STUDY OF THE EXPANSION OF HYDROCARBON-OXYGEN PRODUCTS THROUGH SUPERSONIC NOZZLE

M.A.ELKADY*, M.M.KEMRY*, M.ABDEL AAL**
Mech. Eng.Dept.,Faculty of Eng. Al-azhar University

ABSTRACT

The objective of the present work is to investigate the expansion of steady, isentropic, one-dimensional flow of hydrocarbon- oxygen combustion products through a convergent -dirvergent nozzle.The study includes the development of three models. The first model assumes a frozen gas mixture composition. The second model assumes the equilibrium composition of the gas mixture. The third model considers the actual flow process for which the reactions controlling the mixture composition have finite rates (kinetic model). The continuity, momentum, energy, and state equations are solved numerically along the longitudinal direction of the nozzle. The flow properties and species concentrations are determined for different equivalance ratios and combustion chamber pressures.

The resluts of the present investigation indicate that the flow characteristics determined using the three models are almost identical in the convergent part of the nozzle. While a substational deviation is experinced in the divergent part recommending the use of the kinetic model for accurate simulation of a real flow problem.

* Associate Professor

** Demonstrator

INTRODUCTION

The assessement of the characteristics of a chemically reacting gas flowing through asupersonic nozzle plays a great role in the design and development of many propulsive devices.

Previous work in the field of reacting flow assumes that the flow expanding through a supersonic nozzle may be studied by considering that the mixture tends to follow more or less the compositiom characteristics of equilibrium at the local temperature and pressure until the reactions involved can no longer keep up even approximately ith the rate of change of these variables. The gas then rapidly freezes to a fixed composition for the remainder of the flow. Most real propellants and wind tunnel gas mixtures are more complicated than this insofar as their chemistry is concerned .

In the present work different approaches are investigated for the determination of the characteristics of a chemically reacting gas flowing through a supersonic nozzle. The first approach (frozen model) assumes that the rates of the chemical reactions involved are zero. The second approach (eqilibrium model) assumes that the reactions are attaining equilibrium, in other words their rates are infinte. The third approach (kinetic model) considers the finite rates of the chemical reactions involved.

The hydrocarbon used for the present work is kerosine of the form $C_{12}H_{26}$ burned with oxygen. Eight species are considered to be present in the combustion products in significant quantities.These species are H_2O, H_2, OH, H, CO_2, CO, O_2, and O

The equilibrium composition was determined using the model developed by Vickland et al [1], and amended by Benson et al [2]. The solution procedure for isentropic flow of this model is presented in the section of "Solution procedure". In the remaining part of this section and the section of "governing equations". The model of non-equilibrium flow is only considered. As will be shown, the frozen flow is a special case of this flow.

Concerning the nonequilibrium model the elementary reactions responsible for the formation and decomposition of these species (kinetic scheme), are chosen in accordance with the avaibability and certainity of their kinetic data .

The oxidation of carbon monoxide is represented by the reaction

$$CO+OH == CO_2+H \qquad (1)$$

as all hydrocarbons oxidation eventually involves the oxidation of CO through this reaction [3] .

The termolecular radical recombination reactions are represented by the reactions.

$$O+O+M == O2+M$$
$$H+H+M == H2+M \qquad (ii)$$
$$H+OH+M == H2O+M$$

The chain branching steps are considered to include the following reactions.

$$OH+H2 == H2O+H$$
$$O+H2 == OH+H \qquad (iii)$$
$$H+O2 == OH+O$$

The solution was obtained for a convergent divergent nozzle of conical convergent part of semiangle of $\pi/4$, a conical divergent part of a semianglé of $\pi/12$, and curved throat of radius of curvature of 5.08 cm, and a throat diameter of 2.54 cm.

Three computer programmes were developed to cary out the required calculations for the three approaches.

GOVERNING EQUATIONS

The basic equations governing the non-equilibrium flow are the fluid dynamic equations together with the species continuity relations [4]. The formers are.

