

# SUPERSONIC FLOW OF HYDROGEN AND AIR IN A DUCT WITH VARIABLE AREA

Seung Wook Baek\* and Jong Uck Kim\*\*

(Received May 25, 1992)

A chemically nonequilibrium supersonic flow of hydrogen and air has been investigated in a duct with conically divergent or convergent walls. Elementary reaction schemes of radicals involved in reaction of hydrogen-air have been considered and solved through the CHEMKIN code. The aim was to promote an understanding of characteristics of chemically nonequilibrium supersonic flow by introducing a simple mathematical formulation. The temperature, pressure, and density all were found to decrease for divergent ducts as the flow was accelerated, whereas they increased for a slightly convergent duct or a constant cross-sectional area duct. For the divergent nozzle with a greater degree the flow became chemically frozen. But it was quite necessary to take account of the effect of chemical nonequilibrium in a moderately expanded or all convergent conical ducts. As was expected, it was found that the temperature, pressure and Mach number were reduced for a fuel-lean mixture.

**Key Words:** Chemically Nonequilibrium, Supersonic Flow, Nozzle Flow

## NOMENCLATURE

$A$	: Area
$E$	: Activation energy
$h$	: Mixture enthalpy
$h_i$	: Specific enthalpy of species $i$
$M$	: Mach number
$p$	: Pressure
$R$	: Universal gas constant
$T$	: Temperature
$u$	: Velocity
$\bar{W}_i$	: Molecular weight of species $i$
$\bar{W}$	: Mean molecular weight
$x$	: Spatial coordinate
$y_i$	: Mass fraction
$z$	: Cone angle
$\alpha$	: Enhanced efficiency factor
$\Phi$	: Equivalence ratio
$\rho$	: Density
$\omega_i$	: Molar production of species $i$

### Subscripts

$i$	: Species
$o$	: Initial state

## 1. INTRODUCTION

A hydrogen-fueled supersonic combustion ramjet has been investigated for use in aerospace propulsion systems. Considerable amount of effort has been directed toward exploring

the reacting flow in its combustion chamber with complex chemistry (Drummond et al., 1989 and Jachimowski (1988)). Mixing enhancement problem in such a supersonic combustor was also examined by Drummond et al.(1989) in order to achieve a high combustor efficiency.

Pioneer work in the reacting gas flow through an expanding nozzle was experimentally as well as theoretically accomplished by Wegener(1959). Thereafter, Westenberg and Favin(1963) illustrated the complex chemical kinetics in the supersonic nozzle flow of hydrogen-air with simple elementary reactions. Recently Correa and Mani(1989) presented a model for nonequilibrium combustion of hydrogen in air and studied it in one-dimensional supersonic flow by introducing a systematically simplified model of kinetics. In their study the rotational and vibrational relaxation times were also assumed small compared with the relaxation chemical times. The thermodynamic equilibrium between the internal modes of the molecules was therefore assumed to be valid at the local temperature. The results were then presented by defining the reaction progress variable for a premixed flow of hydrogen-air which has a constant value of mixture fraction.

In this study chemically nonequilibrium supersonic flow of hydrogen and air has been analyzed in a duct with variable area. The full chemical kinetic schemes of hydrogen-air has been incorporated to see the effects of the mixture equivalence ratio and cone angle on the fluid dynamic and thermochemical variables. The results for species concentration were directly presented in terms of mass fraction instead of reaction progress variable as was done in Correa and Mani (1989). They were then discussed in comparison with those obtained in chemically frozen flow.

The aim is to promote an understanding of chemically nonequilibrium flow by using a simple mathematical formulation which retains the essential physical features of the problem. This work is also related to the ignition distance and reaction length in which a supersonic combustion of  $H_2$  and  $O_2$  is completed as was done by Yip(1989).

\*Korea Advanced Institute of Science and Technology Aerospace Engineering Department, 373-1, Kusung-dong, Yuseong-ku, Taejon, Korea

\*\*Agency for Defense Development, Propulsion Division, P.O. Box 35 Taejon, Korea

## 2. THEORETICAL MODELS

The basic assumptions made in this study are as follows :

(1) The flow is steady and quasi-one dimensional flow in a channel of varying area.

(2) The fuel is mixed with air instantaneously at the fuel injection point. Therefore the effect of turbulent mixing on the chemistry cannot be explained.

(3) Thermal and mass diffusion effects are negligible.

