calculations are conducted in the condition of constant volume and energy because these values are the conserved quantities of compressible flow.

Thermodynamical Properties Thermodynamical values such as molar enthalpy at standard state H°_j and molar heat capacity at constant pressure at standard state $C^\circ_{p\,j}$ of each species j are calculated by polynomial equations

$$\frac{C^\circ_{p\,j}}{R_u} = a_{1j}T^{-2} + a_{2j}T^{-1} + a_{3j} + a_{4j}T + a_{5j}T^2 + a_{6j}T^3 + a_{7j}T^4 \tag{5}$$

$$\frac{H_j^\circ}{R_u T} = -a_{1j}T^{-2} + a_{2j}T^{-1}\ln T + a_{3j} + a_{4j}\frac{T}{2} + a_{5j}\frac{T^2}{3} + a_{6j}\frac{T^3}{4} + a_{7j}\frac{T^4}{5} + a_{8j}\frac{1}{T} \tag{6}$$

at fluid dynamics computation, and

$$\frac{C_{p\,j}^\circ}{R_u} = a_{1j} + a_{2j}T + a_{3j}T^2 + a_{4j}T^3 + a_{5j}T^4 \tag{7}$$

$$\frac{H_j^\circ}{R_u T} = a_{1j} + a_{2j}\frac{T}{2} + a_{3j}\frac{T^2}{3} + a_{4j}\frac{T^3}{4} + a_{5j}\frac{T^4}{5} + a_{6j}\frac{1}{T} \tag{8}$$

at chemical model reduction where $a_{ij}(i = 1, ..., 8), A_j, B_j, C_j$ and D_j $(j = 1, ..., ns)$ are constant and different between species. ns is the number of species. This difference of formula of equations are due to the difference of the database used. For the calculations of flame sheet model and chemical equilibrium model, the equations of former forms are used with the data of NASA-CEA[6], and for the calculations of unsteady chemical reaction model, that of latter forms are used with teh data of KUCRS[7].

2.2 Numerical Method for Time Integration

For the flame sheet model and the chemical equilibrium model, there is no need to consider time because these model regards the rate of chemical reactions as infinity. so the time integrations of chemical reaction at those models are conducted simply by replacing temperature, specific heat ratio, viscosity coefficient and averaged molecular weight of each cell at each time step according to internal energy and mass fraction.

For unsteady chemical reaction model, a time integration method is necessary. Because the time integration of chemical reactions becomes very stiff generally, special time integration libraries are used frequently. In these time integration library, LSODE is famous because it has been used in famous chemical reaction library Chemkin-II[9], but Yi et al. used VODE in simulation of a detonation engine[11] and found it useful. Therefore, these two methods are compared in the calculations of homegeneous gas phase ignition.

The absolute and relative differences set in the LSODE and VODE are 10^{-10} and 10^{-12} respectively. The jacobians are not given directly to LSODE or VODE, so differential jacobians are used.

2.3 Reduction Method of Unsteady Chemical Reaction Model

2.3.1 Concept and Valuation Basis of Reduced Model

Although KUCRS[7] can generate chemical reaction mechanisms if a list of reactants (hydrocarbon, oxygen or nitrogen only) is given, the list is too long to be included directly into fluid dynamics calculation. This time, important information from chemical reaction mechanism is only the time history of "temperature", so we reduced the model by the methods modified to operate the reduction fully systematicaly.

The only needed information from chemical reaction model is the time history of temperature, but this paper evaluates each reduced models more simply by the differences of "ignition time" or "equilibrium temperature" from the KUCRS-generated model.

In this paper, "model difference" indicates the larger difference of ignition time or equilibrium temperature, where "ignition time"t_{ign} is defined as the time needed for 0-dimensional homogeneous reactants to reach 400 K higher temperature than the initial one from when they appear suddenly at $t = 0$, on adiabatic and constant volume conditions, and "equilibrium temperature" is the temperature at $t = 10t_{ign}$ on the same condition as the calculation of t_{ign}.

2.3.2 Reaction Reduction using Sensitivity Analysis

Zhu et al performed a reduction of elementary reactions by using sensitivity analysis[4]. In the paper, the sensitivity $S_{j,k,l}$ of reaction$k$ to species$j$ at time grid point t_l has been defined as follows.

$$S_{j,k,l} = \left.\frac{\partial \ln[X_j]}{\partial \ln k_k}\right|_{t=t_l} \tag{9}$$

where k_k is $k_{f,k}$ or $k_{r,k}$, and t_l is lth time grid point. To define "the sensitivity of reaction$k$"B_k, the equation below is used.

$$B_k = \sum_{j\in L}\sum_{l} S_{j,k,l}^2 \tag{10}$$

In this equation, summation of l is done overall time range. The set L is defined as the group whose member's maximum $[X_j]$ overall time is large. The number of species in L is about 10, and includes reactants, products and important radicals.

Originally, the elimination of reactions has been done by the procedure below.

1. From the reactions whose B_j are smaller, calculate the model difference.
2. **If the model difference does not exceed the allowed limit,** remove the reaction. and return to 1.
3. **If the model difference does exceed the allowed limit,** determine whether the reaction is the particular reactions (e.g. chain initiation).
4. **If the reaction is one of the particular reactions,** leave the reaction to the model and return to 1 to determine the next reaction.
5. **If the reaction is not one of the particular reactions,** stop procedure.

