

Kinetic Solution of the Structure of a Shock Wave in a Non-Reactive Gas Mixture

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Abstract. The multi-species Boltzmann equation is numerically integrated to characterize the internal structure of a Mach 3 shock wave in a hard sphere gas. The collision integral is evaluated by the conservative discrete ordinate method of Tcheremissine [1]. There was excellent agreement of macroscopic variables with those of Kosuge, Aoki, and Takata. [2] The effect of species concentration and mass ratio on the behavior of macroscopic variables and distribution functions in the structure of the shock wave is considered for both two and three-species gas mixtures. In a binary mixture of gases with different masses and varying concentrations, the temperature overshoot of the parallel component of temperature near the center of the shock wave is highest for the heavy component when the concentration of the heavy component is the smallest. A physical basis for the temperature overshoot is put forth.

Keywords: Shock Wave Structure, Nonequilibrium, Multi-Species Boltzmann Equation

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INTRODUCTION

There is considerable challenge in the design of aerospace vehicles flying at high altitude in the transitional flow region [3]. In the gas kinetic description, intermolecular collisions change the translational, rotational, vibrational, and electronic energies of the collision partners. For a two-species gas mixture, if the masses are equal ($m^A = m^B$), the translational energy relaxation time (τ_{trans}) is of the order of the mean free time (τ_0) in the equilibrium gas. For elastic collisions, the energy exchange is comparable to the energy of the species before collisions. For $m^A \gg m^B$, $\tau_{trans} \sim \frac{m^A}{m^B} \tau_0$ and for $m^A \ll m^B$, $\tau_{trans} \sim \frac{m^B}{m^A} \tau_0$. When the difference in molecular masses is large, it may be concluded qualitatively that the difficulty in exchanging energy leads to an increase in relaxation time. The work of Tcheremissine [4] outlines the method for the prediction of the macroscopic variables for a Mach 2 shock wave structure consisting of a mixture of two gases. The present study extends a single component Boltzmann flow solver based on the method of Tcheremissine [1] to a multi-species Boltzmann solver and characterize a Mach 3 shock wave structure of inert gas mixtures. The paper generalizes the method so that gas mixtures with more than two species can be treated, that has not been done in earlier studies. One of the objectives of the paper is to provide a better physical insight into the flow physics of shock wave structures. Previous work by Josyula, et al [5] addressed accuracy issues, particularly the requirement of the velocity grid resolution for simulating the internal structure of a shock waves in a single component monatomic gas. The direct numerical integration of the Boltzmann equation for the inert gas mixture is a first step towards extending the solution to inelastic and reactive collisions. The present study is generalized for an inert mixture and considers gas mixtures consisting of two and three species to study the nonequilibrium relaxation in the internal structure of the Mach 3 shock wave. It provides physical insight into the observed physical phenomenon relating to the dynamics of the relaxation of the different species in the shock wave structure.

DISCRETIZED FORM OF MULTI-SPECIES BOLTZMANN EQUATION

The Boltzmann equation expresses the behavior of many-particle kinetic system in terms of the evolution of the particle distribution function. The Boltzmann equation is written as

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial \mathbf{x}} = I(\xi) \quad (1)$$

where the distribution function, $f d\xi d\mathbf{x}$ gives the number of molecules at position \mathbf{x} and velocity ξ at time t . The left hand side of the above equation represents the continuum flow, and the right side denotes the collision term leading to discontinuous jumps in phase space. If the distribution function f is known, the macroscopic variables of the mass, momentum, energy and stress can be obtained by appropriate weighting and integration.

When considering gas mixtures, inelastic collisions and reactive energy exchanges, it is convenient to transform the distribution function from velocity ξ_i to momentum p_i^α variables with $p_i^\alpha = m^\alpha \xi_i$ and $f(\xi, \mathbf{x}, t) \rightarrow f^\alpha(\mathbf{p}^\alpha, \mathbf{x}, t)$. Here p_i^A is the initial momentum of species α . Each species, α , in the system is cast on a grid x_i in the configuration space with κ nodes and a uniform three dimensional grid, p_γ^α in momentum space (the subscript γ denotes a momentum node) with N_0 nodes. Thus the system of species Boltzmann equations takes the form

$$\frac{\partial f^\alpha}{\partial t} + \frac{p_i^\alpha}{m^\alpha} \frac{\partial f^\alpha}{\partial x_i} = I^\alpha \quad \text{for species } \alpha = A, B, \dots \quad (2)$$

The number of species in the gas mixture is denoted by S . The elastic collision integral for species α takes the form

$$I^\alpha = \sum_{j=A}^S \int_{-\infty}^{+\infty} \int_0^{2\pi} \int_0^{b_m} (\tilde{f}^j \tilde{f}^\alpha - f^j f^\alpha) g_{\alpha j} b d\varphi d\mathbf{p}^j \quad (3)$$

Here b_m is the maximum impact parameter with b and φ characterizing the impact for collision between species j and α . The relative velocity $\mathbf{g}_{\alpha,j}$ is $|\frac{\mathbf{p}^j}{m^j} - \frac{\mathbf{p}^\alpha}{m^\alpha}|$. The *tild*e quantities denote the post-collision values.