Momentum equation

$$V\, dv/dz + dp/dz = 0 \qquad (1)$$

Energy equation

$$dh/dz + V\, dv/dz = 0 \qquad (2)$$

Continuity equation

$$\frac{1}{\rho}\frac{d\rho}{dz} + \frac{1}{A}\frac{dA}{dz} + \frac{1}{V}\frac{dV}{dz} = 0 \qquad (3)$$

The species continuity relations are :

$$dF_i /dz = (A/\dot{m})\, d[A_i]_J /dt \qquad (4)$$

where $d[A_i]_J /dt = \Delta\mu_{iJ} \{k_{fJ}\pi\, [A_i]^{\mu'_{iJ}} - k_{bJ}\pi\, [A_i]^{\mu''_{iJ}} \}$ (5)

A perfect gas equation of state is assumed :

$$P = R\, T\Sigma\, F_i \qquad (6)$$

Appropriate forms of the above differential equations are attained by employing the specified area method [ ]; and assuming perfect gas relations :

$$\frac{dV}{dZ} = \frac{V}{M^2-1}\left[\frac{1}{A}\frac{dA}{dZ} - \frac{B}{pVa^2}\right] \qquad (7)$$

$$\frac{d\rho}{dZ} = -\rho\left[\frac{M}{M^2-1}\left[\frac{1}{A}\frac{dA}{dZ} - \frac{B}{pVa^2}\right] + \frac{B}{pVa^2}\right] \qquad (8)$$

$$\frac{dT}{dZ} = -T\left[\frac{(\gamma-1)M}{M^2-1}\left[\frac{1}{A}\frac{dA}{dZ} - \frac{B}{pVa^2}\right]\frac{(\gamma-1)\sum_{i=1}^{n}}{\gamma pV} h_i\sigma_i\right] \qquad (9)$$

where $B = \sum_i^n\left[\gamma R_1 T - (\gamma - 1)\ h_i\right]\sigma_i$

$$P = T\Sigma\ M\ R\ F \qquad (10)$$

$$\frac{dF_i}{dZ} = \frac{A\ \sigma_i}{\dot{m}} \qquad (i=1,2,3,...5) \qquad (11)$$

$$\sigma_{ij} = (d[A_i]_j/dt)\ M_i \qquad (12)$$

The unknown quantites are determined as follows. The flow variables V, p, and T are determined from equations (7) through (9). Five of the species mole fractions are determined from equation (11), the other three species mole fractions are obtained from the following atomic balance relations :

$$(F_{CO} + F_{CO2}) = \text{constant} \qquad (13)$$

$$(2F_{H2O} + 2F_{H2} + F_{OH} + F_H) = \text{constant} \qquad (14)$$

$$(2F_{CO2} + F_{CO} + 2F_{O2} + F_O + F_{H2O} + F_{OH}) = \text{constant} \qquad (15)$$

Finally the pressure is obtained from equation (10) .
The formation of the five equations represented by equation (11) requires the selection of a kinetic scheme The selected kinetic scheme together with the reactions forward and backward rate constants are given in [3] .
This scheme is presented in the section of "introduction" by reactions (i) to (iii) and it is used to formulate the five species rate equations. As an example, appliction of equation (11) for carbon monoxide on the given scheme yields

$$dF_{CO}/dz = (A/\dot{m})\,\rho^2[-k_{fi}\ F_{CO}\ F_{OH} + k_{bi}\ F_{CO2}\ F_H]$$

Equations (7) through (15) forms a set of stiff nonlinear ordinary differential equations in the twelve unknowns namely, temperature T, velocity V, density p, pressure P, and the concentrations of the eight species. This set of equations is integrated numerically using fourth-order Rung-Kutta numerical method [5]. The solution is obtained for various equivalance ratios and different combustion chamber pressures.

It is to be noticed that the governing equations for the frozen flow can be obtained by letting the species source function $\sigma_i = 0$, $(i=1,.....,n)$.

SOLUTION PROCEDURE

Three approaches are considered for the solution of the flow through the nozzle they will be briefly discussed in this section.

To intialise the solution the following procedure is performed. The adiabatic flame temperature in the nozzle inlet is dete-rmined from the known information of the fuel composition, the equivelance ratio ϕ, and the combustion chamber pressure This is performed by trail and error using the Secant numerical method [5] the corresponding equilibrium compisition of combusition chamber products is then determined by appling the equilibrium model (see [6]) after modification to suit the case of the present study. The intial condetions mentioned above are considered to be the same for all invistigated models.