(4) The internal degrees of freedom of the molecules are in equilibrium with the local temperature. But the flow is chemically nonequilibrium.

(5) Heat loss and friction at the walls are neglected.

The steady quasi-one dimensional equivalents of the non-linear conservation equations then have the following form :

Over-all continuity

$$\rho u A = \text{constant} \quad (1)$$

Species continuity

$$\frac{d(\rho y_i u A)}{dx} = \omega_i W_i A \quad (2)$$

Momentum

$$\rho u \frac{du}{dx} + \frac{dp}{dx} = 0 \quad (3)$$

Energy

$$\frac{dh}{dx} + u \frac{du}{dx} = 0 \quad (4)$$

Equation of state

$$p = \rho R T / \bar{W} \quad (5)$$

Mean molecular weight

$$\bar{W} = \left( \sum_i \frac{y_i}{W_i} \right)^{-1} \quad (6)$$

Eq. (1) can be rewritten in following differential form

$$\frac{1}{\rho} \frac{d\rho}{dx} + \frac{1}{u} \frac{du}{dx} + \frac{1}{A} \frac{dA}{dx} = 0 \quad (7)$$

Substituting Eq. (7) into Eq. (2) gives

$$\frac{dy_i}{dx} = \frac{\omega_i W_i}{\rho u} \quad (8)$$

Equation of state (5) can be recast in following differential form

$$\frac{1}{p} \frac{dp}{dx} = \frac{1}{\rho} \frac{d\rho}{dx} + \frac{1}{T} \frac{dT}{dx} - \frac{1}{\bar{W}} \frac{d\bar{W}}{dx} \quad (9)$$

Eqs. (3),(4) and (7)~(9) contain (15) variables in this study : The mixture density  $\rho$ , flow velocity  $u$ , mixture temperature  $T$ , pressure  $p$ , mixture enthalpy  $h = \sum h_i y_i$ , and ten species mass fraction  $y_i$  ( $i=1, 2, \dots, 10$ ). Other variables are : Specific enthalpies of the species  $h_i$ , molar production rates of the species  $\omega_i$ , molecular weights of the species  $W_i$ , cross-sectional area of the duct  $A$ , and the universal gas constant  $R$ .

The model considered a total of ten species ( $H_2, O_2, H_2, H, O, N, OH, HO_2, H_2O, NO$ ) and 32 elementary reaction steps. The reaction scheme and the corresponding rate constants are shown in Table 1. The reverse rate constants are related to the forward rate constants through the equilibrium constants. The CHEMKIN subroutines (Kee, et al., 1980) were used to calculate the molar production rates of the species  $\omega_i$  in Eq. (8).

The governing system of ordinary differential equations

derived above constitutes an initial value problem, once initial values of  $T_o, p_o, y_{i,o}$ , and initial Mach number  $M_o$  are known at the inlet of nozzle. They were solved via the highly reliable code LSODE written by Hindmarsh(1980) which is applicable for the very wide range of stiff initial value problems.

## 3. RESULTS AND DISCUSSION

The solution in this study is begun at the entrance to a divergent section only, since most of the chemical interest is in the divergent section of the nozzle. Even though a non-linear rate of change of the cross-sectional area with respect to axial distance  $dA/dx$  can be chosen as shown in Fig. 1, only a linear variation is considered here. Therefore the nozzle shape may be regarded as conical. The entrance diameter is taken as 5 cm and the nozzle length 50 cm. All calculations were done for four configurations ( $\tan z = -0.005, 0, 0.1, 0.2$ ). A case of  $\tan z = 0$  corresponds to the duct with uniform cross-sectional area, both  $\tan z = 0.1$  and  $0.2$ , divergent duct, and  $\tan z = -0.005$ , a slightly convergent duct.

Unless otherwise specified, all the calculations presented below are carried out for the following conditions : the stoichiometric equivalence ratio of hydrogen-air mixture  $\Phi = 1$ , initial Mach number  $M_o = 3$ , initial mixture temperature  $T_o = 2200$  K, and initial static pressure  $p_o = 0.4$  atm.

