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A computational study of inviscid hypersonic flows using energy relaxation method

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Abstract

Reasonable analysis of hypersonic flows requires a thermodynamic non-equilibrium model to properly simulate strong shock waves or high pressure and temperature states in the flow field. The energy relaxation method (ERM) has been used to model such a non-equilibrium effect which is generally expressed as a hyperbolic system of equations with a stiff relaxation source term. Relaxation time that is multiplied with source terms is responsible for non-equilibrium in the system. In the present study, a numerical analysis has been carried out with varying values of relaxation time for several hypersonic flows with AUSM (advection upstream splitting method) as a numerical scheme. Vibration modes of thermodynamic nonequilibrium effects are considered. The results obtained showed that, as the relaxation time reduces to zero, the solution marches toward equilibrium, while it shows non-equilibrium effects, as the relaxation time increases. The present computations predicted the experiment results of hypersonic flows with good accuracy. The work carried out suggests that the present energy relaxation method can be robust for analysis of hypersonic flows.

Keywords: Hypersonic flows; Energy relaxation method; AUSM; Relaxation time

1. Introduction

A gas can be considered to be in thermodynamic equilibrium, if all the modes of internal energies are in equilibrium with each other. The modes of internal energy are associated with translational motion, rotational motion, vibration, dissociation, electronic excitation, and finally ionization. At hypersonic velocities, the time available for changes in thermodynamic variables can be so small that internal energies are not in equilibrium even though they change from point to point. In fact, these modes are in non-equilibrium all along and trying to attain equilibrium [1].

The proper modeling of non-equilibrium gas dynamics is required in certain regimes of hypersonic flows. For inviscid flow, this gives a system of conservation laws coupled with source terms. Often a wide range of time scales is present in the hypersonic flows, leading to numerical difficulties [2]. In the literature, the relaxation method is introduced as a tool to study different time scales present in most engineering fluid mechanics problems and the numerical scheme used to resolve it.

Jin et al. [3] have shown that the Godunov scheme is not able to resolve all spatial and temporal scales when the relaxation term becomes stiff. Therefore, they have considered a semi-discrete scheme by modifying the Godunov scheme to resolve the scales. Caflisch et al. [4] have found that when the relaxation term becomes very strong and highly stiff, an under-resolved numerical scheme produces spurious results. They have developed a method of line approach that uses a high-order Godunov discretization of the fluxes. This scheme has been studied by Pember [5] and Jin [6] using a method of lines approach com-

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bined with suitable operator splitting techniques. Bereux and Sainsaulieu [7] have studied the importance of considering a fully coupled hyperbolic system with relaxation terms to get accurate solutions and developed a higher order Roe-type numerical scheme. Liotta et al. [8] has presented a generalized central numerical scheme for the model of relaxation with stiff source. Their numerical scheme is the extension of Nassyahu-Tadmor [9] scheme. Pareschi [10] has developed a scheme for an application that involves a hyperbolic system of conservation laws with stiff source terms. His scheme works for all ranges of relaxation time using coarse grid, but does not resolve the small relaxation time. Pareschi and Russo [11] have presented a different second-order uniformly accurate high-resolution non-oscillatory central scheme and avoided the use of Riemann solvers. Lowrie and Morel [12] have shown that hyperbolic systems with stiff relaxation terms remain a challenge for numerical methods. Lowrie has analyzed two semi-discrete and one fully discrete method for the solution of a hyperbolic system with stiff relaxation term. Patil et al. [13] used the relaxation method along with HLLC numerical scheme for the simulation of hypersonic flows. Rao et al. [14] studied the grid-free upwind relaxation scheme for the simulation of inviscid compressible flows.

