

Computation of Hypersonic Shock Waves in Inert Gas Mixtures Using the Generalized Boltzmann Equation

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Abstract. For numerical solution of the Generalized Boltzmann Equation (GBE) for simulating rarefied hypersonic flows in a gas mixture of multiple species, the GBE is formulated in the impulse space. The gas mixtures may consist of both monatomic gases and diatomic gases with arbitrary constituents, concentrations, and mass ratios. The conservative discrete ordinates method of Tcheremissine is applied to validate the solutions against the existing simulations for shock waves in an inert binary mixture of monatomic gases. The method is then exercised for various concentration ratios, mass ratios, and density ratios to evaluate its ability to simulate a wide range of binary gas mixtures. It is also applied to simulate two of the three primary constituents of air (N_2 , O_2 , Ar) in a binary mixture at 1:1 concentrations and at the relative concentrations found in air. These solutions can serve as validation test cases for other methods as well as an important building block in developing complex 3D simulations for shock waves in a mixture of multiple gases.

Keywords: Boltzmann Equation, Shock Wave, Compressible Flow, Hypersonic Flow, Gas Mixtures

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INTRODUCTION

A goal of continued development of direct methods for solving the generalized Boltzmann equation (GBE) is to extend the existing GBE solver to calculate the flowfields of inert gas mixtures of monatomic and diatomic gases in translational non-equilibrium. In general, many gas mixtures include a large number of species, which may also be reacting. The existing classical Boltzmann equation (CBE) and the generalized Boltzmann equation (GBE) solvers have been extensively used by the authors to compute hypersonic shock waves in single specie monatomic and diatomic gases, respectively [1]. The solvers are based upon the conservative discrete ordinates method developed by Tcheremissine [2], which is a completely conservative method for solving the Boltzmann equation. These solvers are extended for computing hypersonic shock waves in an inert binary mixture of monatomic and diatomic gases. For this purpose, the Boltzmann equation is reformulated in the impulse space. The developed code is first validated by computing the shock wave solutions in an inert mixture of two monatomic gases for which computations of Kosuge et al. [3] are available. The code is then employed to compute shock waves in a binary inert gas mixture of a monatomic gas for a range of concentration ratios, diameter ratios, and mass ratios. The mixture is considered to be in translational non-equilibrium only. Finally, the code is employed to compute shocks in a binary gas mixture of monatomic and diatomic gases; the gases are assumed to be the primary constituents of air (N_2 , O_2 , Ar).

SHOCK WAVE SIMULATIONS IN BINARY INERT GAS MIXTURES

So far in the existing literature, direct methods for the solution of the classical Boltzmann equation have only been employed for the computation of shock structures in an inert mixture of two monatomic gases with varying concentrations [3] and for a mixture of two diatomic gases in translational non-equilibrium [1]. Agarwal and Tcheremissine [1] computed the shock structure in an inert binary mixture of two diatomic gases in translational

non-equilibrium at Mach 5; however, they recognized that the inclusion of both the rotational and vibrational energy levels in the calculation of shock structure would be extremely computationally intensive. Therefore, Agarwal et al. [4] developed and validated a two-level rotational energy (2LRT) model for the solution of the GBE for RT relaxations. For example, by introducing the 2LRT model, Tcheremissine and Agarwal and [5] were able to reduce the total number of rotational and vibrational energy levels to 12 from 420 for a Mach 10 shock [5] in a gas in both rotational and vibrational non-equilibrium.

The natural extension of the work of Agarwal and Tcheremissine [1] is to perform additional validations of the solution approach for GBE in impulse space and to conduct simulations of gas mixtures with realistic concentrations. Furthermore, most simulations to date have focused on mixtures of two monatomic or two diatomic gases. In order to eventually simulate realistically gas mixtures such as air containing more than two constituents, it is important to examine the interaction between the diatomic and monatomic gases in a binary gas mixture.