In the basis of three-dimensional delta functions, the distribution function and the collision integral are represented in the form.

$$f^\alpha(\mathbf{p}, \mathbf{x}, t) = \sum_{\gamma=1}^{N_0} f_\gamma^\alpha(\mathbf{p}, \mathbf{x}, t) \delta(\mathbf{p} - \mathbf{p}_\gamma), \quad I^\alpha(\mathbf{p}, \mathbf{x}, t) = \sum_{\gamma=1}^{N_0} I_\gamma^\alpha(\mathbf{x}, t) \delta(\mathbf{p} - \mathbf{p}_\gamma) \quad (4)$$

After determining the expansion coefficients for the collision integral in the Eqns 4, the problem is reduced to solving the coupled system of equations

$$\frac{\partial f_\gamma^\alpha}{\partial t} + \frac{\mathbf{p}_\gamma^\alpha}{m^\alpha} \frac{\partial f_\gamma^\alpha}{\partial \mathbf{x}} = I_\gamma^\alpha \quad \alpha = A, B, \dots S \quad \gamma = 1, 2, \dots N_0 \quad (5)$$

The conservative numerical method of Tcheremissine [4], extended to multiple species, is employed. The eight dimensional collision integral is evaluated on a uniform grid following the method of Tcheremissine [1, 4].

The internal shock structure of the Mach 3 shock wave was simulated in the present study. The Rankine-Hugoniot conditions across the shock wave for $\gamma=5/3$ consist of: downstream (M_d)=0.522, $p_d/p_u=11$, $\rho_d/\rho_u=3$, $T_d/T_u=3.667$. The steady flow is treated as one-dimensional in the configuration space and three dimensional in momentum space. A uniform equilibrium state is assumed far upstream and downstream of a standing normal shock wave. Number conservation, conservation of total momentum and conservation of total energy lead to a generalized set of Rankine Hugoniot relations [2]. The distribution function boundary conditions up and downstream were specified by a drifting Maxwellian. Four cases are presented in this paper. The first three cases have a mass ratio ($m^A : m^B$)=0.5, the same diameter ratio and concentration ratio of species B, $\chi^B=0.1, 0.5$, and 0.9 . The fourth case is a three-species inert gas mixture with $m^A : m^B : m^C=1:0.9:0.8$, $d^A : d^B : d^C=1:1:1$, and $\chi^A : \chi^B : \chi^C=1:2:3$. Note: (1) By convention the nominal mass is that of species A, (2) $\chi^\alpha \equiv \frac{N^\alpha}{\sum_{j=1}^S N_j}$.

RESULTS AND DISCUSSIONS

The shock wave structure in a two- and three-species gas mixture of inert gases was analyzed for a variety of mass ratios and molecular diameters in the hard sphere collision approximation. Validation results are presented initially for the multi-species solver. Fig. 1 shows the individual species' densities and mixture density in the Mach 3 shock wave structure for mass ratio of 0.5, diameter ratio of 1, and for different concentrations of species B. The density is normalized with its upstream value. For all concentrations considered, $\chi^B=0.1, 0.5$, and 0.9 (Fig. 1a, b, and c) the lighter component (species B) transitions earlier from its undisturbed upstream condition to the shock and maintains a slightly higher density than the heavier component throughout the shock wave.

The streamwise velocity component is shown for the Mach 3 shock wave in Fig. 2 for different concentrations of B (χ^B) of 0.1, 0.5, and 0.9 for mass ratio of 0.5, diameter ratio of 1. The velocity of the lighter component, species B, transitions earlier from its undisturbed freestream value to the shock wave for all concentrations considered.

It is noted that for $\chi^B=0.1$ (Fig. 2, the frequency of collisions for A-A particles is highest, followed by A-B, then BB. This behavior governs the differing relaxation times for the collisions between different collision partners, $\tau_{AB} > \tau_{AA}$. The magnitude and trends of velocity and density profiles in the shock wave noted above (Fig. 1 and 2) is evidence of conservation of mass flux in the different gas mixtures. In summary, for a gas mixture with fixed values of mass ratio and diameter ratio, the concentration ratio has very little effect on mixture density, velocity, and temperature. There is, however, an effect of varying the concentration on the individual temperatures, as well as the component temperatures, T_x and T_y , (discussed next).

