福山大学工学部紀要
第27巻 2003年12月

FEM Simulation of Hypersonic Reactive Flows Around Re-entry Capsule

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ABSTRACT

Hypersonic reactive flows are analyzed by FEM(Finite Element Method). Chemical reactions of dissociation for 6 species are introduced into a FEM formulation, and Mach 25 flow field around the re-entry capsule is simulated. By considering the dissociation reaction, atomic distributions of O, N, NO are obtained, and temperature around the capsule decreased compared to the calculation results of ideal gas analysis. In the case of Mach 10 simulation, the dissociation reaction of air was not found.

Keywords: Finite Element Method, Hypersonic flow, Reactive Flow

1. INTRODUCTION

Investigations of hypersonic flow have been made in many countries. It is important to visualize flowfield around the hypersonic vehicle in order to understand the hypersonic phenomena. One of the authors newly developed the electric discharge method[1], and several phenomena such as streamlines around hypersonic vehicles, and shock-wave/boundary-layer interaction have been clarified by its visualization[2][3].

On the other hand, CFD (Computational Fluid Dynamics) approach is effective to know the detail of the hypersonic flowfield. The FEM (Finite Element Method) analysis program based on explicit dynamic method for incompressible fluid has been developed, and simulation examples of ideal gas flow including shock wave have been shown[4][5].

If the Mach number is high, it is important to consider the phenomena of reactive flows such as dissociation and ionization of air. In this study, the equations of reactive gas is introduced into the FEM, and several numerical results are shown.

2.FEM FORMULATION

2.1 Basic equations

The FEM analysis for compressible flow is based on the conservation form of equations. The conservation of mass and momentum is expressed as follows,

$$\frac{\partial \rho}{\partial t} + \{v_k \rho\}_{,k} = 0 \quad \cdots\cdots\cdots (1)$$

$$\frac{\partial (\rho v_i)}{\partial t} + \{v_k (\rho v_i)\}_{,k} = \sigma_{ik,k} \quad \cdots\cdots\cdots (2)$$

where ρ is density, v_i is velocity and σ_{ij} is stress tensor. In this paper, summation convention is applied for the subscripts, and the $(*)_{,i}$ denotes $\partial (*)/\partial x_i$.

In the reactive gas analysis, the chemical reactions of species can not be ignored. In this paper, the m-species which density expressed $\rho^{(1)}$, $\rho^{(2)}$, $\cdots$, $\rho^{(m)}$ is considered. The superscript with bracket (i) represents the i-th species.

The conservation of energy becomes as follows,

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$$\frac{\partial(\rho e)}{\partial t}+\{v_k(\rho e)\}_{,k}=\{v_m\sigma_{mk}\}_{,k}-q_{k,k}\cdots(3)$$
$$-Q_{k,k}$$

where e is total energy per unit mass including kinetic energy, and q_i is heat flux vector. Q_i is defined by next equation.

$$Q_i=\sum_{(k)}V_i^{(k)}h^{(k)} \quad \cdots\cdots(4)$$

$h^{(i)}$ is enthalpy for t-th species, and $V_i^{(k)}$ is diffusion velocity which is given as follows.

$$V_i^{(k)}=-\rho D^{(k)}\{Y^{(k)}\}_{,i} \quad \cdots\cdots(5)$$

where

$$Y^{(i)}=\rho^{(i)}/\rho \quad \cdots\cdots(6)$$

and $D^{(k)}$ is diffusion constant.

Conservation of mass of i-th species is written,

$$\frac{\partial\rho^{(i)}}{\partial t}+\{v_k\rho^{(i)}\}_{,k}=-\{V_k^{(i)}\}_{,k}+W \quad \cdots\cdots(7)$$

where W is source term from reaction.

In this paper, the flow assumed to be laminar, and one temperature model is used. The pressure of mixed gas is calculated by Dalton's law of partial pressure,

$$p=\sum_{(k)}\rho(c_p^{(k)}-c_v^{(k)})T \quad \cdots\cdots(8)$$

where $c^{(k)}_p$ and $c^{(k)}_v$ is specific heart at constant pressure and at constant volume of k-th species respectively. $c^{(k)}_v$ is given,

$$c_v^{(k)}=\frac{3}{2}R^{(k)} \quad c_v^{(k)}=\frac{5}{2}R^{(k)} \quad \cdots\cdots(9)$$

for atomic species, and diatomic species respectively. $R^{(k)}$ is gas constant for k-t species, and $c^{(k)}_p=c^{(k)}_v+R^{(k)}$.