COMPARISONS OF PRESENT SOLUTIONS TO EXISTING SOLUTIONS

Kosuge et al. [3] have presented a detailed evaluation of the properties of one-dimensional shock waves in inert binary gas mixtures of monatomic gases. They presented the results of several simulations and included tabulated data for two of the simulations. Two pairs of Mach numbers and mass ratios were considered – Mach 2 with a mass ratio of 0.25 and Mach 3 with a mass ratio of 0.5. Examples of the results are shown in Figure 1 at Mach 2 for constituent B (concentration equal to 0.1) and a mass ratio equal to 0.25. Figure 2 presents the results at Mach 3 for constituent B (concentration equal to 0.1) and a mass ratio equal to 0.5. The graph on the left shows the behavior of properties for each constituent and the mixture through the shock wave. The graph on the right shows comparison of the present results for the mixture with those of Kosuge et al. Based upon these comparisons, it can be concluded that the current approach produces solutions in good agreement with the results obtained by Kosuge et al. [3].

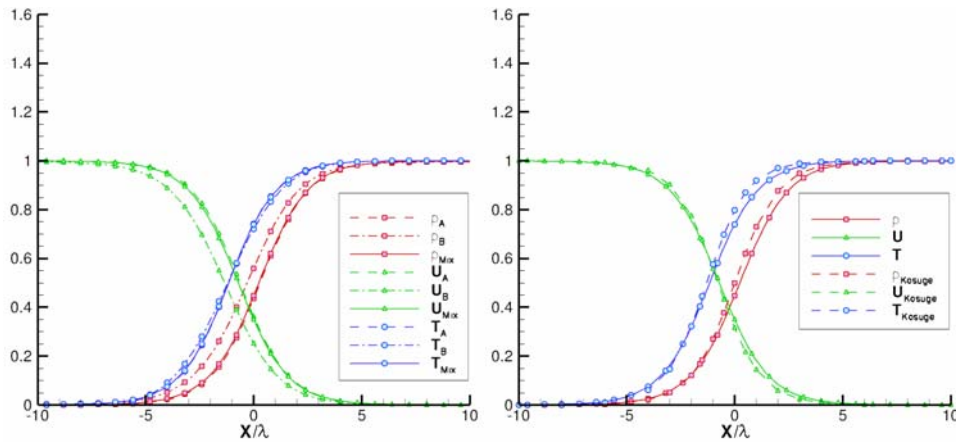


FIGURE 1. Shock wave properties and their comparison with Kosuge et al., B concentration = 0.1, mass ratio = 0.25, M = 2

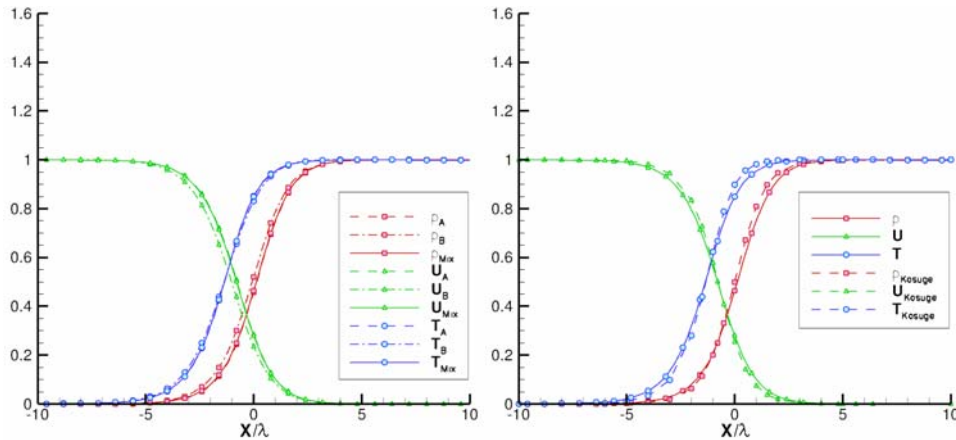


FIGURE 2. Shock wave properties and their comparison with Kosuge et al., B concentration = 0.1, mass ratio = 0.5, M = 3

PARAMETRIC STUDY OF SHOCK STRUCTURE IN BINARY GAS MIXTURES

As demonstrated in the preceding section, the present numerical approach shows good agreement with the results of Kosuge et al. [3] obtained by using the solution method of Sone et al. [6] for the collision integral. In this section, we further demonstrate the solution capability of the present method by performing simulations for a range of mass ratios, diameter ratios, and density ratios. Five values for each ratio are used (0.1, 0.5, 1.0, 5.0, and 10). A total of thirteen simulations are performed at Mach 2. Figure 3 shows the baseline solution for Mach 2 where each ratio is equal to unity. The solutions that were generated by varying only the concentrations of each constituent in the binary mixture resulted in similar solutions since the mass and diameter ratios of the constituents A and B were equal to unity. As expected, these solutions produced results identical to Figure 3