We modify this methods.

First, because $S_{j,k,l}$ can become large even if $[X_j]$ is very small (in this case, the influence to temperature is small), we modify the definition of $S_{j,k,l}$ to the definition of Andrew et al[1].

$$S_{j,k,l} = \frac{1}{\max_l [X_j]} \left. \frac{\partial [X_j]}{\partial a_k} \right|_{t=t_l} \tag{11}$$

where a_k is the coefficient multiplied to the actual reaction rate q_k. In other word, if $a_k = 1$, the reaction rate is equal to the actual one, and if $a_k > 1$, larger than the actual one and if $a_k < 1$, smaller. So ∂a_k is equal to $\partial \ln k_k$. This modification changes the magnitude of $S_{j,k,l}$ small when $[X_j]$ is smaller than that at other time grid point $t = t_{l'}$.

Second modification is the determination of reaction exception. To determine whether the elementary reaction is particular reaction (e.g. chain initiation) or not, one needs chemical knowledge, so this determination is difficult to automate. We modify the procedure.3 to

> "**If the model difference does exceed the allowed limit,** leave the reaction and return to 1 to determine the next reaction."

Due to this modification, elimination of reactions can be conducted fully systematically.

2.3.3 Procedure of Reduction

In this paper, reductions of chemical reaction mechanism are performed along the procedure below.

1. Select several condition points from the condition range where the accuracy of reduced model is wanted to be guaranteed.
2. Remove chemical species until elimination of any chemical species in the model makes the maximum model difference on all the selected conditions exceeds 3%. This operation makes one model.
3. On each selected condition points, conduct the reduction of reactions using sensitivity analysis mensioned above on the reduced model previous step made. In this reduction, the allowed difference is 5%. The number of model this operation makes is equal to the number of selected condition points.
4. Gather all the elementary reactions which the reduced models previous step made used. This operation makes one model.
5. From the reduced model previous step made, remove chemical species until elimination of any chemical species in the model makes the maximum model difference on all the selected conditions exceed 5%. This operation makes one final model.

The limit of maximum model difference (3% and 5% above) can be changed if more precise or rough model is necessary.

Table 1: Scope of Reduction of Chemical Reaction Model

	Lower bound	**Upper bound**
Equivalence ratio ϕ	0.5	2
Initial temperature T_0	900 K	1200 K
Initial pressure p_0	0.1 atm	100 atm

Table 2: Selected Points for Reduction of Chemical Reaction Model

	Selected condition points
Equivalence ratio ϕ	0.5, 1, 2
Initial temperature T_0	900 K, 1200 K
Initial pressure p_0	0.1 atm, 100 atm

2.4 Condition of Calculation

The validation of unsteady chemical reaction modeling is done in the scope Table.1 shows. The range of initial pressure is selected as the range of chamber pressure. The lower boundary of intial temperature is selected in such a way as to ignite at about 0.1 sec, and the upper one is the temperature at which reactants are stable at initial state if existing separately. Selected points to make the reduction model are 3 (equivalence ratio) × 2 (initial temperature) × 2 (initial pressure) = 12 combinations of the condition points Table.2 shows.

The propellants are propylene and oxygen because the future target of this research is to simulate PP/LOX hybrid rocket, and compared with the reaction of methane/air, the reaction between this combination becomes stiff and needs more elementary reactions.

Calculations are conducted on the conditions next: At $t = 0$, pure reactants appear suddenly in the fully mixed state (homogeneous gas). Reaction happens at an adiabatic constant volume container, so density ρ and internal energy e are constant throughout the reaction and reactants ignite voluntarily by using internal energies of themselves.

In this section, calculations are conducted by Intel®Core$^{\text{TM}}$i7-2600K CPU. Only one core of this CPU is used.

2.5 Result and Discussion

Figure.2 show the number of elementary reactions and species that KUCRS-generated model and the reduced model used. The reduced reaction model uses 1/2 species and 1/4 elementary reactions compared to the KUCRS-generated model. All the species the reduced model used are:

> C_3H_6, O_2, CO_2, H_2O, CO, H, OH, O, HO_2, CH_2O, CH_2CHO, aC_3H_5, C_2H_3, aC_3H_5O, CH_2CO, C_3H_6OOHba, C_3H_6cyOab, HCO, C_3H_6OHb, $HOOHOC_3H_5OOb$, HOC_3H_5OOHb, $HOCHOC_2H_3OOHa$, HOC_3H_6OOb, HOC_3H_6OOa, $C_3H_5O_3b$, C_3H_6OHa, C_3H_6OOHab, H_2O_2, C_3H_5OHa, HOCHvCHOa, HOHCCOa, C_2H_3CHO, CH_3, CH_2OH, $HOOC_3H_5aOHb$, CH_3CO, CH_3COCH_2O, HOC_3H_6OOHa, C_3H_7OOa, CH_3COCH_2OOH, H_2, C_2H_5, C_2H_4, aC_3H_4, $C_3H_6O_2a$, $HOOC_3H_5aOHa$, C_3H_5OHb

The notation is that of KUCRS[7].