The solution procedure for the equilibrium model, is performed as follows. The critical pressure at the nozzle throat is assumed. This pressure must lead to a Mach number of unity at throat. The first est- imated value is that obtained using constant specific heat ratio. The composition of the gas mixture as well as the fluid properties at various locations of the nozzle is conducted using the following step by step procedure. The pressure drop for each step is specified in accordance with the number of steps (between inlet and throat), the stagnat- ion pressure (at inlet), and the estimated throat pressure. The flow under isentropic conditions is calculated; starting from inlet till the throat. The Mach number at the throat is then checked with its unity value. If convergence is attained, then solution is established, otherwise another estimated value of the throat pressure is assumed and the above procedure is repeated. The Secant method was employed for determining the throat pressure. It is to be noticed that the above procedure are only carried out in the converging part of the nozzle.No iterations are required in the diverg- ent part of the nozzle where the solution is directly obtained by specifying the pressure at any position. Thus, assume at any location the pressure is specified. The solut- ion at that location is performed as follows. First, the temperature is estimated. The species mole frac- tions are then determined from equilibrium model. The enthalpy is determined for the specified temperature and composition (see Benson [7]). The velocity is calculated from the assumption of constant statgnition enthalpy. The density is calculated from the equation of state. The area can be determined from the relation $A/A^* = \rho^* V^* / \rho V$. Finally, the entropy is calculated; where it is checked with isentropic condition. If the assumption of isentropic flow is specified then the solution is attained, otherwise the above procedure is repeated with another estimated temperature and by appling Secant itteration technique.

The non-equilibrium (kinetic) model is applied in the supersonic portion of the nozzle, after negligibly small intial region of the throat for which the solution of the rate equations is quite sensitive to trunction errors. After several trails it was found that the kinetic model was successful to start solution at an area ratio of about 1.04. It is to be noticed that the solution of all models leads to the same results in the convergent part of the nozzle. This was verified by the present investigation (for the frozen and equilibrium models). The assumption of starting the non-equilibrium solution in the divergent part was made by many investigators; see [4], [8], and [9]. In the non-equilibrium model, equations (7) through (15) are numerically integrated by specifying the step size Z (variable step sizes are employed in the solution). The numeical fourth order Rung Kutta method is employed in the solution of the governing equations.

The flow properties for the case of frozen flow are determined along the nozzle, simply by setting all the forward and backward rate constants equal to zero. The solution starts from the nozzle enterance, and is extended to the nozzle exit. An itteration procedure is performed on the mass flow rate, to give monotonic decrease in temperature and density through- out the nozzle.

RESULTS AND DISCUSSION

The investigation includes the effect of equivalance ratio, and inlet stagnation pressure, on the flow characteristics. Three values of the equivalance ratio are chosen namely; 0.6, 1.0, and 1.5, and two values of the inlet stagnation pressure of 10, and 100 bar are considered. The results of the present investigation are plotted in figures 1 to 7

Fig 1 shows the effect of O on the variation of CO and H2 mol fractions with area ratio down stream of the throat, with an inlet stagnation pressure of 100 bar. From this figure it is clear that, as the area ratio increases substational deviation takes place between the equilibrium solution and kinetic solution. Another important observation is that the kinetic solution is approaching limitting constant values as area ratio increases. This means that the flow at this position is reaching the frozen condition. As shown from the figure, the freezing location depends on the value of ϕ. Fig 2 shows the effect of Pc on the mole fractions of CO and H2 at ϕ=1. The same behavior of frozen condition is declared. The figure indicates that as Pc decrease, the frozen condition comes at earlier values of

A/A*. This is due to the lower value of the temperature attained for lower values of pressure. The results of figures 1 and 2 confirm the work of ref. [4].

Fig 3 shows variations of M, V, and T with A/A* at ϕ =1 and Pc=10 bar for the three models. The solutions of the equilibrium and frozen models lead to compatible results in the subsonic part of the nozzle. Appreciable diviations are observed in the diverging part of the nozzle. By considering that the kinetic model is the most realistic solution, it is clear from the figure that the equilibrium model overestimates the values of T and V and consequently, underestimates the values of M. An important observation is that the difference in solutions of the frozen and kinetic models are of small quantites. The reason for this is that the temperature at an area ratio nearly greater than 10 is not exeeding about 1500 K, (for a satgnation temperature of about 3500 K) where the kinetic model is approaching the freezing condition This behaviour was observed in all investigated conditions; and for this reason the solutions of the kinetic and equilibrium are only introduced in the remaining figures.

Varition of T with A/A* is presented in fig 4 where the effect of ϕ is investigated at Pc=100 bar.Again, substainal diviations are declared between the equilibrium and kinetic solutions. The diviation becomes of larger values for the correct mixture (ϕ =1). This is due to the fact that, in the equilibrium model, the correct mixture results in temperature of high values than those for the incorrect mixtures. As shown from the figure, the temperature predicted by the equilibrium modelis greatly affected by the values of ϕ; while it is of limitted effect for the kinetic solution.

