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Abstract. The generalized hydrodynamic computational models for diatomic gas flows are developed. The rotational nonequilibrium effect is included by introducing excess normal stress associated with the bulk viscosity of the gas. The new models are applied to study the one-dimensional shock structure and the multi-dimensional rarefied hypersonic flow about a blunt body. The general properties of the constitutive equations are also presented through a simple analysis. An excellent agreement with experiment is observed for the inverse shock density thickness.

INTRODUCTION

The study of nonlinear gas transport in rarefied condition [1,2] and microscale gas flows associated with MEMS [3,4] has emerged as an interesting topic in recent years. Along with the DSMC method, high-order fluid dynamic models that come under the general category of the moment method or the Chapman-Enskog method have been developed for this type of problem. However, it is observed that most of fluid equations show some defective behavior of the computed solution for the problem of a very high Mach number or the rapidly expanding flow.

In this study, the generalized hydrodynamic computational model for monatomic gases is extended to diatomic gases. The rotational nonequilibrium effect is taken into account in the present work by introducing excess normal stress associated with the bulk viscosity of the gas. The rotational relaxation mechanisms are not explicitly included on the basis that the rotational energy relaxes at a much shorter time scale than the hydrodynamic relaxation time scale [5]. A new slip model for the diatomic gas and surface molecular interaction is also introduced. The computational models reduce to the models for monatomic gases in the limit of small bulk viscosity. The new models for diatomic gases share the basis of their computational algorithm with the models for monatomic gases. This feature will make it possible to develop the computational code in very efficient way.

Another feature of the present work is that it is based on the hydrodynamic equations, which are proven to be consistent with the second law of thermodynamics. Therefore the corresponding computational models should, in principle, yield solutions for all Knudsen numbers and under any flow condition.

The present paper is organized as follows. First, a generalized hydrodynamic computational model for diatomic gases and slip boundary condition are introduced. We then present the solutions of constitutive equations and CFD algorithms. Finally we apply the present model to the shock structure problem and the two-dimensional hypersonic flow about a blunt body.

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EU'S GENERALIZED HYDRODYNAMICS FOR DIATOMIC GASES

From Eu’s generalized hydrodynamic equations [5–9], a computational model of the conserved and non-conserved variables in diatomic gases can be written as

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}_T = 0,$$

and

$$\dot{\mathbf{I}} q(c\hat{R}) = (1 + f_b \Delta) \dot{\mathbf{I}}_0 + [\dot{\mathbf{I}} \cdot \nabla \hat{u}]^{(2)},$$

$$\Delta q(c\hat{R}) = \Delta_0 + \frac{3}{2} f_b (\dot{\mathbf{I}} + f_b \Delta I) \cdot \nabla \hat{u},$$

$$\dot{Q} q(c\hat{R}) = (1 + f_b \Delta) \dot{Q}_0 + \dot{\mathbf{I}} \cdot \dot{Q}_0.$$  

Here $\dot{\mathbf{I}}_0$, $\Delta_0$, and $\dot{Q}_0$ are determined by the Newtonian law of shear and bulk viscosity and the Fourier law of heat conduction, respectively:

$$\dot{\mathbf{I}}_0 = -2\eta |\nabla u|^2, \quad \Delta_0 = -\eta b \nabla \mathbf{u}, \quad \dot{Q}_0 = -\lambda \nabla \ln T.$$

Notice that the so-called second coefficient of viscosity in Stokes’ hypothesis [10] is equivalent to

$$\eta_b = \frac{2}{3} \eta.$$

All the variables in the aforementioned equations are made dimensionless by introducing the following dimensionless variables and parameters

$$t^* = t/(L/u_r), \quad x^* = x/L, \quad \eta^* = \eta/\eta_r, \quad \lambda^* = \lambda/\lambda_r, \quad u^* = u/u_r, \quad \rho^* = \rho/\rho_r, \quad T^* = T/T_r,$$

$$p^* = p/p_r, \quad E^* = E/E_r, \quad \mathbf{I}^* = \mathbf{I}/(\eta_r u_r/L), \quad \Delta^* = \Delta/(\eta b, u_r/L), \quad Q^* = Q/(\lambda_r \Delta T/L T_r).$$