Figure.3 shows the time histories of various time integration methods and chemical model. This is the condition of $\phi = 0.5$, $T_0 = 900$K and $p_0 = 0.1$atm, which has the largest ignition time which exceeds 0.3 seconds. One can find all of them produce the same result and the differences between models are sufficiently small.

Figure.4 and 5 show the ignition times at different conditions. The crossed points are calculated by KUCRS-generated model, and the lines are calculated by the reduced model. In both calculation, time integrations are conducted by LSODE. The coincidences of the ignition time between the KUCRS-generated model and the reduced model can be confirmed over the wide range of conditions. Similary, the coincidences of equilibrium temperature are also confirmed.

Figure.6 shows the necessary wall clock time of 50 times calculation of time history Figure.3 shows. Here we can find the combination of VODE and the reduced model can calculate about 50 times faster than the combination of LSODE and KUCRS-generated model. (The latter result can be obtained when KUCRS-generated model is inputed directly to Chemkin-II.) This ratio becomes bigger than that of the number of elementary reactions, because by the reduction, the species which can be large amount are eliminated, therefore the stiffness of the time integration becomes small.

Moreover, Figure.7 shows the necessary wall clock time of 10000 times calculation of equilibrium calculation and VODE-reduced unsteady chemical reaction model calculation. From the previous research using the equilibrium calculation, the number of internal iteration is about 15, so this number is used to reproduce real necessary wall clock

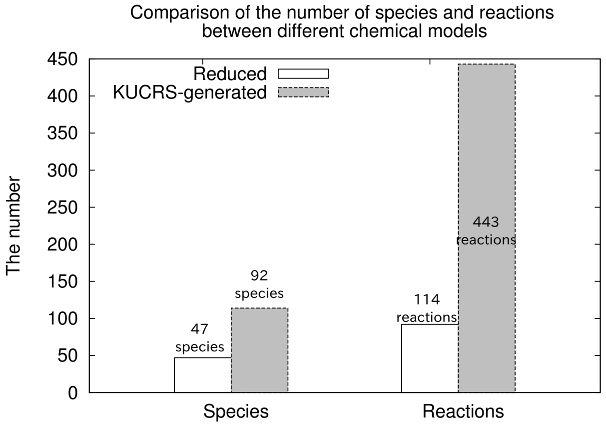

Figure 2: The Number of Elementary Reactions and Species

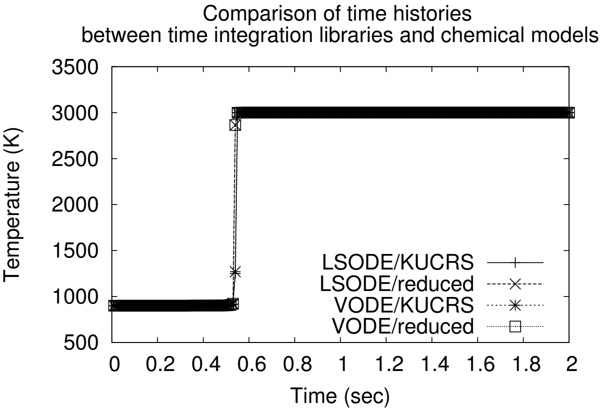

Figure 3: Comparison of Time Histories between Different Time Integration Methods and Chemical Models

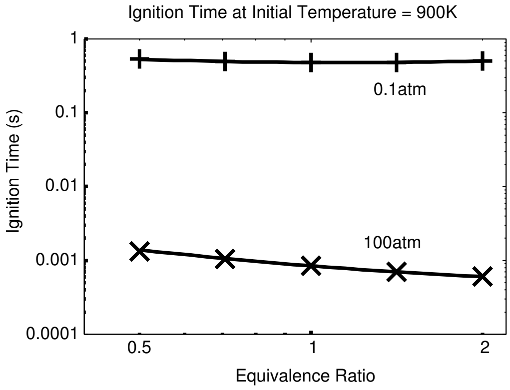

Figure 4: Ignition Delay at $T_0 = 1$

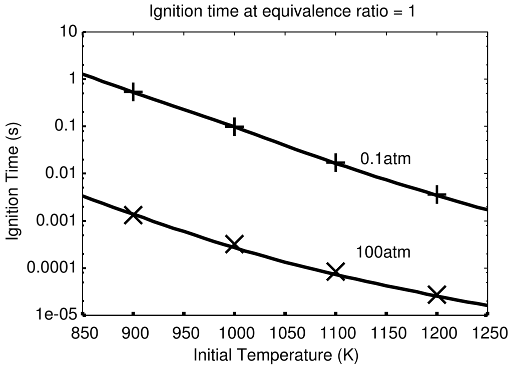

Figure 5: Ignition Delay at $\phi = 1$

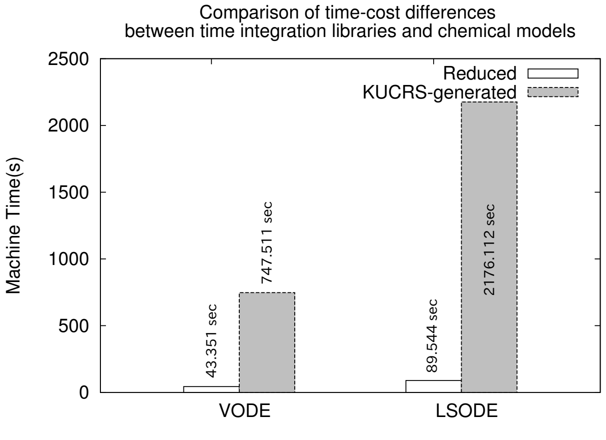

Figure 6: Comparison of Necessary Wall Clock Time between Different Time Integration Methods and Chemical Models