2.2 Matrix Description

The conservation form of 2D basic equations are expressed as following matrix form.

$$\frac{\partial U}{\partial t}+\frac{\partial F_x}{\partial x}+\frac{\partial F_y}{\partial y}+\underline{\frac{F_y}{y}}=\frac{\partial G_x}{\partial x}+\frac{\partial G_y}{\partial y}+\underline{\frac{G_y'}{y}}+S \quad \cdots\cdots(10)$$

where, U, F_i, G_i can be described as follows.

$$U=\begin{bmatrix}\rho\\ \rho v_x\\ \rho v_y\\ \rho e\\ \rho^{(k)}\end{bmatrix} \qquad F_i=v_iU$$

$$G_i=\begin{bmatrix}0\\ \sigma_{ix}\\ \sigma_{iy}\\ v_m\sigma_{mi}-q_i-Q_i\\ -V_i^{(k)}\end{bmatrix} \quad S=\begin{bmatrix}0\\0\\0\\0\\w^{(k)}\end{bmatrix} \quad \cdots\cdots(11)$$

if the problem is axi-symmetric, the underlined term should be considered. G'_y is expressed as follows.

$$G_y'=\begin{bmatrix}0\\ \sigma_{yx}\\ \sigma_{yy}-\sigma_{\theta\theta}\\ v_m\sigma_{my}-q_y-Q_y\\ -V_y^{(k)}\end{bmatrix} \quad \cdots\cdots(12)'$$

The FEM formulation based on weighted residual method becomes finally next form.

$$\int_A w\frac{\partial U}{\partial t}dA=-\int_A w\left(\frac{\partial F_1}{\partial x}+\frac{\partial F_2}{\partial y}\right)dA$$
$$-\int_A\left[\frac{\partial w}{\partial x}G_1+\frac{\partial w}{\partial y}G_2\right]dA+\int_{SP}w\bar{P}dS+\int_A wSdA$$
$$\underline{-\int_A w\left(\frac{F_2'}{y}-\frac{G_2'-G_2}{y}\right)dA} \quad \cdots\cdots(13)$$

where w is weighting function.

2.3 Reaction model

In this study, 5 species (N_2, O_2 N, O, NO) are considered, and next 5 reactions of dissociation are taken into consideration.

① $O_2 + M \rightarrow O + O + M$
② $N_2 + M \rightarrow N + N + M$
③ $NO + M \rightarrow N + O + M$
④ $NO + O \rightarrow N + O_2$
⑤ $O + N_2 \rightarrow N + NO$

$M = N_2,\ O_2,\ N,\ O,\ NO$

The forward reaction rate coefficient k_f is assumed to be next equation.

$$k_f = CT^s \exp(-T_d / T) \quad \cdots\cdots(14)$$

The constants in this equation, C (cm^3/mole), S, $Td(K)$ for these reactions are shown by Park[6], and they are shown in Table 1.

Table 1 Constants for Eq.(14)

Reaction①	C	S	Td(K)
M=N	8.250E+19	-1.000	59,500
M=O	8.250E+19	-1.000	59,500
M=N2	2.750E+19	-1.000	59,500
M=O2	2.750E+19	-1.000	59.500
M=NO	2.750E+19	-1.000	59,500
Reaction②	C	S	Td
M=N	1.110E+22	-1.600	113,200
M=O	1.110E+22	-1.600	113,200
M=N2	3.700E+21	-1.600	113,200
M=O2	3.700E+21	-1.600	113,200
M=NO	3.700E+21	-1.600	113,200
Reaction③	C	S	Td
M=N	4.600E+17	-0.500	75,500
M=O	4.600E+17	-0.500	75,500
M=N2	2.300E+17	-0.500	75,500
M=O2	2.300E+17	-0.500	75,500
M=NO	2.300E+17	-0.500	75,500
Reaction④	C	S	Td
	2.160E+08	1.290	19,220
Reaction⑤	C	S	Td
	3.180E+13	0.100	37,700
Reaction⑥	C	S	Td
	1.530E+11	-0.370	32,000

The reverse rates of these reaction k_r is expressed as

$$k_r = k_f / K \quad \cdots\cdots(15)$$

where K is equilibrium constant, and K is expressed as the function of temperature as next form[6].

$$K(T) = \exp\left(A_1 + A_2 \ln Z + A_3 Z + A_4 Z^2 + A_5 Z^3\right) \quad \cdots\cdots(16)$$

where Z=10,000/T, and the values of constants A_1,..,A_5 are shown in table 2.