Figs. 2~5 show the temperature, pressure, Mach number and density variations for four different nozzle configurations. For divergent ducts ( $\tan z = 0.1$  and  $0.2$ ) the temperature, pressure, and density drop very smoothly along the flow direction as the mixture expands. But the pressure is almost fully expanded in a short distance compared with the others, while the flow is being quickly accelerated downstream. For

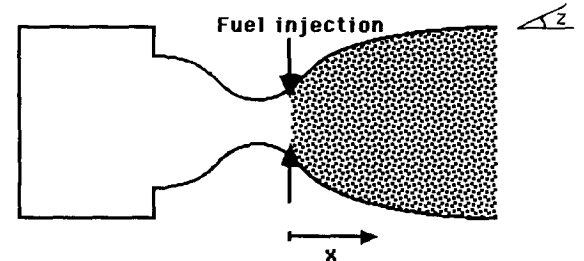


Fig. 1 Schematic of the problem

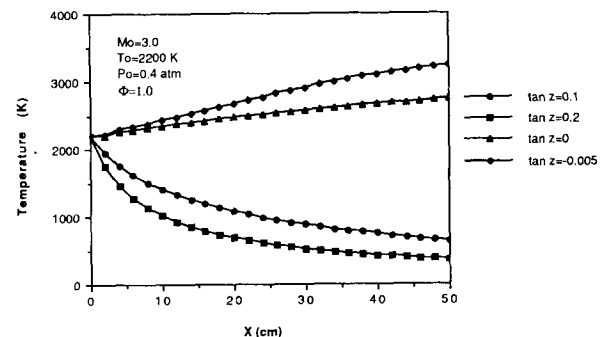


Fig. 2 Temperature variation for  $M_o = 3.0$ ,  $T_o = 2200$  K,  $p_o = 0.4$  atm, and  $\Phi = 1.0$

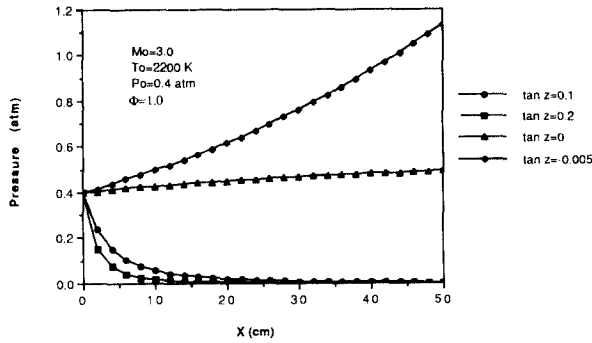


Fig. 3 Pressure variation for  $M_o=3.0$ ,  $T_o=2200$  K,  $p_o=0.4$  atm, and  $\Phi=1.0$

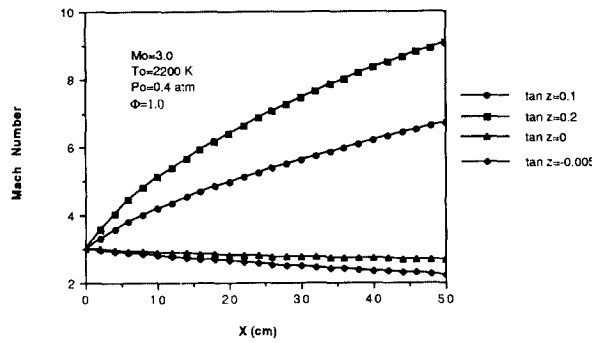


Fig. 4 Mach number variation for  $M_o=3.0$ ,  $T_o=2200$ K,  $p_o=0.4$ atm, and  $\Phi=1.0$

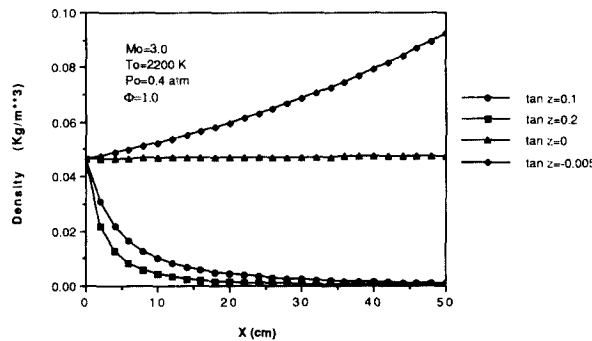


Fig. 5 Density variation for  $M_o=3.0$ ,  $T_o=2200$  K,  $p_o=0.4$  atm, and  $\Phi=1.0$