Fig 5 illustrates the effect of varing the inlet stagnation pressure on the predicted temperature in the supersonic region for correct mixture. From this figure it is clear that the effect of increasing Pc is to increase the temperature. This figure indicates the same trend of fig 4, where the equilibrium predicts temperature of higher values than those predicted by the kinetic solution.

Fig 6, 7 illustrates the variation of the Mach number with area ratio. Fig 6 shows the effect of variation of ϕ (Pc=100 bar), while fig 7 shows the effect of variation of Pc (ϕ=1). Both figures indicates that the equilibrium model underestimates the values of M. This can be concluded from figures 4 and 5, where, the temperature predicted by the equilibrium model is of higher value. Fig 6 indicates that the effect of O (for the same model) is that, as it approaches unity (ϕ=1) the Mach number decreases (M for ϕ=1.5 is not illustrated in the figure because it is approximately coinsides with that for ϕ=0.6). The effect of increasing pressure is to reduce the value of M as declared in fig 7.

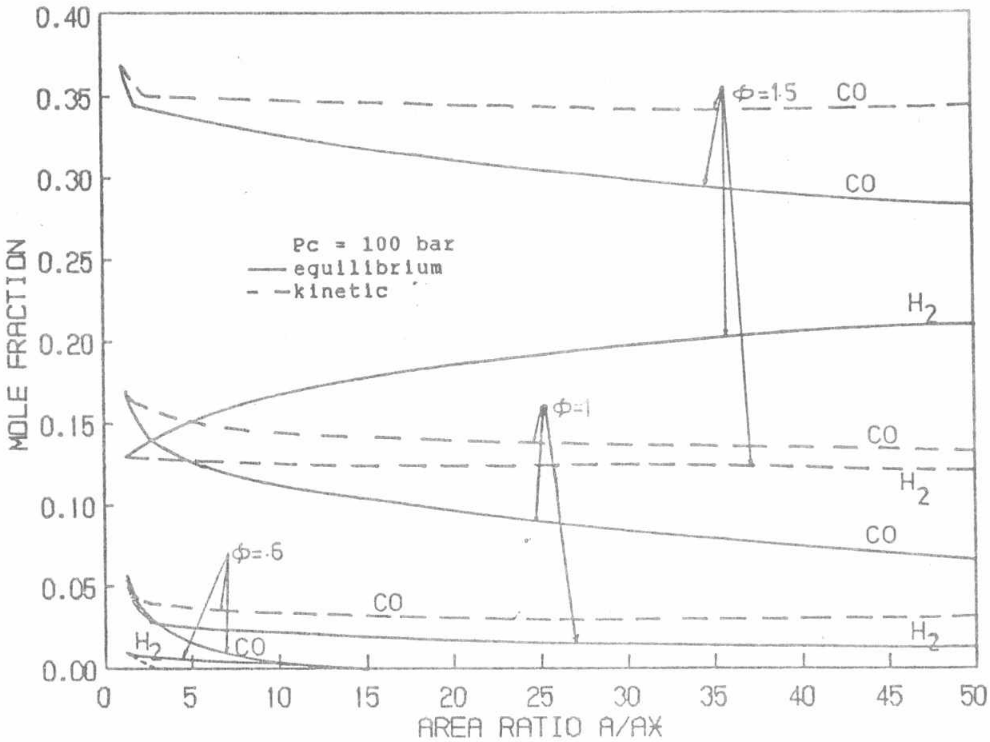

Fig 1 Variation of CO and H2 mole fractions with area ratio for equilibrium and kinetic.