Fig. 3 shows parallel and perpendicular components of temperature (T_x and T_y) and the mixture temperature for the three concentrations, $\chi^B=0.1, 0.5, \text{ and } 0.9$ for mass ratio of 0.5, and diameter ratio of 1. The parallel (T_x) and perpendicular (T_y) components of the temperature are calculated from their corresponding pressure components, $kT_x = \overline{mu'^2} = p_{xx}/n$ and $kT_y = \overline{mv'^2} = p_{yy}/n$. For all three concentrations, there is overshoot of parallel component (T_x) for both the heavier (species A) and lighter species of the gas mixture. The T_x component of the heavier particle (species A) has a greater magnitude and overshoot than that of specie B. It is also noted that the greater the value of χ^B , the higher the overshoot of the T_x for both the heavier species (species A) and lighter species.

Fig. 4 and 5 depict the parallel and perpendicular components of the momentum distribution function for the binary gas mixture (Species A and B) for $\chi^B=0.1, 0.5, \text{ and } 0.9$ for mass ratio of 0.5, and diameter ratio of 1. Species A is the heavier component and Species B the lighter. Comparisons of results of the Species A (heavier) and Species B (lighter) shows that the momentum distribution function of the parallel component is wider, which can be related to the temperature overshoot for the T_x component seen in the preceding figure (Fig. 3). Similarly, on comparing the momentum distribution functions of the parallel components for various values of χ^B , one sees that the width of the distribution function is highest for $\chi^B=0.9$, followed by 0.5 and then 0.1, which can be related to the overshoot of the parallel (T_x) component, the highest for $\chi^B=0.9$, followed by 0.5 and then 0.1 (Fig. 3).

Results for a three-species gas mixture are presented for differing mass ratios, with the same diameter ratio, and variation in concentration ratios for the three species. Fig. 6 shows the velocity distribution function for the three species A, B, and C at different locations in the shock wave. At locations inside the shock wave, $X/\lambda=-0.4$ and $X/\lambda=+2$, one can see a non-Maxwellian distribution. It is noted that for the three-species gas mixture with small variation in mass ratio and identical diameter ratio, the size of the distribution function is found to increase with the concentration ratio.

CONCLUDING REMARKS

A numerical study was performed for the solution of the internal structure of shock waves in monatomic gas mixtures, assuming the hard sphere collision model. The multi-species Boltzmann equation was solved by the conservative discrete ordinate method of Tcheremissine. Macroscopic parameters predicted in the present study for Mach 3 shock wave agree well with those from the previous work of Kosuge, Aoki and Takata. The effect of species concentration and mass ratio in the shock wave was presented by macroscopic variables and distribution functions.

The temperature overshoot of the parallel component near the center of the shock wave is highest for the heavy component when the concentration of the heavy component is the smallest. The relative comparison of the parallel and perpendicular components of momenta shows that the parallel component has a wider distribution, which manifests as a temperature overshoot. The relative magnitudes of the parallel temperature overshoots for different mixture concentrations correspond with the relative magnitudes of widths of parallel component momentum distribution functions.

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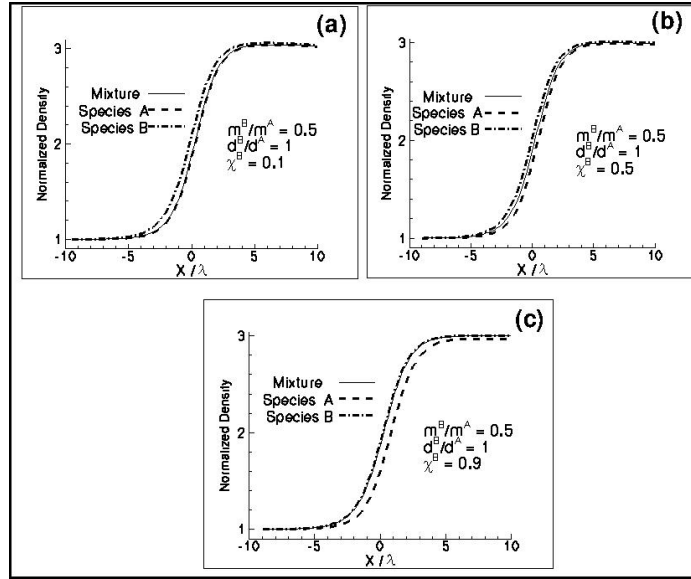