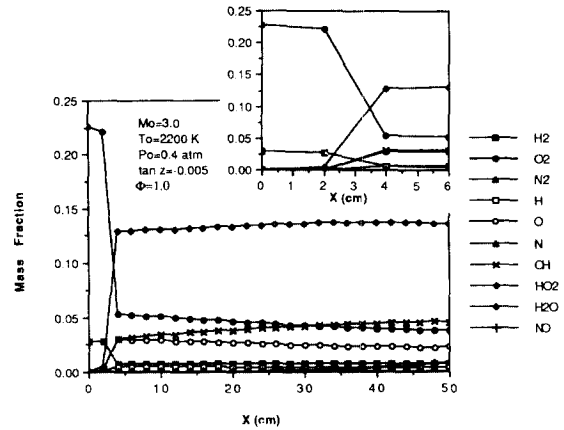


Fig. 6 Mass fraction variation for  $M_o=3.0$ ,  $T_o=2200$ K,  $p_o=0.4$ atm,  $\Phi=1.0$  and  $\tan z=-0.005$

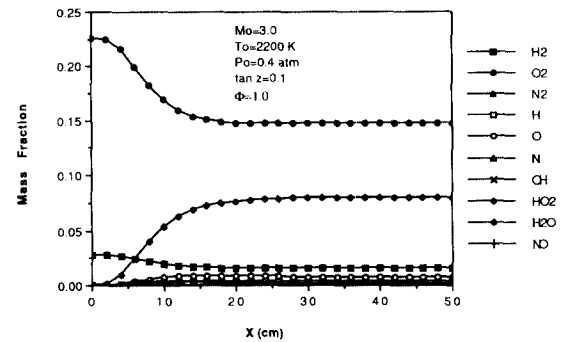


Fig. 7 Mass fraction variation for  $M_o=3.0$ ,  $T_o=2200$  K,  $p_o=0.4$ atm,  $\Phi=1.0$  and  $\tan z=0.1$

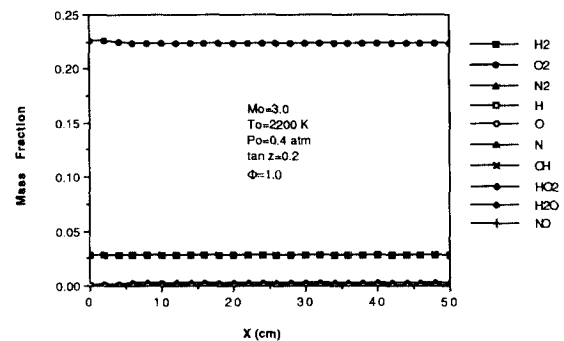


Fig. 8 Mass fraction variation for  $M_o=3.0$ ,  $T_o=2200$ K,  $p_o=0.4$  atm,  $\Phi=1.0$  and  $\tan z=0.2$

a duct with uniform cross-sectional area ( $\tan z=0$ ), the temperature and pressure are seen to sluggishly increase as the mixture is kinetically reacted. But the density just negligibly increases as much as the flow is decelerated. However for a convergent duct ( $\tan^2=-0.005$ ) the temperature is observed to slowly increase and the flow is decelerated as the flow is rapidly compressed. It must also be noted that the increasing rate of the pressure and density is considerably higher than other variables, even if the rate of change of area is very minor.

Figs. 6~8 represent the mass fraction variation of various species for three duct configurations such as  $\tan z=-0.005$ , 0.1 and 0.2 respectively. The mass fraction of nitrogen molecule is just insignificantly dissociated from its initial

value of 0.745. Therefore it is not shown in the figure for a pictorial clarity of other species. In general these figures illustrate the complex behavior of the gas composition as the mixture flow is expanded or compressed along the axial direction. A common characteristic is such that the  $H_2$ -air mixture is more dissociated as the angle of the conical wall  $z$  is diminished. Fig. 8 plotted for the case of  $\tan z=0.2$ , however, shows a simple trend, in which all the species are seen to nearly maintain their initial values all the way to the exit. In other words the mixture is almost chemically frozen because the temperature drops rapidly due to the substantial expansion to a greater degree. Subsequently there is also no obvious change found even in the magnified plot of the mean molecular weight as shown in Fig. 9. But for ducts with the

slope of  $\tan \alpha = 0$  and  $-0.005$ , there exists a visual variation in the mean molecular weight, even though the absolute value of its change is minor.

