HYPERSONIC NOZZLE FLOW ANALYSIS USING EQUILIBRIUM CHEMISTRY MODEL

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ABSTRACT

For high speed flows particularly those in hypersonic regime, the assumption of ideal gas is no longer valid and inclusion of chemistry model is necessary for accurate computations. A computer code is developed which performs computations both with ideal gas law and equilibrium chemistry model, the later one gives accurate results particularly for high density flows, where reaction rates are high. Computations are performed for compressible, steady, inviscid flow within a nozzle. The computer code uses Steger and Warming flux vector splitting scheme to solve the gas dynamic equations. Equilibrium chemistry model is implemented in the code by entering high temperature equilibrium air properties using polynomial correlations of the calculated and tabulated data. The results are presented using both the ideal gas law and equilibrium chemistry model and compared with the experimental and published data. At low mach numbers, both models gave precise results. However, at very high mach numbers ideal gas law over predicted the post shock temperature while the equilibrium chemistry model accurately predicted the post shock temperature. Also at very high mach numbers equilibrium chemistry model predicted a drop in the specific heats ratio distribution and increase in density distribution in post shock regions as compared to ideal gas law. However the effect on the post shock pressure is minimal. Thus the equilibrium chemistry model is found to be better suited to high temperature gas dynamics as compared to Ideal gas Law.

INTRODUCTION

For high speed flows particularly those in hypersonic regime, the assumption of ideal gas is no longer valid. That is due to the high temperatures associated with such flow fields. As a consequence of high temperatures, molecules will dissociate and may ionize. Therefore, the effect of chemistry must be accounted for if a reasonable computation is to be carried out. The underlying assumption of ideal gas law is that specific heat coefficients are constant and, hence specific heat ratio γ is also constant. For example, a value of γ =1.4 is used for air. In addition the internal energy is expressed solely as a function of temperature. For a chemically reacting flow the internal energy must be a function of temperature as well as pressure. The ratio of specific heats is no longer constant and a new definition of γ is required. For flow fields where chemical reaction rates are extremely high, the reactions take place instantaneously. Thus reaction is completed before fluid has a chance to move downstream. Such a flow is called *equilibirium* or more precisely *chemical equilibirium*. For a wide range of applications, the utilization of an equilibirium chemistry model will provide an accurate solution. That is particularly true for high-density flows where a sufficient number of molecular collisions take place and reaction rates are high. In this paper solution method for such flow fields with *equilibrium chemistry* model is presented.

NOMENCLATURE

- u Velocity of fluid [m/s]
- ρ Density of fluid [kg/m³]
- S Area $[m^2]$
- P Pressure $[N/m^2]$
- e_t Total energy [J/kg]
- Q Conservative variable vector
- E Flux vector
- E⁺ Positive flux vector
- E⁻ Negative flux vector
- H Source terms vector
- x Cartesian coordinate
- Δx Spatial step size [m]
- Δt Temporal time step [sec]
- γ Ratio of specific heats
- a Speed of sound [m/sec]
- D Damping term
- ϵ_{e} Damping coefficient
- M Mach number
- T Temperature [K]
- t Time [sec]
- n Iteration level
- R Gas constant of the mixture
- A Flux jacobian matrix
- A⁺ Positive flux jacobian matrix
- A Negative flux jacobian matrix
- u_i Free stream velocity
- T_i Free stream temperature
- P_i Free stream pressure

GEOMETRY

The nozzle with cross-sectional area defined by following relation is selected for the analysis [1].

(1)
$$S(x) = 1.398 + 0.347 \tanh (0.8x-4)$$

Inflow \longrightarrow Outflow

FIG.1 Geometry of the problem

The nozzle entrance is located at x=1.2cm and nozzle exit at x=8.0cm

INITIAL AND BOUNDARY CONDITIONS

The inflow boundary conditions are set by specification of the inlet Mach number, temperature, and pressure. The outflow boundary condition is set by specification of pressure so as to position a normal shock at x=4.0cm.In order to demonstrate the differences in the computed flow fields by ideal law gas model and equilibrium chemistry model, inlet pressures of 79.8 N/m² and 26500 N/m² (corresponding to altitude of 50Km and 10 Km) are used. The inlet temperature is set to a fixed value of 230.44K, which is about the average value of the temperatures at the two altitudes. To start the solution, initial conditions are specified by specifying flow variables everywhere in the domain to be that of inflow conditions.