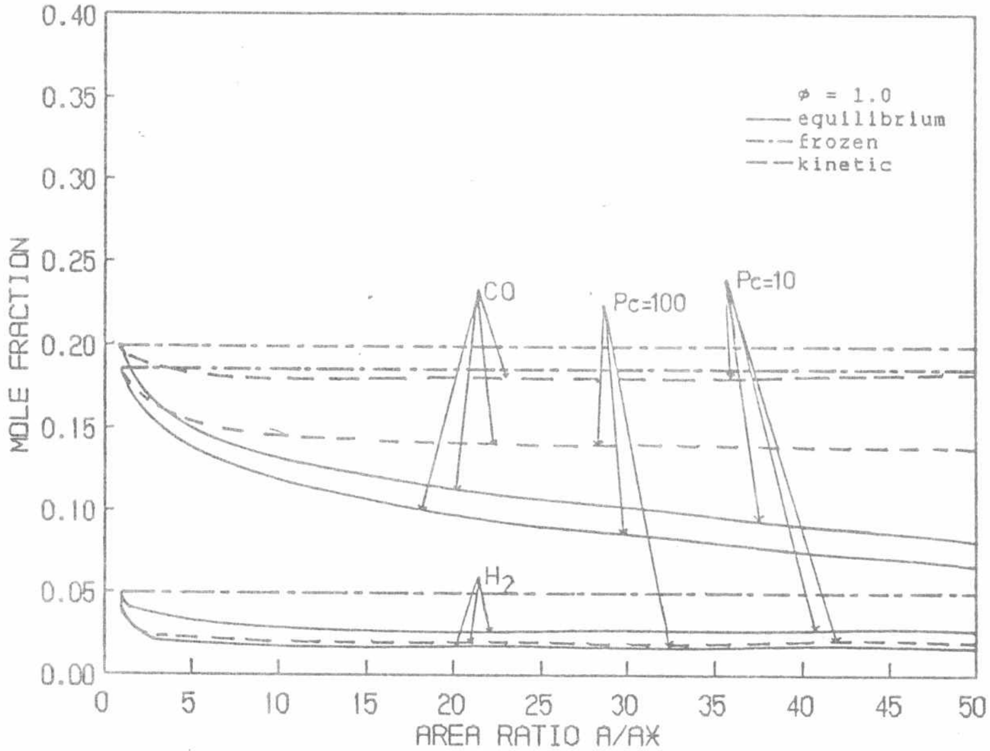

Fig 2 Variation of CO and H2 mole fractions with area ratio for three models, φ = 1.0