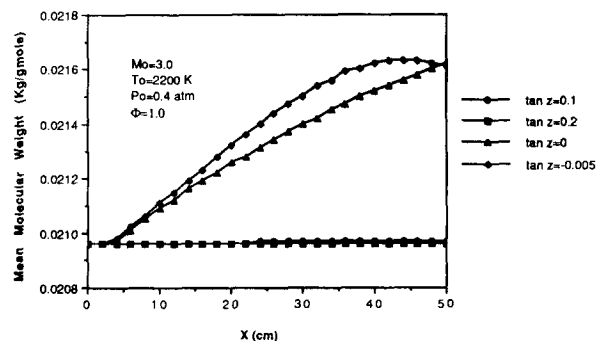
In Figs. 6 and 7 appreciable amount of atomic H, O and radical OH is respectively observed resulting from the controlling three body reactions listed in Table 1. As the duct angle  $\alpha$  is reduced, the required nozzle length, within which the combustion tends toward completion, decreases and less hydrogen remains after the completion of combustion as shown in Figs. 6~8. This tendency is in a good agreement with the fact that the pressure and temperature should be kept high enough for a fast and complete combustion.

Figs. 10~13 illustrate the comparison of temperature, pressure, Mach number, and density between chemically nonequilibrium and chemically frozen flows for three different nozzle shapes ( $\tan \alpha = -0.005, 0.1$  and  $0.2$ ). Frozen flow solutions were obtained from the same chemically nonequilibrium program simply by setting all the molar production rates  $\omega_i$  equal to zero. As mentioned above, between two flows only a marginal difference could be found in each figure for  $\tan \alpha = 0.2$ . Therefore a supersonic chemical flow in the divergent nozzle with a greater degree is considered to be chemically frozen. However there exists a significant difference for the case of  $\tan \alpha = -0.005$ . Especially the temperature and pressure in the chemically nonequilibrium flow deviate more significantly from those in the chemically frozen flow. The energy produced by the hydrogen oxidation results in much higher temperature in the chemically nonequilibrium flow. Density as well as pressure is also higher in the nonequilibrium flow. But the velocity becomes lower in the nonequilibrium flow to satisfy the mass continuity. The results obtained for  $\tan \alpha = 0.1$  show a similar trend, although its diversion is smaller, in temperature and Mach number. Consequently the effect of chemical nonequilibrium must be taken into account to predict the supersonic chemical flow inside a moderately expanded or all convergent conical ducts. But in all the other supersonic flows expanded more than moderate the reaction may be considered to be chemically

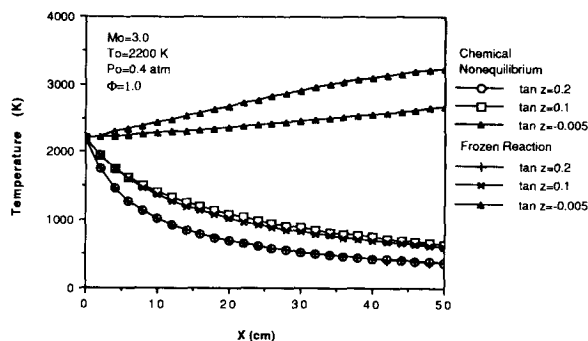
**Table 1** Rate constants for elementary reactions  $k = aT^b \exp(-E/RT)$

No.	Reaction	a	b	E
1	$H_2 + O_2 = 2OH$	$1.7 \times 10^{13}$	0	47780
2	$H_2 + OH = H_2H + O$	$5.2 \times 10^{13}$	0	6500
3	$H + O_2 = OH + O$	$1.22 \times 10^{17}$	-0.907	16620
4	$O + H_2 = OH + H$	$1.8 \times 10^{10}$	1	8826
5	$H + O_2 + M = HO_2 + M$ $\alpha$ of $H_2O = 20$	$2.0 \times 10^{15}$	0	-870
6	$OH + HO_2 = H_2O + O_2$	$1.2 \times 10^{13}$	0	0
7	$H + HO_2 = 2OH$	$6.0 \times 10^{13}$	0	0
8	$O + HO_2 = O_2 + OH$	$1.0 \times 10^{13}$	0	0
9	$2OH + O = H_2O$	$1.7 \times 10^5$	2.03	-1190.
10	$H_2 + M = 2H + M$ $\alpha$ of $H_2O = 5$	$2.23 \times 10^{12}$	0.5	92600
11	$O_2 + M = 2O + M$	$1.85 \times 10^{11}$	0.5	95560
12	$H + OH + M = H_2O + M$ $\alpha$ of $H_2O = 20$	$7.5 \times 10^{23}$	-2.6	0
13	$H + HO_2 = H_2 + O_2$	$1.3 \times 10^{13}$	0	0
14	$O + N_2 = NO + N$	$1.4 \times 10^{14}$	0	75800
15	$N + O_2 = NO + O$	$6.4 \times 10^9$	1	6280
16	$OH + N = NO + H$	$4.0 \times 10^{13}$	0	0