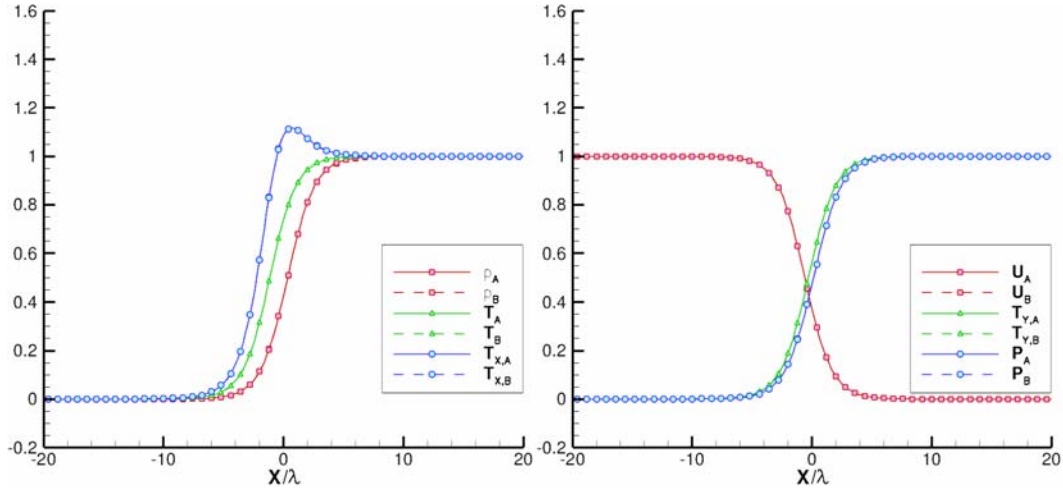


FIGURE 3. Baseline shock structure in a binary gas mixture at Mach 2; $m_B/m_A = 1$, $d_B/d_A = 1$

An example of the solutions for the non-unity mass ratios is presented in Figure 4. These solutions demonstrate that as the mass of a constituent becomes lighter, with respect to the other constituent in the mixture, the lighter constituent begins to experience changes in its properties further upstream than the heavier constituent. Another important note from the mass ratio parametric study is that extremely small mass ratios ($m_B/m_A = 0.1$) or extremely large mass ratios ($m_B/m_A = 10$) require smaller time steps in order to obtain convergent solutions.

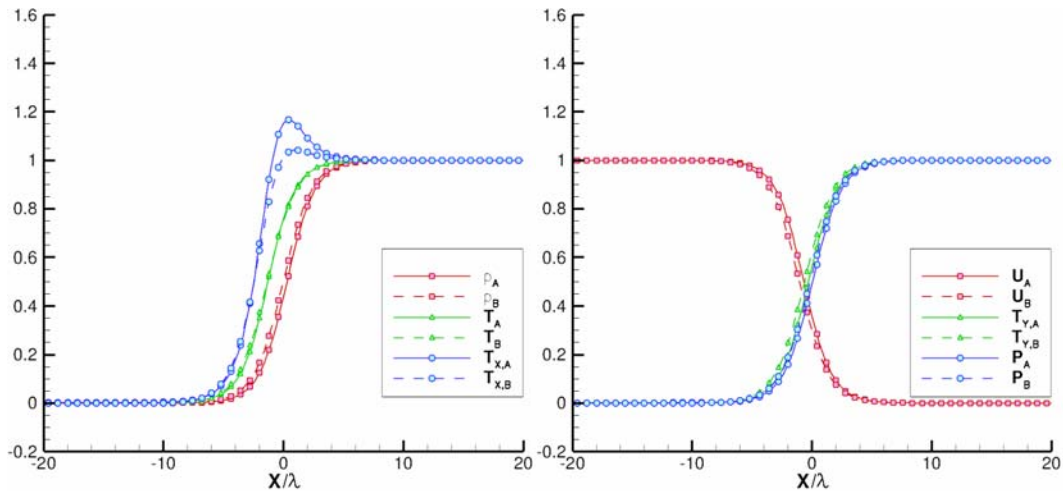


FIGURE 4. Shock structure in a binary gas mixture with $m_B/m_A = 0.5$ and $d_B/d_A = 1$ at Mach 2