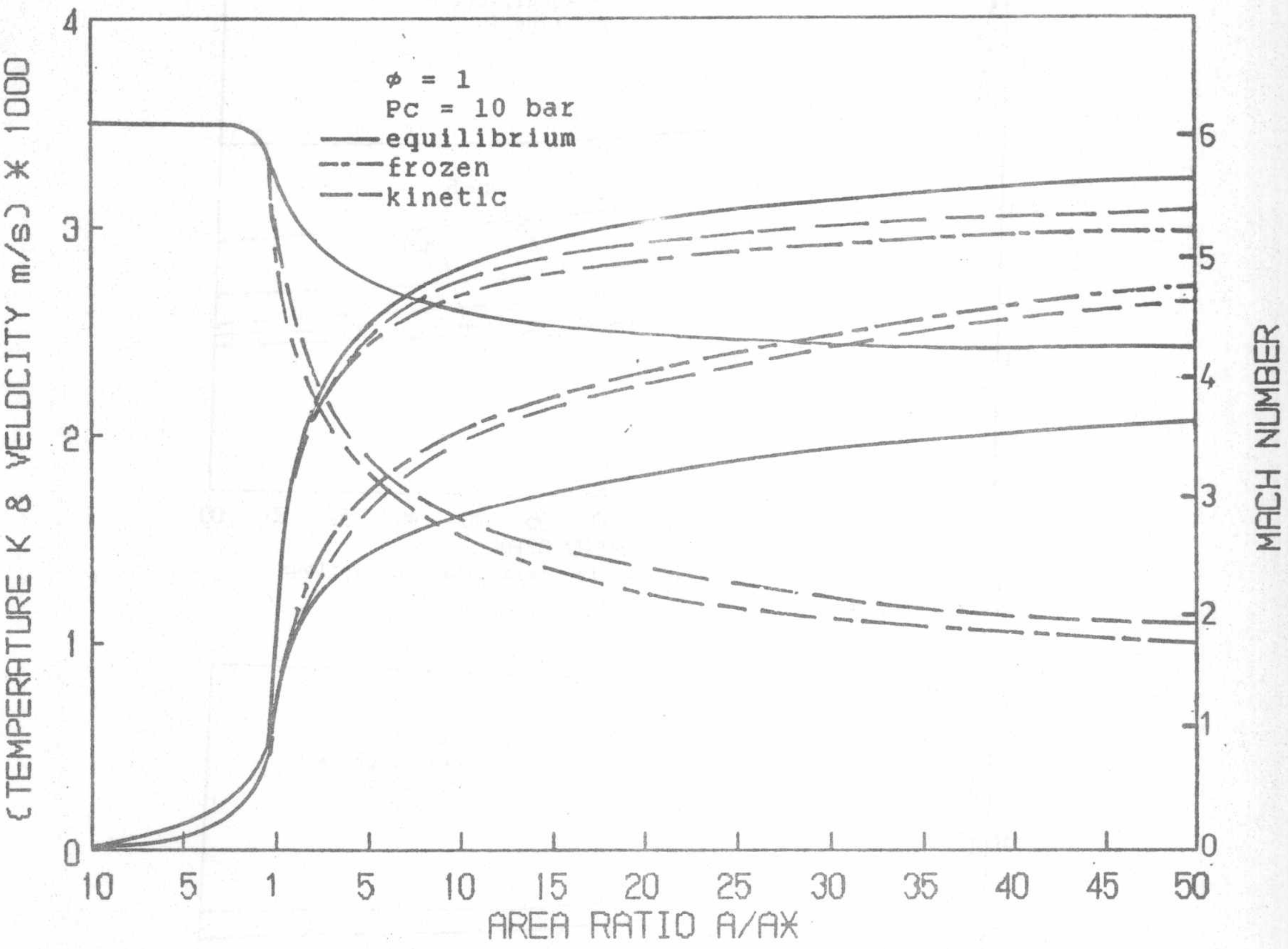

Fig 3 Temperature, velocity, and Mach number with the area ratio for the three modele.

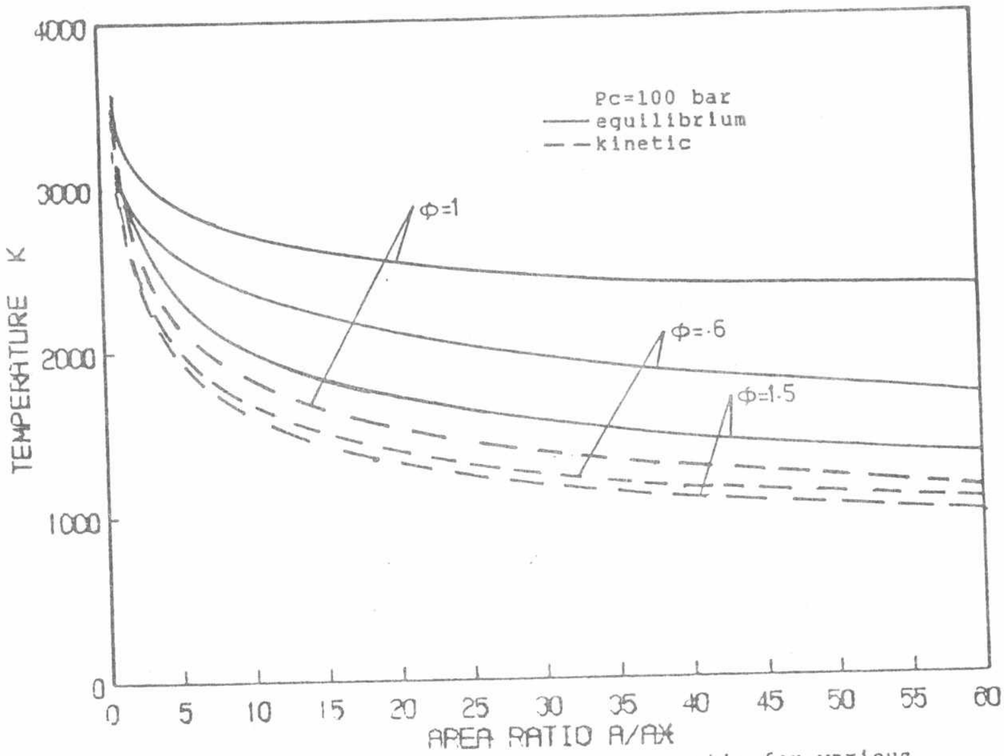

Fig 4 Variation of temperature with area ratio for various equivalance ratios.