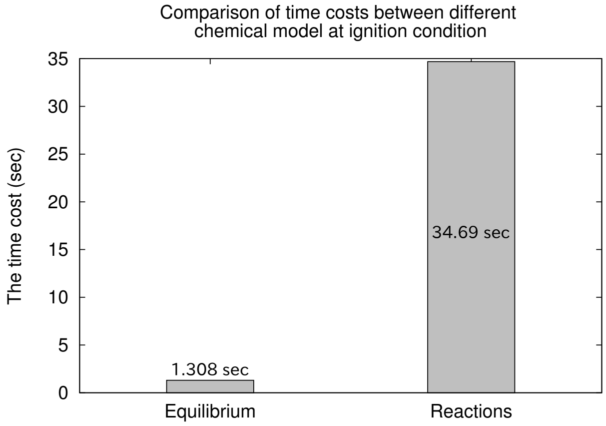

Figure 7: Comparison of Necessary Wall Clock Time between Different Chemical Models at Ignition Condition

times of equilibrium calculation in the CFD. In the calculation of VODE-reduced model, Δt is set to 10^{-6} seconds which is a general time step in the global time step and Newton-Raphson time integration. These two types of methods are compared at the middle of ignition at the same condition used at the calculation Figure.3 shows. From Figure.7, the difference of necessary wall clock times of two model are 26.5 times, which is one order of magnitute so that one can find the calculation using this VODE-reduced model is not unrealistic.

3. Simulation of Boundary Layer Combustion

3.1 Governing Equations

In this paper, at fluid dynamic calculation, the speed of chemical reactions is supposed as infinity. Therefore, the information of chemical species are represented only by mass fraction ξ such as

$$\xi = \frac{m_f}{m_o + m_f} \tag{12}$$

where m_f and m_o is mass of fuel and oxydizer at the point each other. So the extended two-dimensional laminar Navier-Stokes equations are

$$\frac{\partial Q}{\partial t} + \frac{\partial (F_c - F_v)}{\partial x} + \frac{\partial (G_c - G_v)}{\partial y} = 0 \tag{13}$$

where Q, F, G and S are defined as

$$Q = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \\ \rho \xi \end{pmatrix}, \quad F_c = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho E + p)u \\ \rho \xi u \end{pmatrix}, \quad G_c = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho E + p)v \\ \rho \xi v \end{pmatrix} \tag{14}$$

$$F_v = \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ u\tau_{xx} + v\tau_{xy} - q_x \\ \rho D \frac{\partial \xi}{\partial x} \end{pmatrix}, \quad G_v = \begin{pmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ u\tau_{yx} + v\tau_{yy} - q_y \\ \rho D \frac{\partial \xi}{\partial y} \end{pmatrix} \tag{15}$$

where ρ is the density, u and v are the velocity components of x and y direction each other, E is the total energy, p is the pressure. p is calculated from the equations follows.

$$p = \rho R_u T / MW \tag{16}$$

where R_u is universal gas constant, MW is averaged molecular weight and T is temperature. The normal and shear stresses τ in F_v and G_v are represented as follows.

$$\tau_{xx} = \mu\left(\frac{4}{3}\frac{\partial u}{\partial x} - \frac{2}{3}\frac{\partial v}{\partial y}\right), \quad \tau_{xy} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right), \quad \tau_{yy} = \mu\left(\frac{4}{3}\frac{\partial v}{\partial y} - \frac{2}{3}\frac{\partial u}{\partial x}\right) \tag{17}$$

The energy fluxes q_x and q_y are

$$q_x = -k\frac{\partial T}{\partial x}, \quad q_y = -k\frac{\partial T}{\partial y} \tag{18}$$

μ is the mixture viscosity coefficient, k is the mixture thermal conductivity and D is the mixture mass diffusivity. The relationships of these parameters can be represented by Schmidt number Sc and Prandtl number Pr

$$\mathrm{Sc} = \frac{\mu}{D}, \quad \mathrm{Pr} = \frac{\mu c_p}{k} \tag{19}$$

where c_p is averaged specific heat per unit mass. In this paper, it is assumed as $\mathrm{Sc} = \mathrm{Pr} = 1$ and the thermal conductivity k and the mass diffusivity D are calculated from the viscosity coefficient μ.