Hyperbolic system of equations with stiff relaxation method are being identified in the recent literature as a novel method of predicting long time behavior of systems such as gas at high temperatures (real gas) having two time scales, one for thermodynamic processes and the other fluid dynamics processes. This has been done following the Coquel and Perthame model [15] which has two separate conservation laws for energy each with a source term. One equation of conservation law is for equilibrium energy due to translational motion of molecules and the other for advection energy due to all other effects. This method of modeling the thermodynamics in high-speed flows is energy relaxation method (ERM), which is modeled as a hyperbolic system of equations with stiff relaxation source term. Based on this study, it is seen that high enthalpy hypersonic flows can be modeled as hyperbolic equations with relaxation terms. The investigation of hypersonic flows commences with identifying suitable numerical schemes for their robustness and use in high-speed flows. The present work considers the advection upstream splitting method (AUSM) [16] as a suitable numerical scheme for simulation of hypersonic flows as they can work in extremely large range of flow speeds and give accurate shocks with minimal diffusion. In the present work, the effect of relaxation time on the performance of this scheme for several hypersonic flow fields has been studied.

2. Energy relaxation method

The Euler equation for a real compressible inviscid fluid is given by,

$$\begin{aligned} &\partial_t \rho + \nabla \cdot (\rho U) = 0 , \\ &\partial_t (\rho U) + \nabla \cdot (\rho U \otimes U) + \nabla p = 0 , \\ &\partial_t E + \nabla \cdot (E + p) U = 0 , \end{aligned} \tag{1}$$

where, $(x, t) \in R_d \times R^+$, $U = (u_1, ...,u_d)^T$, the velocity vector, d the space dimension. The associated state space is given by $U: R_d \times R^+ \rightarrow \Omega$. In the above system, ρ is the density, p the pressure and E volumetric energy. Normally closure of the above system is done by the thermally perfect calorically perfect (TPCP) gas model, which is applicable for mono-atomic gases for an entire temperature regime. For polyatomic gases, the thermodynamic model must consider an inelastic energy transfer in microscopic collisions. Microscopic collision at high temperature reflects the temperature dependency of the heat capacity. At such condition, the specific internal energy e is a nonlinear function of the temperature. A gas requiring a more complex thermodynamic model than the TPCP will be termed a real gas. In local thermodynamic equilibrium, the system is closed by the constitutive relation,

$$p = p(\rho, e), E = \tfrac{1}{2} \rho U^2 + \rho e . \tag{2}$$

As the temperature varies over a wide range, the gas will not be in local thermodynamic equilibrium. The pressure p considered as a function of only a part of e, while another part of e is governed by a rate equation. In such a case, nonlinearity involved in the pressure law $p = p(\rho, e)$ strongly influences the flow dynamics and significant difficulty arises over the numerical resolution of Eq. 1 .

Coquel and Perthame [15], in their energy relaxation method (ERM) have relaxed the energy of the Euler equation for real gas simulation to preserve the correct flow dynamics. They have split the specific internal energy $e = e_1 + e_2$ to relax the nonlinearities in the pressure law. The internal energy e_1 governs a

simple pressure law (polytropic law), while e_2 shows the nonlinearities which are advected by the flows. The Euler equation after relaxing the energy is shown below:

$$\begin{aligned}
&\partial_t \rho + \nabla \cdot (\rho U) = 0 ,\\
&\partial_t (\rho U) + \nabla \cdot (\rho U \otimes U) + \nabla p_1(\rho, e) = 0 ,\\
&\partial_t E_1 + \nabla \cdot [(E_1 + p_1) U] = \frac{1}{\varepsilon}\rho[e_2 - F(\rho, e_1)] ,\\
&\partial_t e_2 + \nabla \cdot (\rho e_2) = -\frac{1}{\varepsilon}\rho[e_2 - F(\rho, e_1)] ,
\end{aligned} \tag{3}$$

where, $E_1 = \frac{1}{2}\rho U^2 + e_1$, ε is relaxation time and equilibrium value of F is functions of the ρ and e_1. The simple pressure law can be stated as $p_1(\rho, e_1) = (\gamma_1 - 1)\rho e_1$ with $\gamma_1 > 1.0$. In short, the principle of ERM is to find a pressure law and an internal energy function $F(\rho, e_1)$, such that the system (Eq. 1) can be recovered as relaxation time $\varepsilon \to 0$, from the relaxation system (Eq. 3). This requires an additional condition called consistency condition,

$$\begin{aligned}
&e = e_1 + F(\rho, e_1), p_1[\rho, e_1 + F(\rho, e_1)]\\
&= p_1(\rho, e_1) = (\gamma_1 - 1)\rho e_1 .
\end{aligned} \tag{4}$$