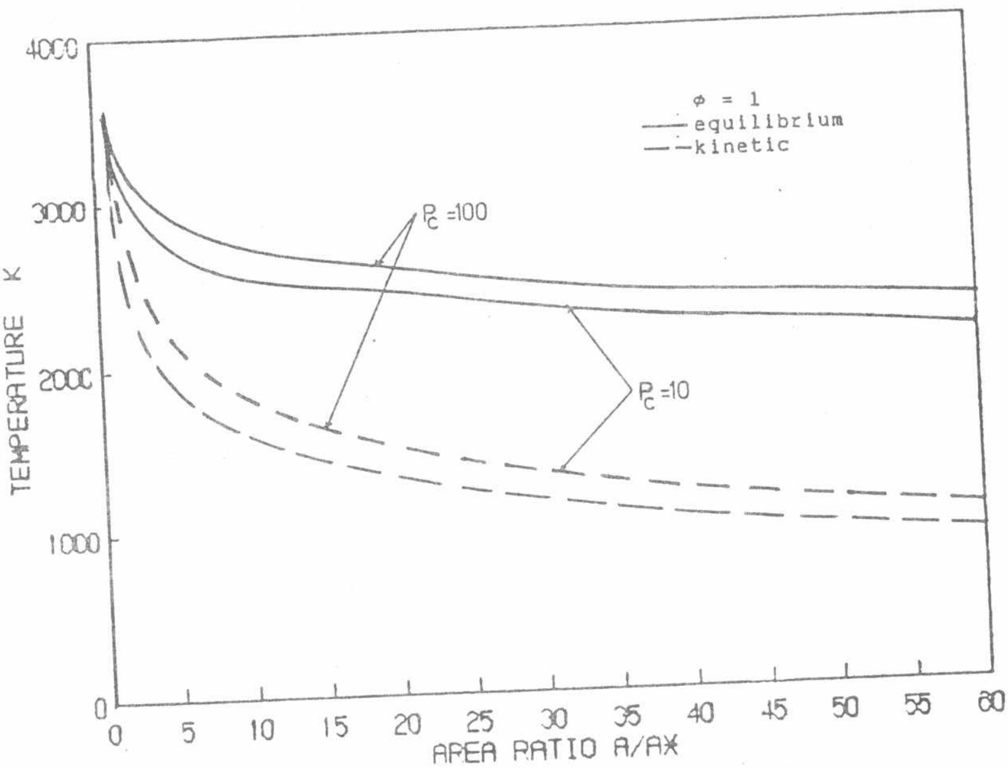

Fig 5 Variation of temperature with area ratio for varrious combustion chamber pressure.

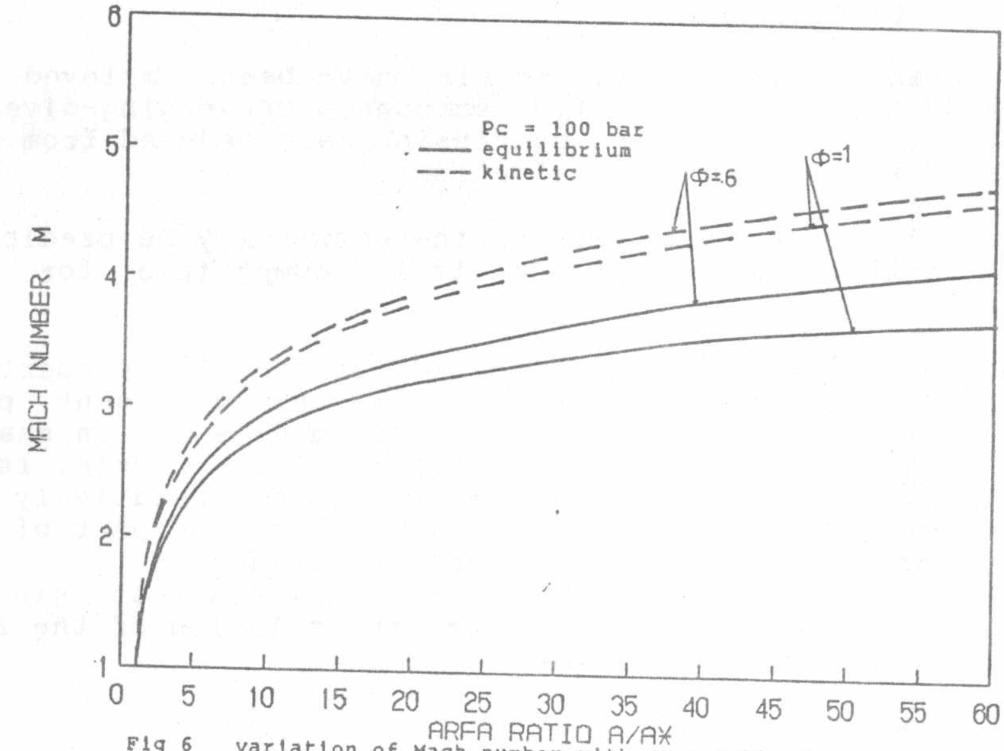

Fig 6 variation of Mach number with area ratio for various equivalance ratios.