An example of the solutions for the non-unity diameter ratios is presented in Figure 5. These solutions demonstrate that, when the diameter ratio of two constituents becomes significantly different from unity, the

thickness of the shock increases. Furthermore, the smaller diameter constituent, with respect to the other constituent in the mixture, begins to experience changes in its properties earlier than the larger diameter constituent.

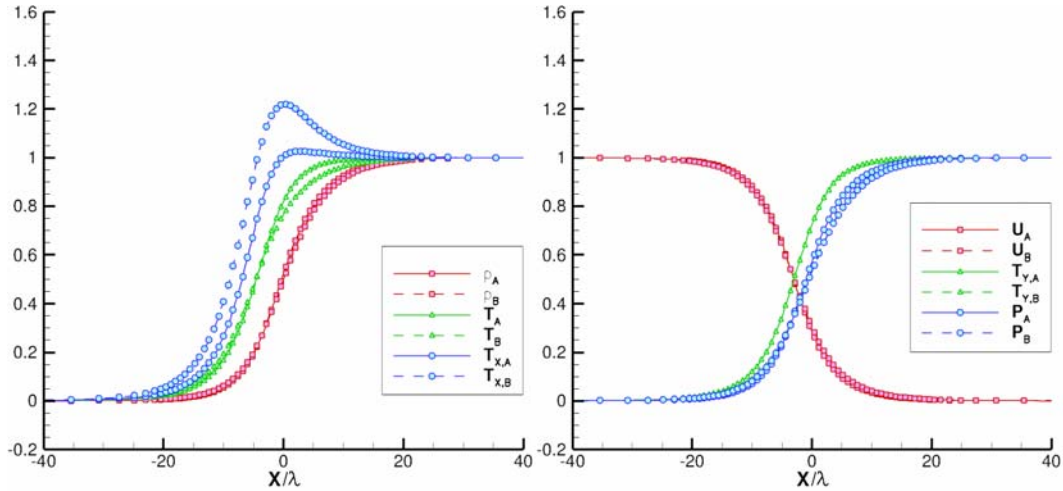


FIGURE 5. Shock structure in a binary gas mixture with $m_B/m_A = 1$ and $d_B/d_A = 0.1$ at Mach 2

The parametric study performed in this section demonstrates that the code is able to handle molecular constituent properties that are far from unity. For the application to immersed bodies, the most relevant gas mixture is air. As a gas mixture, air is relatively well conditioned for the present code since it has mass and diameter ratios of different constituents close to unity. The next section presents the behavior of a one-dimensional shock wave for a binary gas mixture comprised of two of the three primary constituent of air (N_2 , O_2 , Ar).

SHOCK WAVE SOLUTIONS FOR BINARY GAS MIXTURE OF AIR CONSTITUENTS

Historically, there are hardly any solutions for shock waves in a mixture of gases representative of the constituents of air. Furthermore, simulations of gas mixtures have been limited to two constituents of similar atomic structure (i.e. two diatomic gases or two monatomic gases). This section presents solutions for binary mixtures of two of the three primary constituents of air at 1:1 concentration and concentrations representative of those in air. Table 1 presents a summary of the key parameters used in the simulations. The Van der Waals radius can be used to approximate the diameter of the molecule in the collision integral. The rotational and vibrational degrees of freedom for argon can be neglected since it is monatomic. A solution for each mixture was generated at Mach 2 and Mach 5. All figures presented in this section are for the Mach 5 shock wave for the concentration ratios as found in the air. All constituent gases are assumed to be non-reacting.