The consistency conditions are satisfied for any given γ_1, where the value of γ_1 is greater than 1. In addition to consistency condition, it is required to recover the entropy inequality at equilibrium. So it needs the characterization of the adiabatic exponent γ_1 as shown below,

$$\begin{aligned}
&\gamma_1 > \sup_{\rho,e} \Gamma(\rho, e), \Gamma(\rho, e) = 1 + p_e(\rho, e)/\rho\\
&\gamma_1 > \sup_{\rho,e} \gamma(\rho, e), \gamma(\rho, e) = p_e . (\rho/p) + p_e/\rho.
\end{aligned} \tag{5}$$

The above condition is called a sub-characteristic condition. This condition provides stability to the system and it suggests that the speed of sound for internal energy e_1 must be greater than the real speed of sound in the fluid. The above theory justifies that the energy splitting seems natural and simple.

3. Numerical Implementations

Simulation of hypersonic flow problems encounters all kinds of complications, the details are given in [1]. Thus, there is a need to choose a numerical scheme, from amongst the available schemes that is inherently robust and at the same time less dissipative, accurate but efficient and lastly requiring less storage and less expense [17]. AUSM numerical schemes seem to share these properties and hence are popular with researchers for investigation of hypersonic flows. The present work proposes to extend this numerical methods to simulate hypersonic flow past a three- dimensional domain. The implementation of energy relaxation method into an AUSM scheme is explained below.

3.1 AUSM inviscid flux formulation

Liou and Steffen [16] have developed an AUSM scheme to overcome the deficiencies of the other existing upwind methods. The motivation for designing a new upwind scheme has come from the observation of numerical smearing at the location where an eigenvalue changes sign at the shock or approaches zero in the boundary layer. Liou et al. [16] in their scheme have treated the inviscid flux into two physically distinct parts i.e. convective and pressure fluxes. The convective flux is associated with the advection speed, while pressure flux with the acoustic speed. The AUSM scheme accurately captures a shock and contact discontinuity. This scheme satisfies the entropy condition and preserves positivity. The AUSM scheme has been modified to take care of the extra equation of energy relaxation method which is treated similarly to the continuity term. Fluxes along the faces are calculated as a summation of plus and minus flux at the face.

$$f = f^+ + f^- \tag{6}$$

where,

$$f^+ = \begin{pmatrix} \rho a\, Max(0, M) \\ \rho a\, Max(0, M) u_x + p1^+ \\ \rho a\, Max(0, M) u_y + p1^+ \\ \rho a\, Max(0, M) u_z + p1^+ \\ \rho a\, Max(0, M) h_T \\ \rho a\, Max(0, M) e_2 \end{pmatrix}$$

$$f^- = \begin{pmatrix} \rho a\, Min(0, M) \\ \rho a\, Min(0, M) u_x + p1^- \\ \rho a\, Min(0, M) u_y + p1^- \\ \rho a\, Min(0, M) u_z + p1^- \\ \rho a\, Min(0, M) h_T \\ \rho a\, Min(0, M) e_2 \end{pmatrix}$$

Implementation of ERM into the AUSM scheme has shown that the numerical scheme is not altered thus this is a simple approach. The non-equilibrium

equation can be completely ignored while using a numerical scheme as it is. The additional non-equilibrium equation is evolved as if it is a mass equation weighted with non-equilibrium energy density.