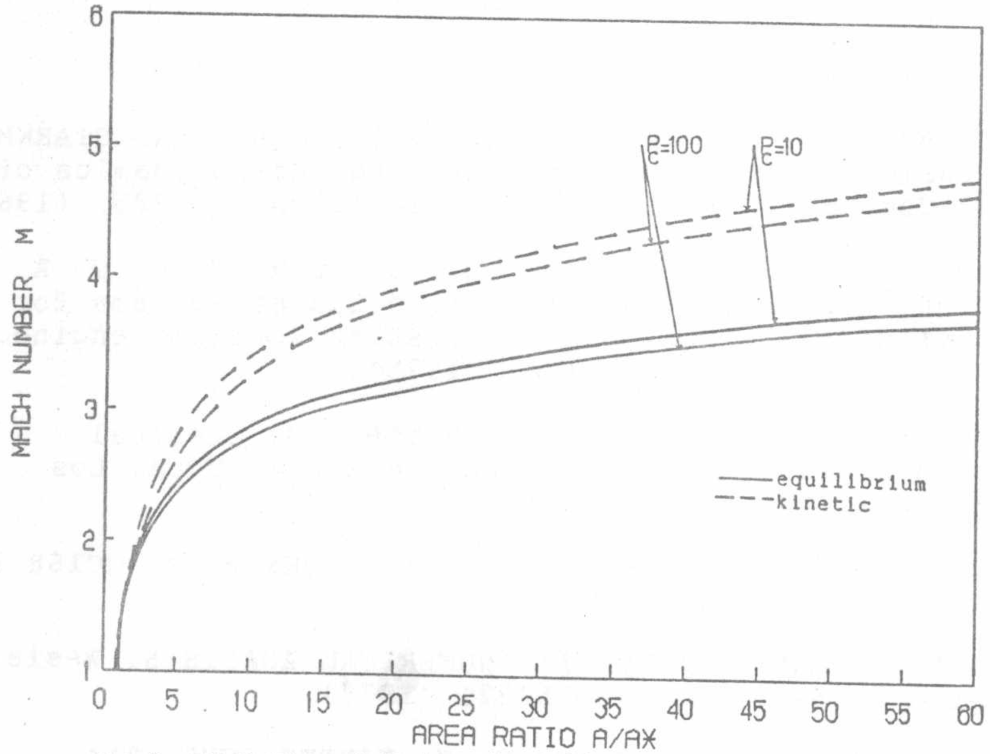

Fig 7 Variation of Mach number with area ratio for various combustion chamber pressures

CONCLUSIONS

In the present study three models have been employed for predicting the isentropic flow through a converging-diverging nozzle. The following conclusions are dedused from the results of the present investigation .

The flow in supersonic part of the nozzle may be predicted by any of three models, since it is compatiple for all models .

Substantial diviations are observed for the flow properties as predicted by the three models in the divergent part nozzle . The non-equilibrium and frozen models are in nearly good agreements in the divergent part of the nozzle. It is expected that this agreement is due to the relatively low temperature exihbites in most of the diverging part of the nozzle. For the case of the present investigation .
From the above declarations it is concluded that kinetic model is the recommended one for the solution of the flow under high temperature levels.

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NOMENCLATURE

A	cross sectional area .
[Ai]	volume based concentration of species i.
a	speed of sound.
Fi	mass based concentration of species i.
I	chemical species, (I=1,.......n).
IJ	species interaction J.
J	chemical reaction (J=1, m).
KfJ	forward rate constant of reaction J.
KbJ	backward rate constant of reaction J.
Kp	equilibrium constant = KfJ/KbJ.
M	Mach number.
Mi	molecular weight of species i.
P	pressure in bar.
Pc	combustion chamber pressure.
R	universal gas constant.
Ri	characteristic gas constant of species i.
T	temperature K
V	velocity m/s.
Z	distance along the flow direction m.
γ	specific heat ratio
μiJ	stoichiometeric coefficient of species i in reaction J.
μiJ	stoichiometeric coefficient of species i in reaction J.
μiJ	iJ - iJ
π	the products a1 a2 an
	density of the mixture.
σ	species source function of species i.
ϕ	equivalance ratio .
*	denotes critical (i.e. sonic) property.