Thermodynamical values are calculated by the chemical model discussed before. Transport properties of the mixture μ is defined by Wilke formula such as

$$\mu = \sum_{i=1}^{ns} \frac{X_i \mu_i}{X_i + \sum_{j=1, j\neq i} X_i \phi_{ij}} \tag{20}$$

$$\phi_{ij} = \frac{1}{4}\left(1 + \left(\frac{\mu_i}{\mu_j}\right)^{1/2}\left(\frac{MW_j}{MW_i}\right)^{1/4}\right)^2\left(\frac{2MW_j}{MW_i + MW_j}\right)^{1/2} \tag{21}$$

3.2 Numerical Method and Calculation Environment

Numerical calculations are conducted by author's original cord.

3.2.1 Spatial Discretization

Spatial discretization of governing equations(13) has been done by finite volume method. Evaluation of fluxes are done by SLAU, and by using MUSCLE, third-order accuracies are obtained. Evaluation of viscous fluxes are done by the second-order central differences.

3.2.2 Time Integration

Time integration of fluids dynamics and chemical reactions are calculated separately.

Generally, the simulation of reactive gas flow is very unstable, so time step cannot be set large when using ordinal time integration scheme. In this paper, Newton-Raphson method is used at time integration. Newton-Raphson method is iterative method. In this paper, this is used to obtain $n+1$th $Q \equiv Q^{n+1}$ which satisfies

$$\frac{3Q^{n+1} - 4Q^n + Q^{n-1}}{2\Delta t} + \frac{\partial(F_c^{n+1} - F_v^{n+1})}{\partial x} + \frac{\partial(G_c^{n+1} - G_v^{n+1})}{\partial y} = 0 \tag{22}$$

When calculating Q^{n+1}, 0th estimation of $Q^{n+1} \equiv \hat{Q}^0$ is set to Q^n, and $m+1$th estimation of $Q^{n+1} \equiv \hat{Q}^{m+1}$ is calculated from $\hat{Q}^m$as follows.

$$\frac{3\hat{Q}^{m+1} - 4Q^n + Q^{n-1}}{2\Delta t} + \frac{\partial(\hat{F}_c^{m+1} - \hat{F}_v^m)}{\partial x} + \frac{\partial(\hat{G}_c^{m+1} - \hat{G}_v^m)}{\partial y} = 0 \tag{23}$$

$$\Delta t = t_{n+1} - t_n \tag{24}$$

where $\hat{\iota}^m$ $(\iota = F_c, G_c, F_v, G_v)$ represents the quantity ι calculated by regarding $\hat{Q}^m$ as Q. In addition, to estimate $\hat{F}_c^{m+1}$ and $\hat{G}_c^{m+1}$, the relations of

$$\hat{F}_c^{m+1} \sim \hat{F}_c^m + \frac{\partial F_c}{\partial Q}\Delta\hat{Q},\ \ \hat{G}_c^{m+1} \sim \hat{G}_c^m + \frac{\partial G_c}{\partial Q}\Delta\hat{Q} \tag{25}$$

$$(\Delta\hat{Q} = \hat{Q}^{m+1} - \hat{Q}^m) \tag{26}$$

are used, so final formula is:

$$\left(\frac{3}{2\Delta t} + \frac{\partial}{\partial x}\frac{\partial F_c}{\partial Q} + \frac{\partial}{\partial y}\frac{\partial G_c}{\partial Q}\right)\Delta\hat{Q} + \left(\frac{3\hat{Q}^m - 4Q^n + Q^{n-1}}{2\Delta t} + \frac{\partial(\hat{F}_c^m - \hat{F}_v^m)}{\partial x} + \frac{\partial(\hat{G}_c^m - \hat{G}_v^m)}{\partial y}\right) = 0 \tag{27}$$

So if $\Delta\hat{Q}$ becomes nearly zero, first term of equation(27) becomes nearly zero. Therefore, by substituting Q^{n+1} for $\hat{Q}^m$ at equation(27), equation(22) is obtained. Equation.(27) are simultaneous linear equations because the first term is the multiplication of matrix and vector. To calculate this equation, LU-SGS method is used.

In this paper, the number of iterations about m at each time step n is fixed to 20. This method is compared with two-step Runge-Kutta method, that is

$$Q^{n+1/2} = Q^n - \frac{1}{2}\Delta t\left(\frac{\partial(F_c^n - F_v^n)}{\partial x} + \frac{\partial(G_c^n - G_v^n)}{\partial y}\right) \tag{28}$$

$$Q^{n+1} = Q^n - \Delta t\left(\frac{\partial(F_c^{n+1/2} - F_v^{n+1/2})}{\partial x} + \frac{\partial(G_c^{n+1/2} - G_v^{n+1/2})}{\partial y}\right) \tag{29}$$