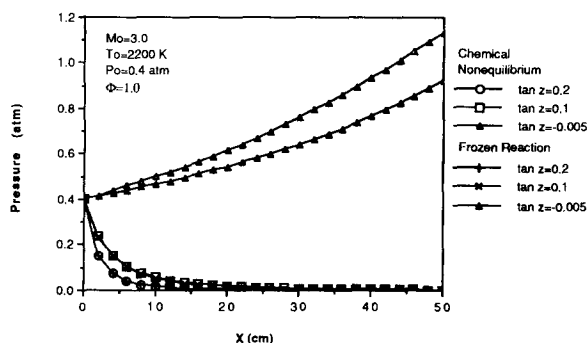
Bimolecular rate constants are given in units of  $cm^3/(mol \cdot s)$ , and termolecular rate constants in units of  $cm^6/(mol \cdot s)$ . The unit of E is cal/mole. M stands for the third-body and  $\alpha$  is the enhanced efficiency factor.



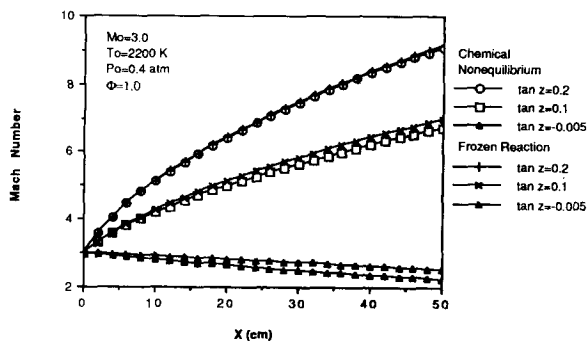
**Fig. 9** Mean molecular weight variation for  $M_o = 3.0$ ,  $T_o = 2200K$ ,  $p_o = 0.4$  atm, and  $\Phi = 1.0$



**Fig. 10** Comparison of temperature variation between chemically nonequilibrium flow and chemically frozen flow



**Fig. 11** Comparison of pressure variation between chemically nonequilibrium flow and chemically frozen flow



**Fig. 12** Comparison of Mach number variation between chemically nonequilibrium flow and chemically frozen flow

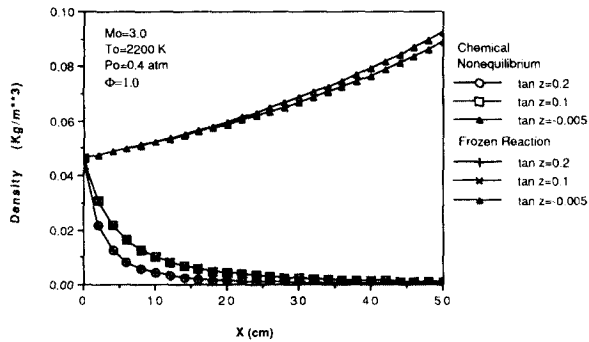


Fig. 13 Comparison of density variation between chemically nonequilibrium flow and chemically frozen flow

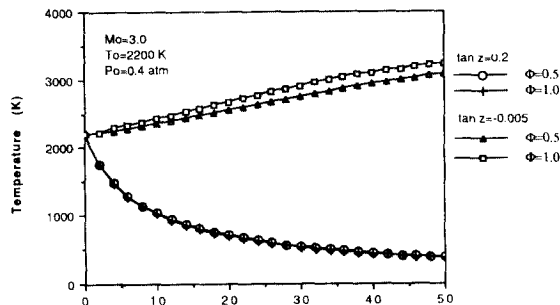


Fig. 14 Comparison of temperature variation for equivalence ratio  $\Phi=0.5$  and  $1.0$