NUMERICAL FORMULATIONS

The Euler equations for a quasi one-dimensional flow may be expressed as:

Continuity,

(2)
$$\frac{\partial}{\partial t}(\rho S) + \frac{\partial}{\partial x}(\rho s) = 0$$

Momentum,

(3)
$$\frac{\partial}{\partial t}(\rho dS) + \frac{\partial}{\partial x}\left[(\rho d^2 + p)S\right] - p\frac{dS}{dx} = 0$$

Energy,

(4)
$$\frac{\partial}{\partial t}(\rho e_t S) + \frac{\partial}{\partial x}[(\rho e_t + p)uS] = 0$$

Where S is the cross-sectional area.

Combining all the above equations and expressing them in the flux vector form we get,

(5)
$$\frac{\partial}{\partial t}(SQ) + \frac{\partial E}{\partial x} - H = 0$$

Where

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho e_t \end{bmatrix}, E = S \begin{bmatrix} \rho u \\ \rho u^2 + p \\ (\rho e_t + p)u \end{bmatrix} \quad H = \frac{dS}{dx} \begin{bmatrix} 0 \\ p \\ 0 \end{bmatrix}$$

Generally two approaches are available for the numerical analysis of differential equations such as Euler or Navier-Stokes equations. These are implicit and explicit formulations. In the explicit formulation time derivative is approximated by a forward difference approximation, and is given by;

(6)
$$S \frac{Q^{n+1} - Q^n}{\Delta t} + \left(\frac{\partial E}{\partial x}\right)^n - H^n = 0$$

The second approach is the implicit formulation, in which the time derivative is approximated by a first order backward difference approximation given by;

(7)
$$S\frac{Q^{n+1}-Q^n}{\Delta t} + \left(\frac{\partial E}{\partial x}\right)^{n+1} - H^{n+1} = 0$$

The change in flow properties per time step is defined as

$$\Delta Q = Q^{n+1} - Q^n$$

 ΔQ is known as delta formulation and the FDE is commonly formulated in terms of it.

This method is based on flux vector E, which is the product of matrices A and Q.Here A, is the flux jacobian matrix and is given as,

(8)
$$A = S \begin{bmatrix} 0 & 1 & 0 \\ \left(\frac{\gamma - 3}{2}\right)u^2 & -(\gamma - 3)u & (\gamma - 1) \\ -\frac{ua^2}{\gamma - 1} + \left(\frac{1}{2}\gamma - 1\right)u^3 & \frac{a^2}{\gamma - 1} + \left(\frac{3}{2} - \gamma\right)u^2 & \gamma u \end{bmatrix}$$

Then the Eigen values and Eigen vectors of the flux jacobian matrix are determined. The flux vector E possesses the homogeneous property; therefore it may be split into sub vectors such that each sub vector is associated with positive or negative values of flux jacobian matrix. For a subsonic flow two of the Eigen values is positive and the third one is negative therefore the flux jacobian matrix is split according to

$$(9) \qquad A=A^++A^-$$

And the flux vector E may be split according to

(10)
$$E^+=A^+Q$$

$$(11) \quad E = A Q$$

For a supersonic flow, all the three Eigen values are positive and, therefore

(12)
$$A^{+}=A$$

(13) $A^{-}=0$

On the basis of splitting of flux vector E equation (6) is written as

(14)
$$S\frac{\Delta Q}{\Delta t} + \frac{\partial}{\partial x} \left(E^{+} + E^{-}\right)^{n} - H^{n} = 0$$

Either a first order or a second order approximation can be used for the spatial derivative.