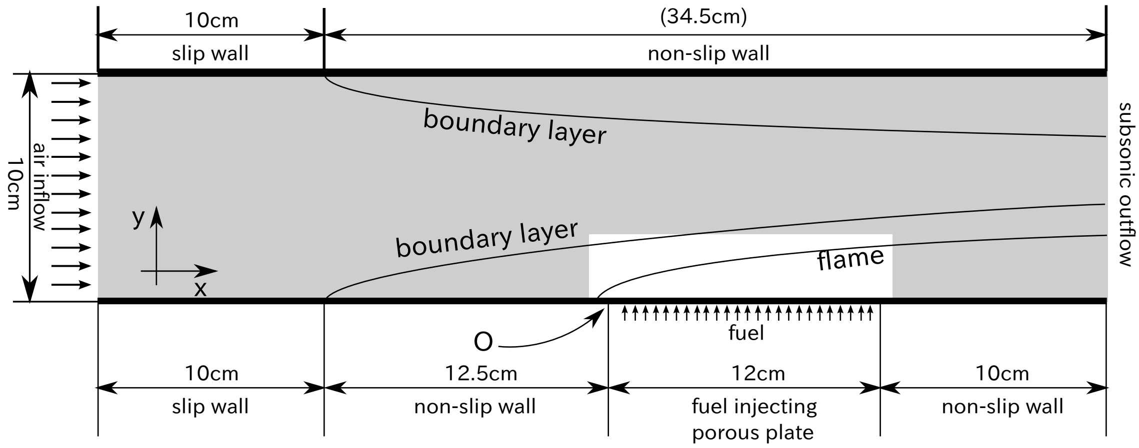

Figure 8: Calculation Area

3.3 Condition of Caluculation

The experiment of Hirano et al.[2] is simulated. Figure.8 shows the two-dimensional calculation area. The number of grids is 488(horizontal) × 199(vertical). The point O is the origin. Upper bound is non-slip wall, and lower bound is slip wall, non-slip wall and porous wall from which fuel injected at the speed of 2 cm/sec. Uniform air flow is injected from left side boundary at the speed of 60.3 cm/sec (subsonic). Right side wall is subsonic outflow boundary, and the pressure at left and right side boundary is set to 1 bar. Because the cited experiment uses a convergent section before the porous wall, there are no given data of the velocity of air inflow from the left boundary and the length of the forward non-slip wall of lower boundary. So these are set in such a way that the non-combustion velocity data coincidents with the calculated data.

In the calculation, the gray area in Figure.8 is consideres as buffering area, and only results of white area are visualized. The gradients of temperature and pressure at porous wall is set to zero.

The calculations to evaluate two time integration methods, i.e. two-step Runge-Kutta methods and Newton-Raphson method, are started from the converged flow field calculated by flame sheet model. The time of this field is set to $t = 0$.

At $t = 0$, the chemical model is suddenly changed from the flame sheet model to the chemical equilibrium model, and two different time history of flow field by different time integration scheme are compared. Grobal time step is used and courant numbers are set to 0.5 at Runge-Kutta method and 20 at Newton-Raphson method. These numbers are the largest numbers in the calculations which can be sustain stability at each time integration methods.

Calculations are conducted by using 60 cores of the super computer of Japan Aerospace Exploration Agency. The theoretical arithmetic capacity is 2.4 TFLOPS. Message Passing Interface is used for parallel computation.

3.4 Result and Discussion

Figure.9 shows the distribution of x-component velocity of the experiment of Hirano et al. and the calculation. Those two datas are in good agreement. Because this calculation sets the velocity of air inlet flow as 60.3 cm/sec and the length of the forward non-slip wall as 12.5 cm, these two values are used at the computations below.

Figure.10 and 11 shows the converged flow field which uses the flame sheet model. The temperature rises up to 2000 K, and the flame is constructed between the fuel-rich zone and the oxydizer-rich zone. From the velocity field, the acceleration at the high temperature zone can be seen. This flow field is used as the initial condition of calculation using the chemical equilibrium model.

At the beginning of calculations, shock waves from the flame zone are observed. This is because of the change of chemical model at $t = 0$.

At Figure.12 and Figure.13, velocity fields at $t = 2.49 \times 10^{-4}$ sec calculated by different time integration schemes are shown. Figure.12 is the result calculated by the Newton-Raphson method and the number of time step is 400, and Figure.13 is the result calculated by the two-step Runge-Kutta method and the number of time step is 16000. We can see the shock waves originally generated by the chemical model change and reflected from the lower and right boundary.

Though the calculation using Newton-Raphson methods uses 40 times larger courant number, but judged from