The asterisks are omitted from the aforementioned equations for the notational brevity. The matrices and other variables are defined as

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho \mathbf{u} u + \rho \mathbf{I} \\ (\rho E + \frac{\rho \mathbf{u} \cdot \mathbf{I}}{\lambda + \rho \mathbf{I}}) \mathbf{u} + \frac{\lambda}{\lambda + \rho \mathbf{I}} \mathbf{Q} \end{pmatrix}, \quad \mathbf{F}_v = \frac{1}{\text{Re}} \left( \begin{array}{c} \mathbf{I} + f_b \Delta \mathbf{I} \\ \mathbf{F} \end{array} \right),$$

$$\dot{\mathbf{I}} \equiv \frac{N_a}{p} \dot{\mathbf{I}}, \quad \dot{\Delta} \equiv \frac{N_a}{p} \Delta, \quad \dot{Q} \equiv \frac{N_a}{p} \mathbf{Q}, \quad \nabla \hat{u} \equiv -2\eta |\nabla \mathbf{u}|, \quad \epsilon \equiv \frac{1}{\text{Pr} \text{Ec} T_r/\Delta^2},$$

and $q(c\hat{R})$ is a nonlinear factor defined by

$$q(c\hat{R}) = \frac{\sinh(c\hat{R})}{c \hat{R}}, \quad \hat{R}^2 \equiv \dot{\mathbf{I}} \cdot \dot{\mathbf{I}} + \frac{4}{5 f_b} \dot{\Delta}^2 + \dot{Q} \cdot \dot{Q}.$$
\[ c = \left[ \frac{2\sqrt{\pi}}{5} A_2(\nu) \Gamma(4 - 2/(\nu - 1)) \right]^{1/2}, \]  

has a value between 1.0138 (Maxwellian) and 1.2232 (\( \nu = 3 \)), where \( \nu \) is the exponent of the inverse power law for the gas particle interaction potential. The \( \eta, \eta_b, \) and \( \lambda \) are the Chapman-Enskog shear viscosity, bulk viscosity, and thermal conductivity. They can be expressed as \( \eta = T^s, \ \eta_b = f_b \eta, \ \lambda = T^{s+1} \) where \( s = \frac{1}{2} + 2/(\nu - 1) \).

For a perfect gas the following dimensionless relations hold

\[ p = \rho T, \ \rho E = \frac{p/\gamma M^2}{\gamma - 1} + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u}. \]  

A composite number, which is defined by

\[ N_\delta \equiv \frac{\eta r u_r}{p_r} = \frac{M^2}{R_0} = Kn M \sqrt{\frac{2\gamma}{\pi}}, \]

measures the magnitude of the viscous stress relative to the hydrostatic pressure, so that it indicates the degree of departure from equilibrium. As \( N_\delta \) becomes small, the Newtonian law and the Fourier law are recovered from the constitutive relations (2), (3), and (4):

\[ \Pi = \Pi_0, \ \Delta = \Delta_0, \ Q = Q_0. \]

If the Stokes’ hypothesis, which is nothing but neglecting the bulk viscosity, is applied, they reduce to the well-known Navier-Stokes-Fourier constitutive equations:

\[ \Pi = \Pi_0, \ Q = Q_0. \]

For a diatomic gas, \( \gamma = \frac{7}{5} \) and \( Pr = \frac{14}{19} \) through Eucken’s relation

\[ Pr = \frac{4\gamma}{9\gamma - 5}. \]

**A GAS-SURFACE INTERACTION MODEL**

For slip models for the gas-surface molecular interaction, the so-called Langmuir’s slip model has been studied in the previous works [11,12]. They can be expressed, in the dimensional form, as

\[ u = \alpha u_w + (1 - \alpha) u_r \]  
\[ T = \alpha T_w + (1 - \alpha) T_r \]

where

\[ \alpha = \frac{\beta_p}{1 + \beta_p}. \]  