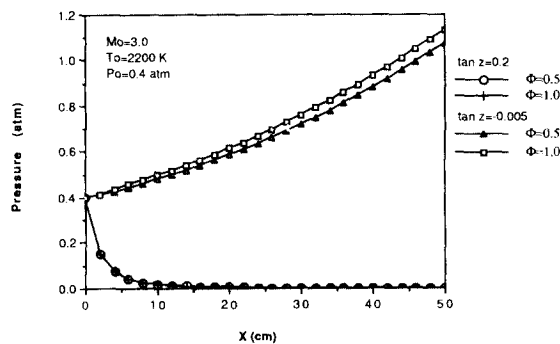


Fig. 15 Comparison of pressure variation for equivalence ratio  $\Phi=0.5$  and  $1.0$

frozen.

Figs. 14~15 show the comparison of temperature and pressure, for two different duct shapes ( $\tan z = -0.005$  and  $0.2$ ), when the equivalence ratio  $\Phi$  is changed from 1 (stoichiometric mixture) to 0.5 ( $H_2$  lean mixture). The mixture temperature, pressure and Mach number for a slightly convergent duct ( $\tan z = -0.005$ ) are lowered for  $\Phi=0.5$ . But there is no illustrative difference for the case of  $\tan z = 0.2$ , since the flow becomes chemically frozen aforementioned.

### 4. CONCLUSIONS

In this study a chemically-nonequilibrium supersonic premixed flow of hydrogen and air has been examined in a duct with conically divergent or convergent configurations. The practical application could be found in a hydrogen-fueled

supersonic combustion ramjet. A multiple chemical kinetic scheme of hydrogen-air has been incorporated into the formulation in order to see the effects of dissociation and recombination on the thermal-fluid variables. The governing system of ordinary differential equations were integrated by using the stiff initial value problem solver LSODE. The results for chemically nonequilibrium flow were then compared with those for chemically frozen flow.

It was found that the temperature, pressure, and density all decreased for divergent ducts as the flow was accelerated. However, they increased for a slightly convergent duct or a constant cross-sectional area duct as the flow was decelerated. Except for the divergent nozzle with a greater degree, in which the flow became chemically frozen, the chemically nonequilibrium results deviated from the solutions obtained from the chemically frozen flow. The more reduced the cone angle is, the larger the deviation. Therefore more radicals were produced when the supersonic mixture flow was compressed rather than expanded. Consequently it is clear that the finite-rate dissociation-recombination chemistry plays an important role in the supersonic combustion. As was expected, the temperature, pressure and Mach number were reduced as the mixture became fuel-lean.

### ACKNOWLEDGEMENT

It is our pleasure to acknowledge support for this work from the Korean Agency for Defense Development under the Long-Range Fundamental Research Fund.

### REFERENCES

Correa, S.M. and Mani, R., 1989, "Nonequilibrium Model for Hydrogen Combustion in Supersonic Flow," J. of Propulsion and Power, Vol. 5, pp. 523~528.

Drummond, J.P., Carpenter, M.H., Riggins D.W. and Adams, M.S., 1989, "Mixing Enhancement in a Supersonic Combustor," AIAA Paper No. 89~2794.

Hindmarsh, A.C., 1980, "LSODE : Livermore Solver for Ordinary Differential Equations," Lawrence Livermore Lab. Transaction No. 3342.

Drummond, J.P., Rogers, R.C. and Hussaini, M.Y., 1986, "A Detailed Numerical Model of a Supersonic Reacting Mixing Layer," AIAA Paper No. 86~1427.

Jachimowski, C.J., 1988, "An Analytical Study of the Hydrogen-Air Reaction Mechanism with Application to Scramjet Combustion," NASA TP 2791.

Kee, R.J., Miller, J.A. and Jefferson, T.H., 1980, "CHEMKIN : A General-Purpose, Problem-Independent, Transportable, Fortran Chemical Kinetics Code Package," Sandia Report 80~8003.

Wegener, P.P., 1959, "Supersonic Nozzle Flow with a Reacting Gas Mixture," Physics of Fluids, Vol. 2, pp. 264~275.

Western, A.A. and Favin, S., 1963, "Complex Chemical Kinetics in Supersonic Nozzle Flow," 9th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh.

Yip, T., 1989, "Ignition Delay and Characteristic Reaction Length in Shock Induced Supersonic Combustion," AIAA/ASME/SAE/ASEE 25th Joint Propulsion Conference, Monterey, AIAA Paper No. 89~2567.