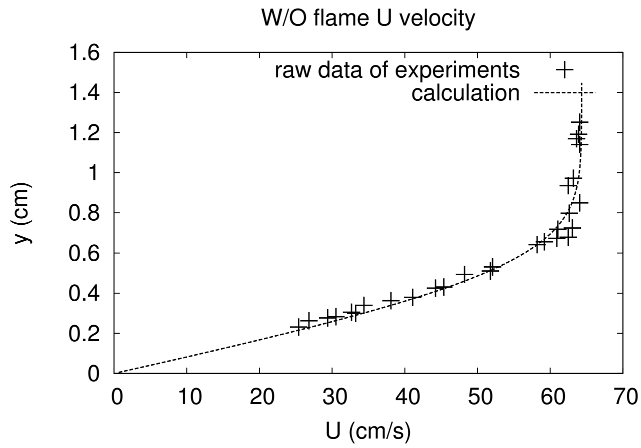

Figure 9: Velocity of x-direction of Non-Combustion Flow

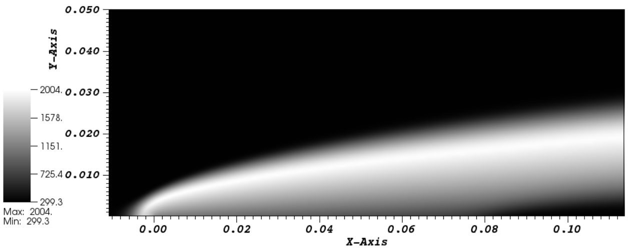

Figure 10: Initial Distribution of Temperature

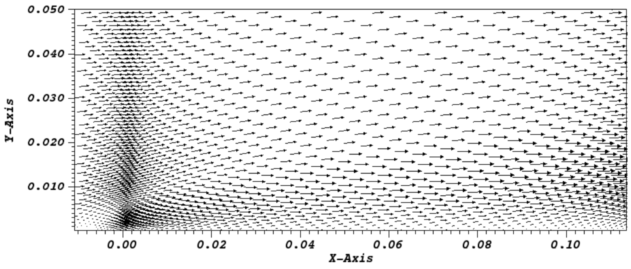

Figure 11: Initial Distribution of Velocity

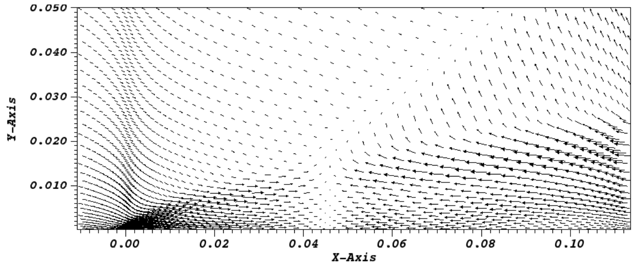

Figure 12: The Flow Field of Two-Step Runge-Kutta Method at 16,000 step

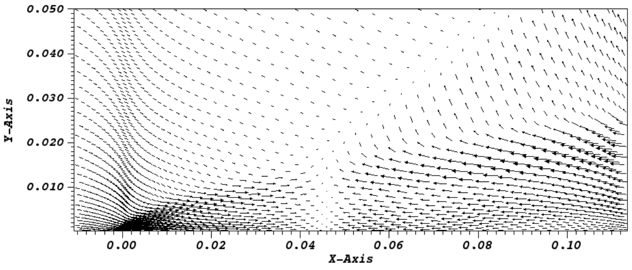

Figure 13: The Flow Field of Newton-Raphson Method at 400 step

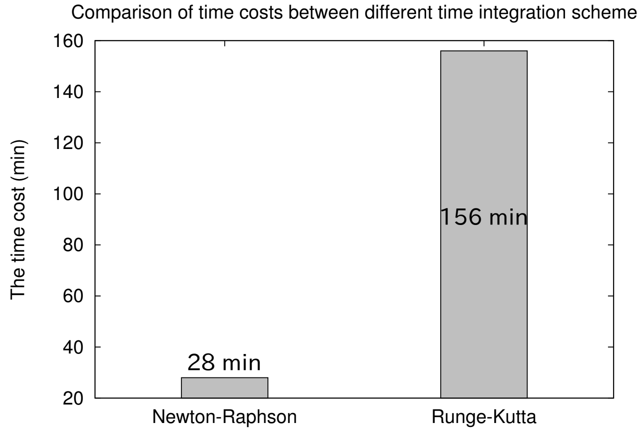

Figure 14: The Comparison of necessary wall clock time betweeen different time integration methods

these two fields, time accuracy and the stability of the calculation using Newton-Raphson method are seem to be almost same as that using Runge-Kutta method. Therefore we can find that the Newton-Raphson methods whose courant number is 20 can produce the same results as the two-step Runge-Kutta methods whose courant number is 0.5 produces.

Figure.14 shows the necessary wall clock times to obtain the results shown at Figure. 12 and 13. These result indicates that the calculation using Newton-Raphson method is 5.6 times faster than one using Runge-Kutta method.