TABLE 1. Gas Mixture Properties for Air

Constituent	Mole Fraction	Atomic Weight (g/mol)	Van der Waals Radius (pm)
N_2	0.78084	28.0134(4)	225
O_2	0.20946	31.9988(6)	206
Ar	0.00934	39.948(1)	188

N_2 and O_2 Mixture

The first binary mixture of air constituents considered is that of N_2 and O_2 . The mass ratio equals 1.1423 and the diameter ratio equals 0.9156. The solutions for the 1:1 concentration reaffirm the conclusion drawn from the parametric study above that the lighter constituent (N_2) begins experiencing changes in properties earlier in the shock wave structure. Additionally, the change in concentration ratio does not have a significant impact on the shock structure. Figure 6 presents an example of the results for N_2 and O_2 .

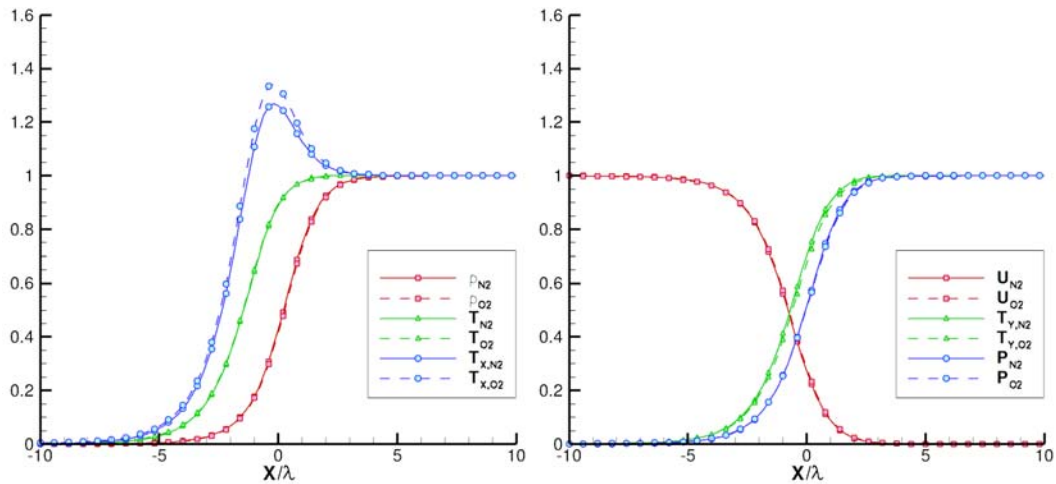


FIGURE 6. Shock wave properties in a mixture of nitrogen and oxygen (as in air) at Mach 5

N₂ and Ar Mixture

The second binary mixture of air constituents considered is that of N₂ and Ar (a diatomic and a monatomic gas respectively). The mass ratio equals 1.4260 and the diameter ratio equals 0.8356. The gases are assumed to be non-reacting. It is interesting to note that the shock thickness has increased compared to the N₂/O₂ mixture simulation. This increase can be attributed to the change in the diameter ratio, as also noted in the section on parametric study. Additionally, the tendency for the lighter constituent to begin experiencing changes earlier in the shock wave holds. Figure 7 presents an example of the results for N₂ and Ar.

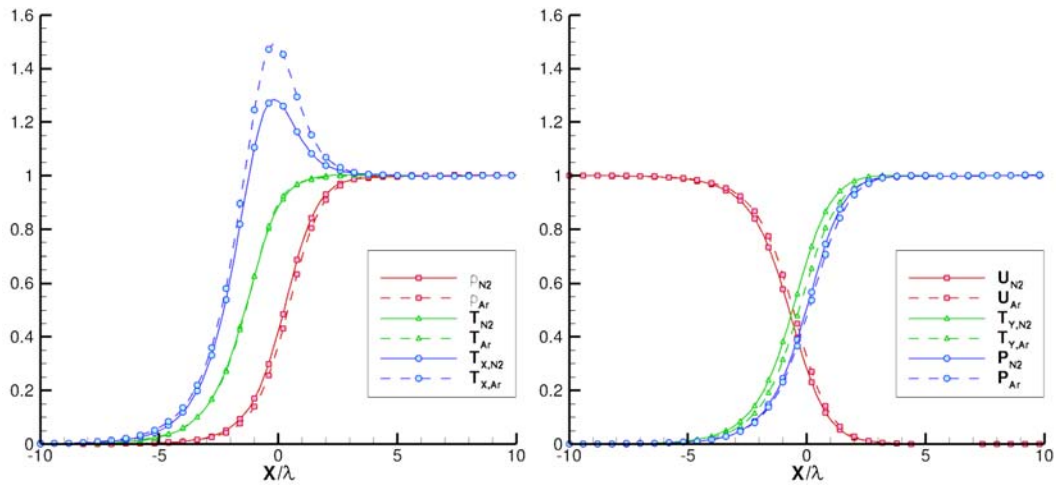


FIGURE 7. Shock wave properties in a mixture of nitrogen and argon (as in air) at Mach 5