The solution procedure of Euler equations (equation 1) for the hypersonic flow examples using the relaxation method is carried out as explained below,

First step

Given an approximate solution to the original Euler equations at a discrete time t^n,

$$U^n = \left(\left[\rho, \rho u_x, \rho u_y, \rho u_z, E_1, \rho e_2 \right]^T \right)^n . \quad (7)$$

Evaluates e^n, ρ^n, pressure $p^n = p\ (\rho^n,\ e^n)$, internal energies $e_1^n = p^n / (\gamma_1 - 1)\ \rho^n)$ and $e_2^n = e^n - e_1^n$.

Second Step

The relaxed Euler equations are integrated in time from t^n to t^{n+1} in the equilibrium limit ($\varepsilon \rightarrow 0$).

Third Step

U^{n+1} is obtained as shown below:

$$U^{n+1} = \left(\left[\rho, \rho u_x, \rho u_y, \rho u_z, (E_1 + \rho e_2) \right]^T \right)^{n+1} . \quad (8)$$

4. Results and discussion

A 3-dimensional finite volume code for structured meshes has been considered for the present simulation. The present code uses an explicit time marching scheme and calculates numerical fluxes by using the modified AUSM. Second order accuracy is achi-eved by calculating variables reconstructed by using the MUSCL approach and limiting fluxes by min-mod limiter. The code uses thermally perfect calorically perfect gas laws but can be used with any gas as long as R, C_p, C_v and k are made available. The code is capable of supporting a number of boundary conditions including adiabatic and isothermal walls. In the present simulation, a thermally perfect and calorically imperfect (TPCI) model for two molecular vibrating gases is considered [18]. Temperature T is calculated by the implicit expression by using the Newton Raphson method as shown below:

$$p(\rho, e) = \rho RT,\ \rho e = \rho C_{cv}^{tr} T + \rho \left(\frac{\alpha \Theta_{vib}}{\exp(\Theta_{vib}/T) - 1} \right), \quad (9)$$

with $C_v^{tr} = R/ (\gamma_{tr} - 1)$, $\gamma_{tr} = 1.4$, $\Theta_{vib} = 10^3$ K, and $\alpha = R$.

The relaxation equation has a source term that is multiplied by a large positive constant called a relaxation time ε. This term is responsible for the non-equilibrium of the system. In the present work, relaxation time is numerically studied, by carrying out numerical experiments with varying values of relaxation time for several flow examples. The equilibrium limit corresponds to the speed at which solution marches / progresses in the domain. Thus, the relaxation time corresponds to the speed of sound. Numerical experiments are carried out with various relaxation times such as speed of sound/ 10.0, 100.0, 1000.0 and 10000.0.

4.1 One-dimensional shock tube flow

In this test case, we simulate the Riemann shock tube problem with two molecular vibrating gases considered as the equation of gas for the computation. The initial conditions for shock tube problem are shown in Fig. 1 and Table 1 [18].

Fig. 2 shows, the variation of density for the different relaxation times. As the relaxation time tends to zero, we get the equilibrium solution. The peak value of density is higher compared to the value given in literature. However, for a finite value of relaxation time, the density plot shows the intermediate stages before coming to equilibrium. Domain of the shock tube has been increased to show the non-equilibrium effect. Moreover, the variation of pressure (Fig. 3) and velocity (Fig. 4) plot shows a similar effect of relaxation time as observed in the case of density. Fig. 5 shows the relaxation time effect for the Mach number. For very small relaxation time, the Mach number plot shows equilibrium solution. The shock distance for the equilibrium state is more than the observed for finite value of relaxation time. Thus, the sub-characteristic condition is satisfied. The effect

Table 1. Initial conditions for shock tube problem.

State	Density	Velocity	Internal energy
Left	0.066	0.0	7.22×10^6
Right	0.030	0.0	1.44×10^6

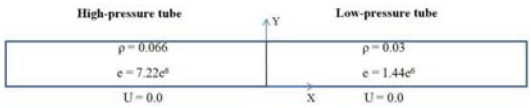

Fig. 1. Initial conditions for shock tube flow.