Table 2 Constants for Eq.(16)

	A1	A2	A3	A4	A5
Reaction ①	2.855	0.988	-6.181	-0.023	-0.001
Reaction ②	1.858	-1.325	-9.856	-0.174	0.008
Reaction ③	0.792	-0.492	-6.761	-0.091	0.004
Reaction ④	-2.063	-1.480	-0.580	-0.114	0.005
Reaction ⑤	1.066	-0.833	-3.095	-0.084	0.004
Reaction ⑥	-7.053	-0.532	-4.429	0.150	-0.007

3. Results and discussion

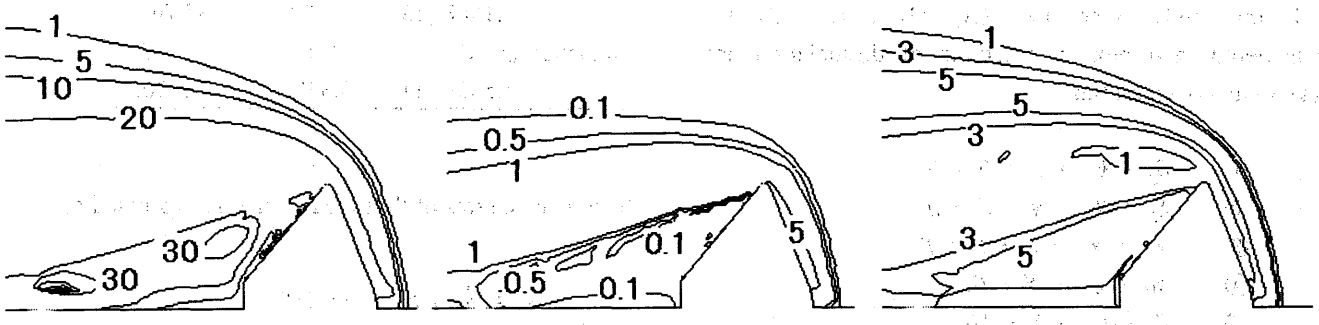
3.1 Simulation Condition

In this paper, the simulation conditions are chosen as the same as experimental conditions in Fukuyama University. That is, density $\rho = 4.5 \times 10^{-3}$ kg/m^3, pressure p=70 Pa. The capsule model used in this paper is the same as used by using ideal gas simulation[5]. In this case of this calculation, the number of nodes is 2700, and number of elements is 2590.

3.2 Simulation results of M25

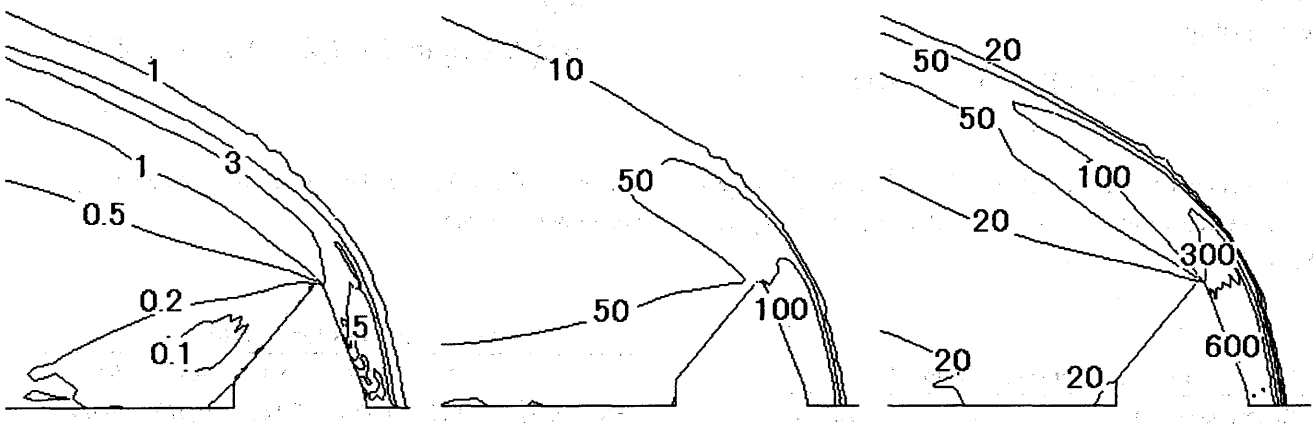
In the case of Mach number 25 simulation, the velocity is 3750 m/s and dt is set at 0.8×10^{-7} s.