FIGURE 1. Density distribution in a Mach 3 shock wave with hard sphere collision model for mass ratio of 0.5, diameter ratio of 1, and concentration as (a) $\chi^B=0.1$, (b) $\chi^B=0.5$, (c) $\chi^B=0.9$

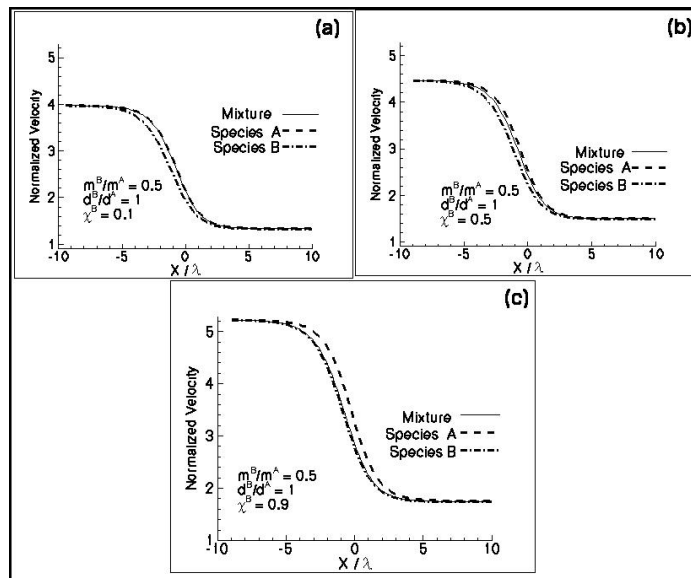


FIGURE 2. Streamwise velocity distribution in a Mach 3 shock wave with hard sphere collision model for mass ratio of 0.5, diameter ratio of 1, and concentration as (a) $\chi^B=0.1$, (b) $\chi^B=0.5$, (c) $\chi^B=0.9$

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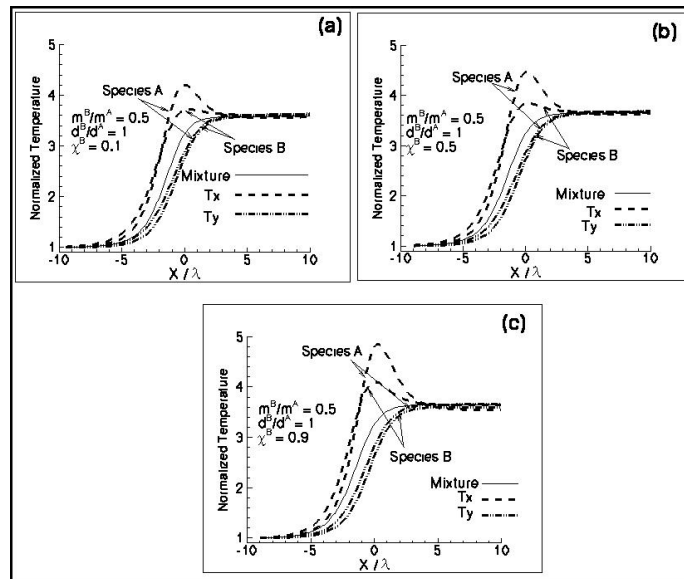


FIGURE 3. Temperature distribution in a Mach 3 shock wave with hard sphere collision model for mass ratio of 0.5, diameter ratio of 1, and concentration as (a) $\chi^B=0.1$, (b) $\chi^B=0.5$, (c) $\chi^B=0.9$

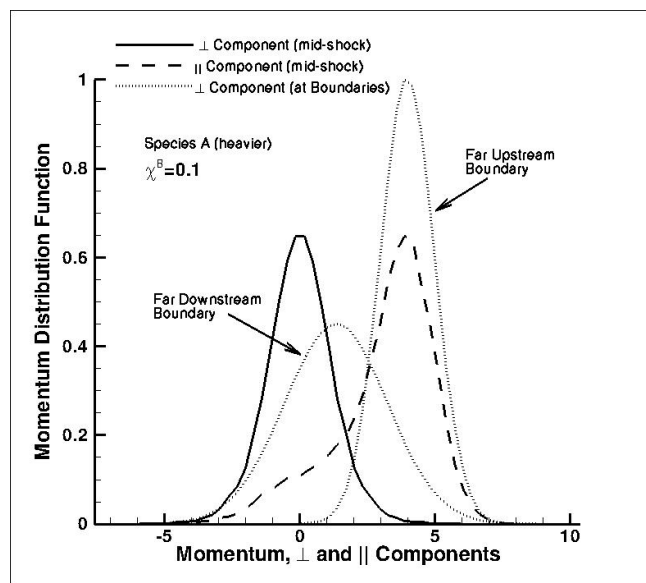


FIGURE 4. Components of momentum distribution function in a Mach 3 shock wave with hard sphere collision model for mass ratio of 0.5, diameter ratio of 1, $\chi^B=0.1$, for Species A (heavier)