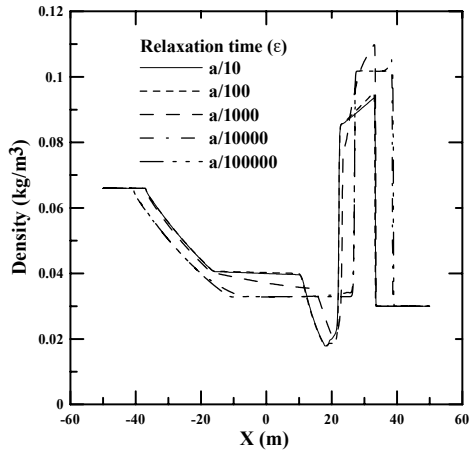

Fig. 2. Density plot for shock tube.

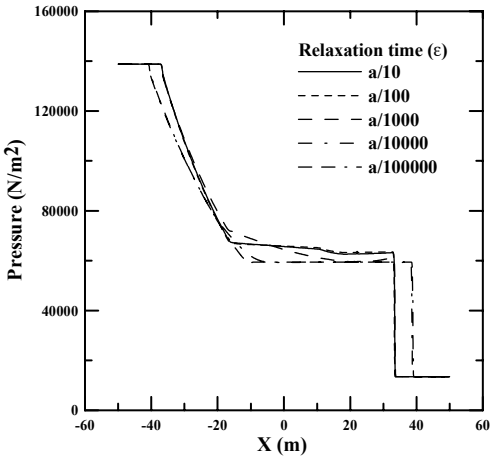

Fig. 3. Pressure plot for shock tube.

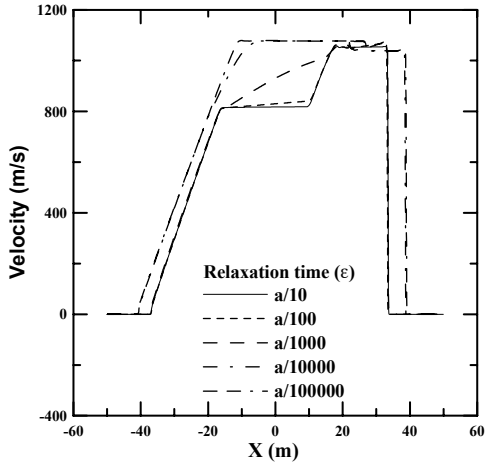

Fig. 4. Velocity plot for shock tube.

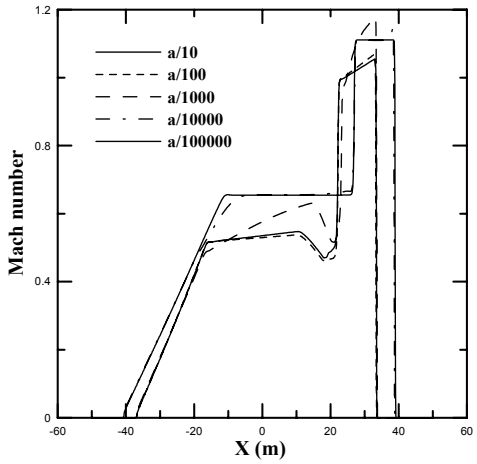

Fig. 5. Mach number plot for shock tube.

of source term is observed as minimum and maximum peak values in all the plots.

4.2 Two-dimensional flow past circular cylinder

A circular cylinder with diameter 90mm is considered for the validation of the numerical scheme, AUSM with ERM. Free-stream flow properties selected are P^{∞} = 687Pa, T^{∞} = 694K, u^{∞} = 4776, ρ^{∞} = 0.00326, Twall = 300K and Mach number as 8.78. Fig. 6 shows the computational domain with boundary conditions considered for this case. Grid size of 181x181 is considered for computations. Present numerical results are compared with the experiment data [19] for the pressure on the surface of the cylinder. A computation has been performed with relaxation time equal to a/10000.0. Fig. 7 shows the comparison of predicted pressure with the experiment data [19] over the cylinder surface. Experiment data for pressure values are available till angle 50. Present results correctly predict the pressure values over the surface of the cylinder.