A first order approximation for the space is given by

$$(15) \Delta Q = -\frac{1}{S} \left(\frac{\Delta r}{\Delta x} \right) \left[E_i^+ - E_{i-1}^+ + E_{i+1}^- - E_i^- \right] + \frac{1}{S} \left(\frac{\Delta r}{\Delta x} \right) H_i$$

While for a second order approximation the FDE is given by

$$(16) \Delta q = -\frac{1}{s} \left(\frac{\Delta r}{2\Delta x} \right) \left[E_{t-2}^{+} - 4E_{t-1}^{+} + 3E_{t-1}^{+} - 3E_{t-1}^{-} - 4E_{t+1}^{-} - 4E_{t+2}^{-} \right] + \frac{1}{s} \left(\frac{\Delta r}{\Delta x} \right) H_{t}^{-}$$

However it is clear from the above equation that at the second point the term E_{i-2}^+ , and at the second last point the term E_{i+2}^{-} will not be applicable. To solve this

problem first order equation is used for the second and second last grid point, while for all the other grid points the second order equation is used.

In the above equations the terms E^+ and E^- have been used which are given by

$$(17)_{E^{+}=S} \frac{\rho}{2\gamma} \begin{bmatrix} 2\gamma u + a - u \\ 2(\gamma - 1)u^{2} + (u + a)^{2} \\ (\gamma - 1)u^{2} + [(u + a)^{3}]/2 + [(3 - \gamma)(u + a)a^{2}]/[2(\gamma - 1)] \end{bmatrix}$$

and

$$(18) E^{-} = S \frac{\rho}{2\gamma} \begin{bmatrix} u-a \\ (u-a)^{2} \\ [(u-a)^{3}]/2 + [(3-\gamma)(u-a)a^{2}]/[2(\gamma-1)] \end{bmatrix}$$

The solution of equation of fluid motion provides velocity u, density ρ and total energy et from which internal energy can be determined.

With the ideal gas assumption the remaining variables pressure and temperature are determined with the following relations

(19)
$$p = \rho e (\gamma - 1)$$

(20)
$$T = \frac{p}{\rho R}$$

In the above formulations the value of γ was kept constant.

In the equilibrium chemistry model the values of velocity u, density ρ , total energy e_t internal energy e are determined by solution of equation of fluid motion but after that an effective γ denoted herein by $\hat{\gamma}$ is computed from the following relation;

$$\begin{array}{l} & \begin{pmatrix} & & \\ (21) & \gamma = a_1 + a_2 Y_1 + a_3 Z_1 + a_4 Y_1 Z_1 + a_5 Y_1^2 + a_6 Z_1^2 + a_7 Y_1 Z_1^2 + a_8 Z_1^3 + \\ & \frac{a_9 + a_{10} Y_1 + a_{11} Z_1 + a_{12} Y_1 Z_1}{1 + \exp\left[\left(a_{13} + a_{14} Y_1\right)\left(Z_1 + a_{15} Y_1 + a_{16}\right)\right]} \\ \text{Where} \qquad Y_1 = \log\left(\frac{\rho}{1.292}\right) \\ \text{and} \qquad Z_1 = \log\left(\frac{e}{78408.4}\right) \end{array}$$

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The corresponding units for the variables in the relation above are:

$$\binom{N}{m^2}$$
 for pressure, $\binom{kg}{m^3}$ for the density,

and $\binom{m}{\sec^2}$ for the internal energy .Once $\hat{\gamma}$ has been

computed, the equation of state is used to compute the pressure, i.e.;

(22)
$$p = \rho e \begin{pmatrix} \wedge \\ \gamma - 1 \end{pmatrix}$$

Now, the temperature (in units of Kelvin) is evaluated from the following relation;

$$\begin{aligned} &(23) \log \left(\frac{T}{151.78}\right) = b_1 + b_2 Y_2 + b_3 Z_2 + b_4 Y_2 Z_2 + b_5 Y_2^2 + b_6 Z_2^2 + b_7 Y_2^2 Z_2 + b_8 Y_2 Z_2^2 + b_8 Y_2 Z_2^2 + b_1 Z_2 + b_1$$

The coefficients appearing in relations (21) and (23) are taken from reference [2].