4. Estimation of Wall Clock Time needed for Simulation using Unsteady Chemical Model

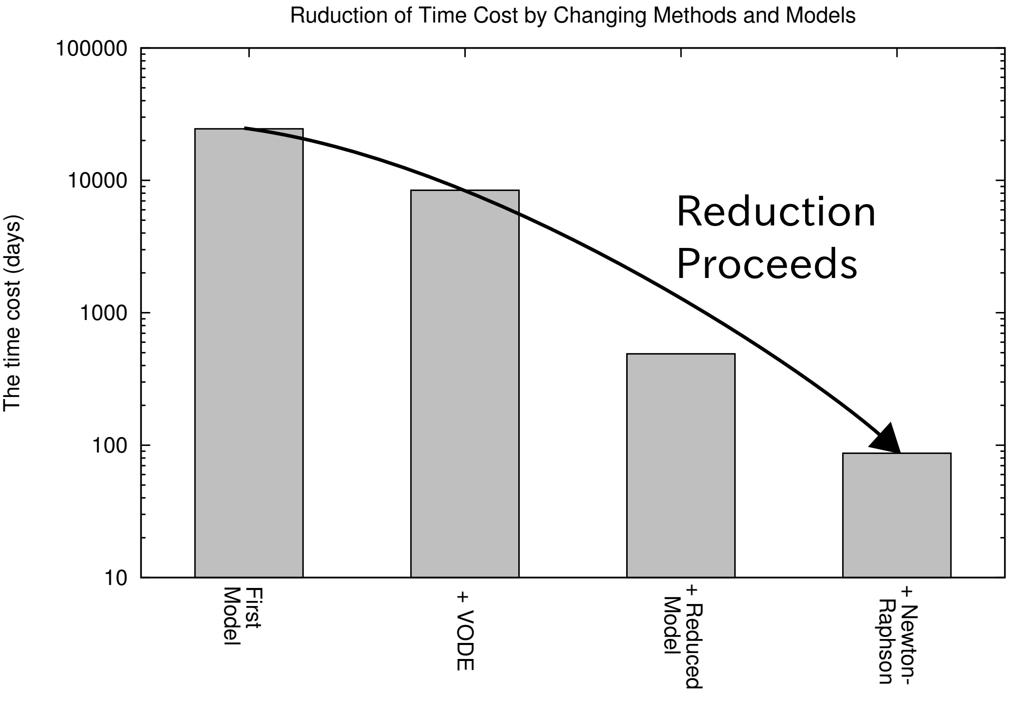

Figure 15: The Reduction of Necessary Wall Clock Time by Changing Methods and Models

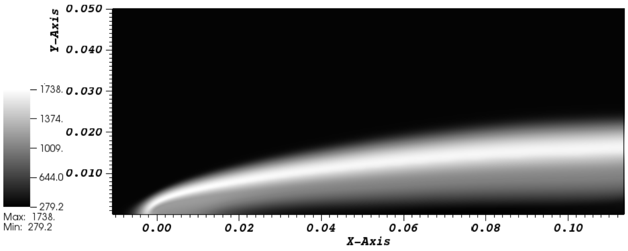

Figure 16: Distribution of Temperature at $t \sim 0.28$ seconds

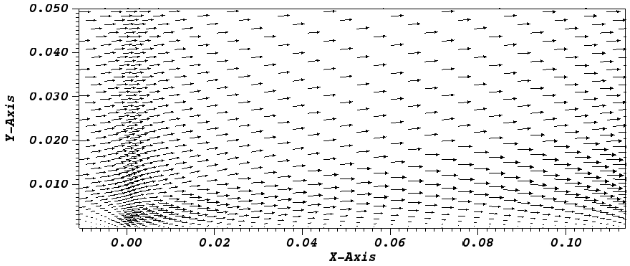

Figure 17: Distribution of Velocity at $t \sim 0.28$ seconds

The length of porous plate is 12 cm and the velocity of air inflow is 60 cm /sec, therefore the physical time necessary for the stream to pass over the porous plate is about 12(cm) / 60(cm/sec) $\sim 2 \times 10^{-1}$ second.

In this research, if the chemical equilibrium model is used, the time difference used at the calculation which use Newton-Raphson method and two-time Runge-Kutta method is about 10^{-6} sec and 2.5×10^{-8} seconds respectively, and each methods can proceeds 2500 steps and 18000 step each other per hour after initial disturbances vanished.

Therefore, the wall clock time necessary to proceed 0.2 sec physical time will be

$$(2 \times 10^{-1})/(2.5 \times 10^{-8})/18000 = 440\text{hours} = 18\text{days} \tag{30}$$

If the Chemkin-II which uses LSODE and KUCRS-generated model, this will be 18 days × 26.5 × 50 = 24500 days = 66 years.

By the use of the cost reductions this paper suggests, the necessary wall clock time is reduced as Figure.15 shows. At last, the 0.2 sec calculation with VODE-reduced model and Newton-Raphson method needs 87 days.

When the calculation in Figure.13 is proceeded further, the results of Figure. 16 and 17 are obtained. Figure. 16 and 17 shows the distributions of temperature and velocity of succeeding at $t = 0.28$ sec. Though $t = 0.28$ seconds passed, the flow has slight vibrations and is not converged yet, so more physical time will be necessary for the convergence of the ignition process.

Therefore, for the simulation of ignition process on boundary layer combustion, more cost reduction will be necessary.

5. Summary and Future works

In order to reduce the wall clock time necessary for the simulation of ignition, two methods are conducted.

For the chemical model, By using modified reduction method and proper selection of time integration method, the wall clock time necessary for the unsteady chemical reactions becomes 1/50 of that of original.

For the fluid dynamics, it is confirmed that Newton-Raphson method using large courant number has a good stability and time accuracy, and can calculate 5.6 times faster than two-step Runge-Kutta method using small courant number.

Finally the wall clock time needed for the simulation using unsteady chemical model is estimated, and the necessity of more cost reduction is guessed.

In future works, three approach will be taken to reduce the necessary wall clock time. Because this simulates flows of low-Mach number, the pre-conditioner of Weiss et al.[10] for example will be needed. Moreover, the non-reflecting boundary will be needed because in this calculation boundaries of calculating area are not so far from the reacting area. Direct inputs of jacobian to VODE at chemical model will also make this calculation faster.

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