Real gas flow over a two-dimensional circular cylinder of 76.2mm diameter (Holden, 1988) has been carried out. Boundaries of computational domain at upstream and far field are located at unity and 3.5 times the radius of cylinder (Fig. 8). Free stream conditions considered are, a pressure of 855Pa, density 0.0234kg/m^3 and total temperature 1725K. Mach number of 8.0 is selected for this example. A mesh of 101 × 101 is used. Fig. 9 shows the coefficient of pressure over the surface of the cylinder. Coefficient of pressure is nearly the same for all relaxation times except at the stagnation region.

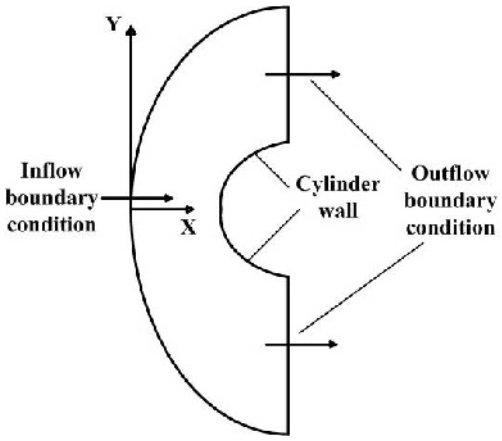

Fig. 6. Computational domain for2-D Cylinder (dia. 90mm).

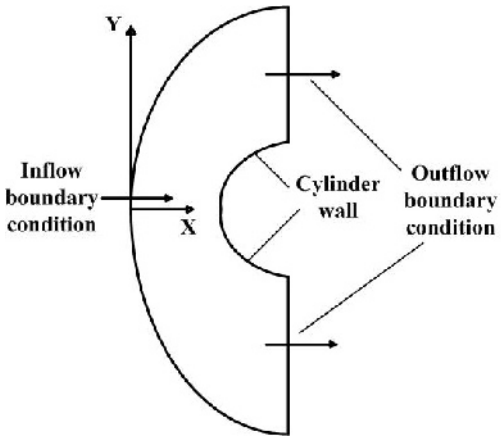

Fig. 8. Computational domain for 2-D Cylinder (dia. 76.2mm).

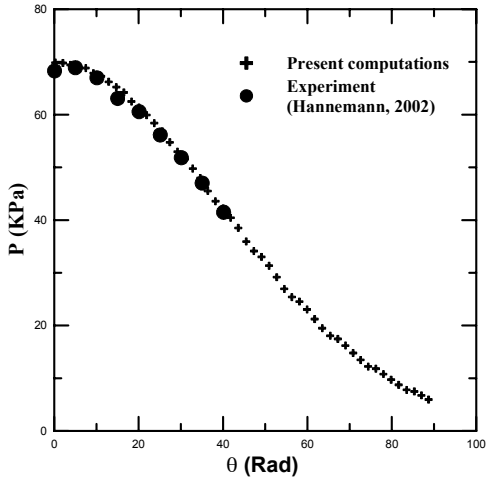

Fig. 7. Comparison of Cp with experiment data over the surface of 2-D cylinder (Mach = 8.78).

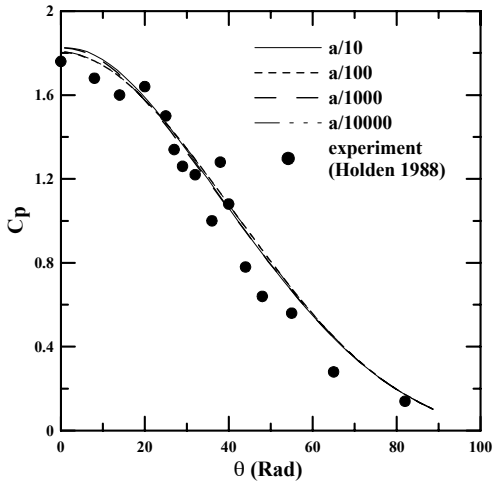

Fig. 9. Variation of relaxation time for the Cp: 2-D cylinder (Mach = 8.0).