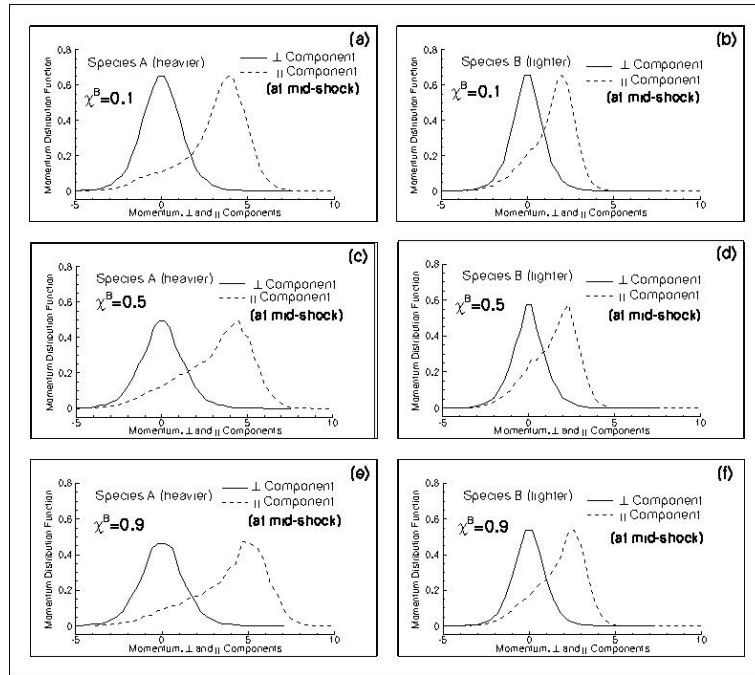


FIGURE 5. Components of momentum distribution function in a Mach 3 shock wave with hard sphere collision model for mass ratio of 0.5, diameter ratio of 1, for (a) Species A (heavier), $\chi^B=0.1$, (b) Species B (lighter), $\chi^B=0.1$, (c) Species A (heavier), $\chi^B=0.5$, (d) Species B (lighter), $\chi^B=0.5$, (e) Species A (heavier), $\chi^B=0.9$, (f) Species B (lighter), $\chi^B=0.9$

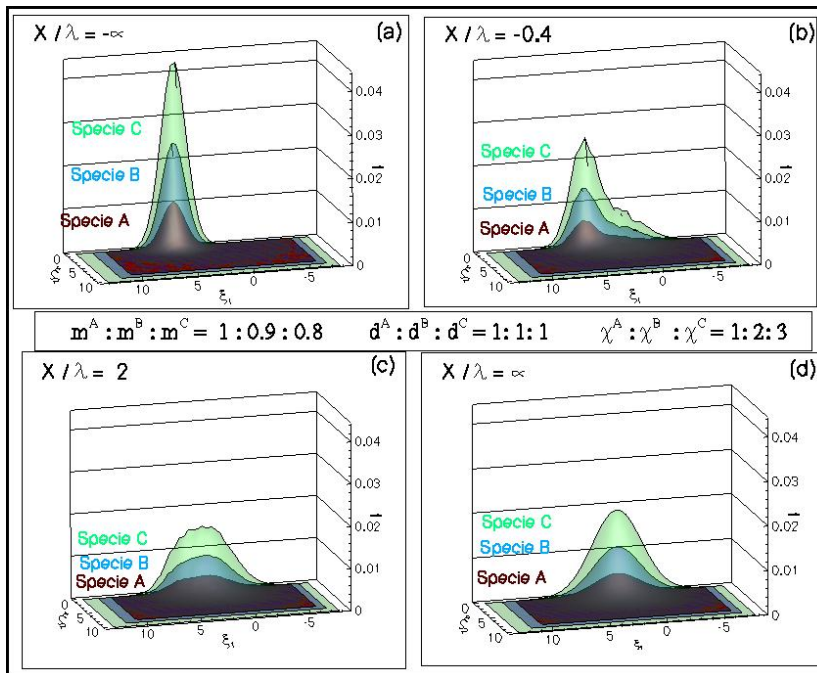


FIGURE 6. Velocity distribution function inside a Mach 3 shock wave with hard sphere collision model, (a) $x/\lambda=-\infty$, (b) $x/\lambda=-4$, (c) $x/\lambda=2$, (d) $x/\lambda=\infty$