Figure 1 shows the calculated O, N, NO distributions. It is found that atomic oxygen O is distributed around



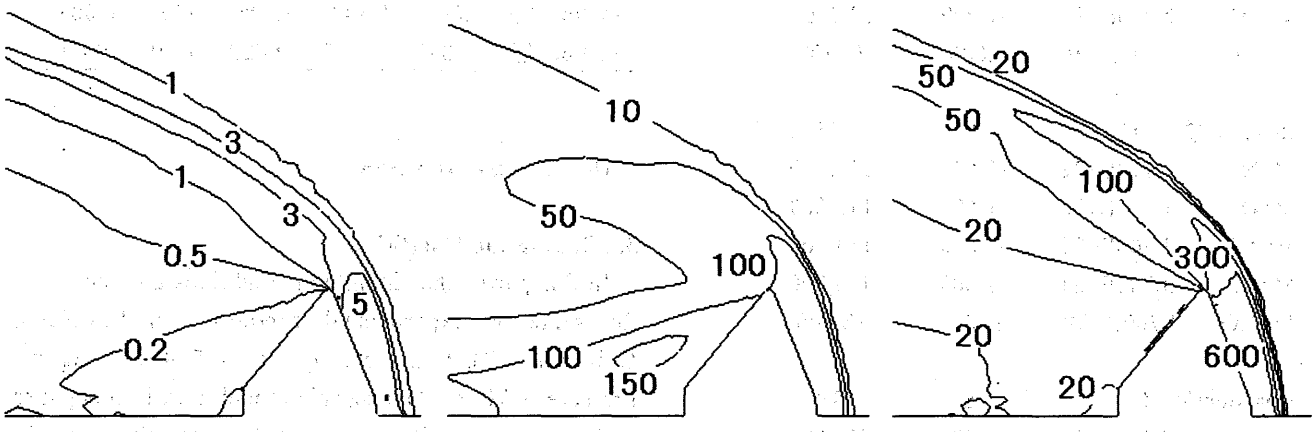
(a) O (b) N (c) NO

Fig.1 O, N, NO distribution $\rho^{(i)}/\rho$ (%) (M25)



(a) ρ/ρ_∞, (b) T/T_∞, (c) p/p_∞.

Fig.2 Simulation results for reacting gas. (M25)



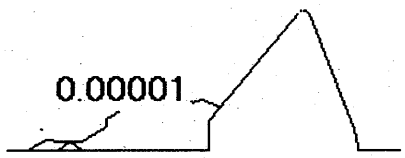
(a) ρ/ρ_∞, (b) T/T_∞, (c) p/p_∞.

Fig.3 Simulation results for ideal gas. (M25)

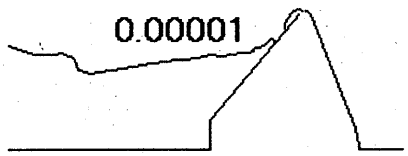
capsule. The N and NO distribution is not obvious.

Figure 2 shows the distribution of density, temperature and pressure. It is found that temperature is 100 times larger than T_∞ so, the temperature around the capsule is about 5000K. Therefore, the dissociation of oxygen molecule is appeared.

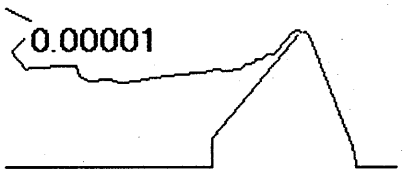
Figure 3 shows the ideal gas simulation results of ρ/ρ_∞, T/T_∞, p/p_∞. Comparing this figure to Fig.2, the



(a) O



(b) N



(c) NO

Fig.4 Simulation results of M10. $\rho^{(i)}/\rho$ (%)

effect of reacting gas calculation is found. That is, although the density and pressure distributions are not so difficult from Fig. 2, the temperature is higher than Fig. 2. It is found that the dissociation of oxygen molecule lower the temperature.

3.3 Simulation results of M10

In the calculation of Mach number 10, the velocity is set 1500 m/s, and $dt=2.0\times10^{-7}$ s. Other simulation conditions are same as the Mach 25 calculation.

The obtained O, N and NO distribution is shown Fig.4. It can be said that these atomic distribution is almost zero. In addition, the density, temperature and pressure distributions are the same as the ideal gas simulation. Therefore, in the case of simulating Mach number 10 flow under the condition of gun tunnel in Fukuyama University, the gas can be treated as ideal gas.

4. Conclusions

In order to analyze the hypersonic flow around the space vehicle, flow simulation considering reactive flow is conducted. The following remarks are obtained.

1) The FEM simulation program for reacting gas flow including dissociation is developed.
2) In the Mach number 25 simulation, the reacting gas effect for the O distribution is found. Temperature around the capsule decreased by considering dissociation, but shock shape, pressure distribution is not obviously changed comparing the results of ideal gas simulation.
3) In the Mach 10 simulation the dissociation of air is not found.

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