There is a small change in Cp values near the stagnation region. At stagnation, high temperature and pressure is observed. Thus, real gas modeling is effective near stagnation and the present relaxation method could capture the real gas effects. Figs. 10 and 11 show the density and Mach contour plot over the surface of the cylinder. The present numerical scheme has captured the bow shock accurately. Fig. 12 shows the Mach number plot along the stagnation line. The present numerical scheme has captured the shock clearly. As expected, minimum Mach number is observed at the stagnation point.

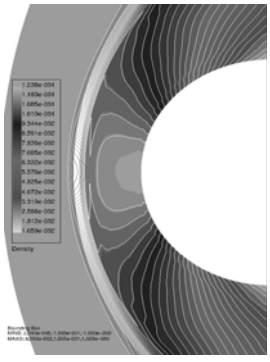

Fig. 10. Density contour plot over the surface of 2-D Cylinder (Mach = 8.0).

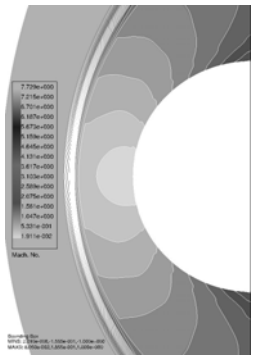

Fig. 11. Mach contour plot over the surface of 2-D Cylinder (Mach = 8.0).

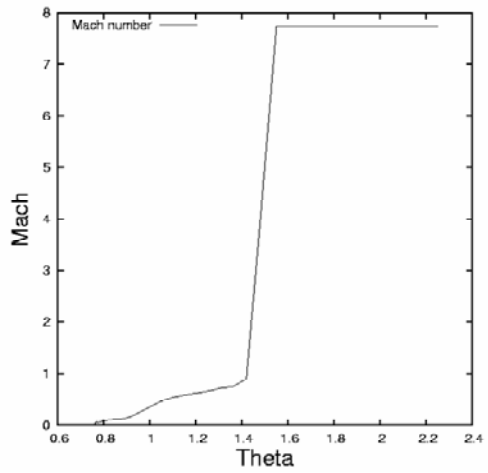

Fig. 12. Mach number plot along the stagnation line of cylinder.

4.3 Three-dimensional flow over re-entry vehicle

A complex geometry, similar to that of a ballistic reentry vehicle has been considered for numerical simulation. This vehicle configuration consists of a blunt bicone with 20/25 degree cone angles. Total length is 3.19 and base diameter 3.97 times the nose radius respectively (Fig. 13). Patil et al. [13] have done numerical experiments with ERM along with HLLC Scheme. Three dimensional grid of size 91 x 75 x 44 is used (Fig. 14). The freestream pressure and temperature are 833 Pa and 63K respectively. Freestream Mach number of 5.0 with 4.66 angle of attack is considered in the present computation. A comparison of wind tunnel (Kalimuthu, 2003) test data with the energy relaxation method (ERM) for coefficient of pressure over the surface of reentry configuration is shown in Fig. 15. Maximum pressure

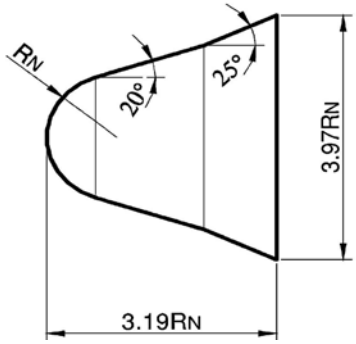

Fig. 13. Reentry vehicle.