The equilibrium chemistry model is implemented into the equation of fluid motion by computing the flow field at the first time step by specified γ . The solution of the gas dynamic equation provides the value of ρ and e. Now the equilibrium model is used to determine a new $\hat{\gamma}$. The computation for the next time level is carried with the newly computed value of $\hat{\gamma}$. The procedure continues until the solution converges.

RESULTS AND DISCUSSION

Ouasi one-dimensional numerical simulation of flow within a nozzle is performed with ideal law gas and equilibrium chemistry model. Simulation is performed with hypersonic inlet Mach number of 20.Twenty one equally space grid points are distributed along the nozzle. The inflow boundary conditions are set by specifications of inlet Mach number, temperature, and pressure. The outflow boundary condition is set by specification of pressure so as to position a normal shock at x=4.0cm. This outlet pressure is obtained analytically. The isentropic relations are used to determine the properties from inlet to a position just before the normal shock at x=4.0cm then the normal shock relations are used to determine the properties just behind the shock wave then again isentropic relations are used to determine the properties upto the outlet.

Fig.2 shows the specific heats ratio γ distribution with both models. It is clear that ratio of specific heats γ does not remain constant in hypersonic regime with inclusion of chemistry effects as opposed to ideal law gas in which this ratio is assumed constant. In the pre-shock region its value remains constant as that of ideal law gas since temperature is too low to initiate chemical reactions. On the other hand in the post shock region chemical reactions are enhanced and due to changes in chemical composition, thermodynamic properties are modified and γ undergoes a drastic decrease across the shock wave from 1.4 to 1.156.

For validation purpose temperature right behind the shock wave is compared with the published post shock temperature values at altitudes of 10Km and 50Km as shown in Fig.3 and Fig.4 [1].Density and pressure distributions are also obtained at hypersonic Mach number of 20 to study the effects on these variables. It is clear from Fig.5 that chemical phenomena cause density to increase.Fig.6 shows the effect of chemistry on the post shock pressure however this effect is minimal. It shows that inclusion of chemistry effects cause post shock temperature to fall, density to increase and almost no effect on pressure as compared to the values obtained by ideal law gas.



Temperature Distribution



FIG .3 Temperature Distribution for inlet Mach number of 20 at 10Km



FIG .4 Temperature Distributions for inlet Mach number of 20 at 50 Km



FIG.5 Density Distribution for inlet Mach number of 20





FIG.6 Pressure Distribution for inlet Mach number of 20

The effect of inlet Mach number on the results is also investigated. Since the post shock temperature ratio becomes larger with the Mach number, chemical processes are expected to be enhanced as the Mach number is increased. The simulations are performed with different inlet Mach number of 8,10,12,20.In all the cases outlet pressure is adjusted to position normal shock at x=4.0cm which is obtained analytically by the procedure described before. At low Mach number the post shock temperature obtained by both models have nearly same value. However with the increase in Mach number this difference increases as shown in Fig.7, 8, 9, 10. The equilibrium model predicts an enhancement of the chemical phenomena with increasing Mach number. This effect is clearly evident at Mach number of 20 from the difference between the post shock temperatures by both models.



number of 8



FIG.8 Temperature Distribution for inlet Mach number of 10

Temperature Distribution



of 12



FIG.10 Temperature Distribution for inlet Mach number of 20

CONCLUSIONS

- 1) Inclusion of chemistry effects in simulation of hypersonic flow cause specific heat ratio to decrease.
- Inclusion of chemistry effects in simulation of hypersonic flow results in higher density ratio, lower temperature ratio across the shock wave. The effect on the post shock pressure is minimal.
- 3) At low altitudes flows are mostly in chemical equilibrium and can be accurately computed by equilibrium chemistry model.
- 4) At a given altitude chemical reactions are enhanced with increasing Mach number.

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