O₂ and Ar Mixture

The third binary mixture of air constituents considered is that of O₂ and Ar. The mass ratio equals 1.2484 and the diameter ratio equals 0.9126. The results for these simulations are similar to those obtained from the N₂/Ar mixture simulation. The shock wave thickness is greater than that obtained from the N₂/O₂ mixture simulation. One would not expect the shock wave thickness to be significantly different between the N₂/Ar simulation and the O₂/Ar simulation since the diameter ratios are similar. Additionally, O₂ is the lighter gas compared to Argon. Therefore, O₂ has a tendency to experience changes in constituent properties earlier in the shock, as demonstrated previously. Figure 8 presents an example of the results for O₂ and Ar.

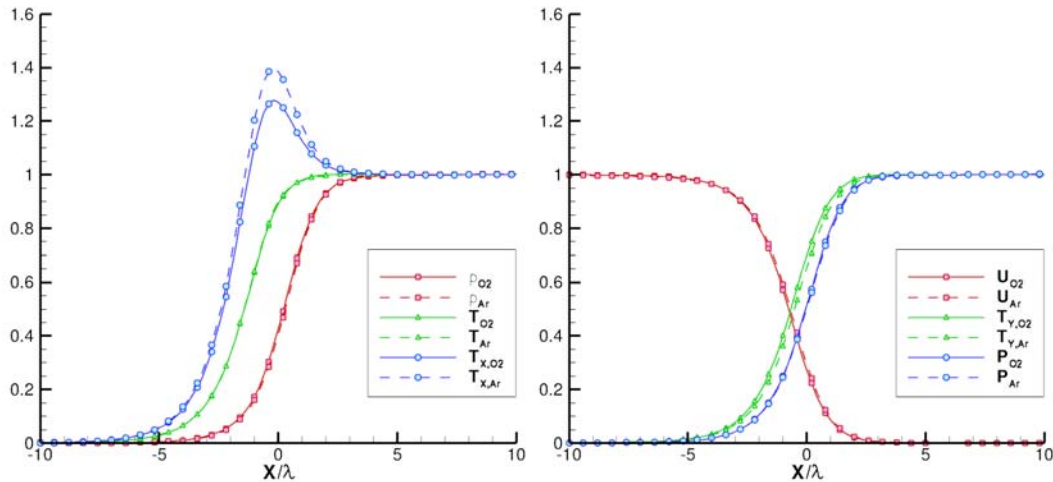


FIGURE 8. Shock wave properties in a mixture of oxygen and argon (as in air) at Mach 5

SUMMARY

A direct method of Tcheremissine has been applied for solving the Boltzmann equation in an impulse space for computation of shock waves in a binary mixture of non-reacting monatomic and diatomic gases in translational non-equilibrium. The method has been validated by comparing the present solutions with those of Kosuge, Aoki and Takata for a binary mixture of inert monatomic gases using a different numerical method due to Sone. A parametric study of the performance of the current method has been performed to evaluate its capability for computing shock waves in binary inert mixtures for various mass ratios, concentration ratios, and diameter ratios. It is demonstrated that the current method is able to handle a wide range of mass, diameter, and concentration ratios without any numerical difficulty. The method is also applied to a non-reacting mixture of two of the air constituents (diatomic nitrogen, diatomic oxygen, and monatomic argon). Two different concentration ratios were used – 1:1 and relative concentrations of these gases in air. The behavior of shock waves in a mixture representative of air constituents is computed. The present work can be extended to compute shock waves in a mixture of multiple non-reacting gases in rotational and vibrational non-equilibrium using the generalized Boltzmann equation.

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