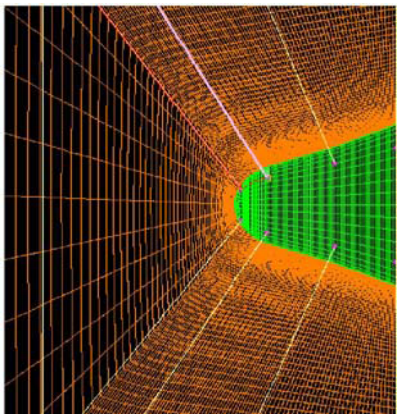

Fig. 14. Volume grid over Reentry vehicle.

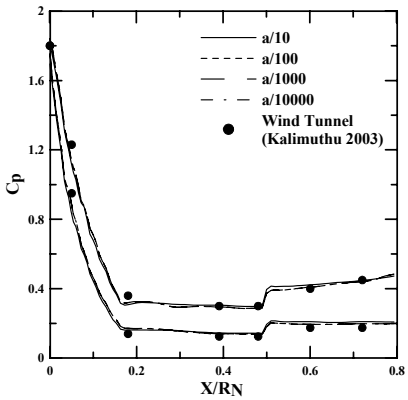

Fig. 15. Comparision of C_p over the surface of Reentry vehicle with wind tunnel data (Mach =5.0, α = 4.66).

at the stagnation is slightly over-predicted. Variation of relaxation time does not have any effect on the pressure values on the surface of the vehicle except near the second shock location (Fig. 15). Density contour plot on the surface of reentry vehicle is

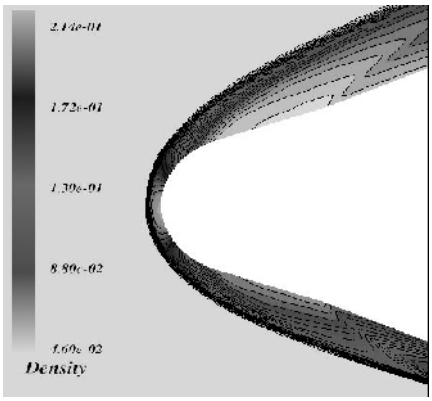

Fig. 16. Density contour plot over Reentry vehicle (Mach =5.0, α = 4.66).

shown in Fig. 16. Bow shock and shock at the second cone are well captured.

5. Conclusions

An energy relaxation method for a compressible real gas has been implemented into the solver with the AUSM numerical scheme. The AUSM numerical scheme has been modified to incorporate the additional energy equation arising from ERM. A numerical simulation for several flow problems were carried out to show that relaxation methods could be applied to any gas over a wide range of conditions. The numerical simulation, that was performed shows good comparison with experimental data available in the literature. The result shows that as the relaxation time tends to zero, the solution marches towards equilibrium. The prediction of hypersonic flows has no effect of relaxation time variation. The work carried out suggests that an energy relaxation method incorporating AUSM is a robust numerical scheme for the analysis of hypersonic flows.

Nomenclature

a : Speed of sound
C_p : Coefficient of pressure/specific heat at constant pressure (J/kg K)
C_v : Specific heat at constant volume (J/kg K)
E : Total energy (N/m^2)
e : Specific internal energy (m^2/s^2)
e_1 : Specific internal energy governed by polytropic law (m^2/s^2)
e_2 : Specific internal energy advected in the flow (m^2/s^2)
F : Internal energy function
M : Mach number
p : Pressure (N/m2)
p,e : Derivative of pressure with respect to internal energy
p,ρ : Derivative of pressure with respect to density
t : Time (s)
T : Temperature (K)
U : Conservation vector

Greek Symbols

Θ : Global temperature of relaxed system (K)
ρ : Density (kg/m^3)
γ : Specific heat ratio
γ_1 : Specific heat ratio corresponding to e_1
ε : Relaxation time

Subscript

vib : Vibration
x : x-component
y : y-component
z : z-component

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