The parameter \( \beta \) depends on the wall temperature \( T_w \) and the interfacial interaction parameters. By imagining the gas–surface molecule interaction process as a chemical reaction, it is possible to express the parameter \( \beta \) in the form

\[ \beta = \frac{AI_r}{k_B T_w} \exp \left( \frac{D_e}{k_B T_w} \right) \cdot \frac{\ell}{l_r}, \]

where \( A \) is the mean area of a site, and \( D_e \) is the potential parameter. These parameters can be inferred from experimental data or theoretical consideration of intermolecular forces and the surface–molecule interaction. The \( k_B \) is the Boltzmann constant. \( \ell \) is a mean collision distance between the wall surface and the gas molecules.
at all angles. If the reference mean-free-path is taken equal to \( \ell \), then the parameter reduces to, after some manipulation,

\[
\beta = \sqrt{\frac{\pi}{32}} \frac{A}{c^2 d_{\text{STP}}^2} \left[ \frac{T_r}{273} \right]^2 \frac{T_r}{T_w} \exp \left( \frac{D_e}{k_B T_w} \right) \frac{1}{p_r},
\]

where \( d \) represents the diameter of the molecule.

This model can be easily extended to the case of the adsorption of a diatomic gas such as nitrogen on a metallic surface. If we assume multimolecular (double) layer on solid surfaces, the resulting relation of \( \alpha \) simply becomes

\[
\alpha = \frac{\sqrt{3p}}{1 + \sqrt{3p}}.
\]

For an \( N_2 \)-Al molecular interaction model, similar data can be used

\[
D_e = 1.32 \text{ kcal/mol}, \quad d_{\text{STP}} = 3.794 \times 10^{-8} \text{ cm}.
\]

**COMPUTATIONS OF CONSTITUTIVE EQUATIONS**

In general, the constitutive equations (2), (3) and (4) consist of ten equations of \( (\Pi_{xx}, \Pi_{xy}, \Pi_{xz}, \Pi_{yy}, \Pi_{yz}, \Pi_{zz}, \Delta, Q_x, Q_y, Q_z) \) for known 14 parameters \( (p, T, \nabla u, \nabla v, \nabla w, \nabla T) \). Owing to the highly nonlinear terms, it is, however, not obvious how to develop a proper numerical method for solving the equations. Nevertheless, it can be shown that they can be solved by a numerical method in the case of a one-dimensional problem.

In the case of a two-dimensional problem the stress and heat flux components \( (\Pi_{xx}, \Pi_{xy}, \Delta, Q_x, Q_y, Q_z) \) on a line in the two-dimensional physical plane induced by thermodynamic forces \( (u_x, v_x, T_x) \) can be approximated as the sum of two solvers: one on \( (u_x, 0, T_x) \), and another on \( (0, v_x, 0) \). It can be shown that the equations for the first solver, which describe compression and expansion of gas, are given by

\[
\hat{\Pi}_{xx} q(c \hat{R}) = (\hat{\Pi}_{xx} + f_b \hat{\Delta} + 1)\hat{\Pi}_{xx0},
\]

\[
\hat{\Delta} q(c \hat{R}) = [3(\hat{\Pi}_{xx} + f_b \hat{\Delta}) + 1]\hat{\Delta}_0,
\]

\[
\hat{Q}_x q(c \hat{R}) = (\hat{\Pi}_{xx} + f_b \hat{\Delta} + 1)\hat{Q}_{x0},
\]

where

\[
\hat{R}^2 = \frac{3}{2} \hat{\Pi}_{xx} + \frac{4}{5f_b} \hat{\Delta}^2 + \hat{Q}_{xx}^2, \quad \hat{\Delta}_0 = \frac{3}{4} f_b \hat{\Pi}_{xx0}.
\]

The following relation between the \( xx \)-component of the shear stress and the excess normal stress can be found from the first two equations

\[
\hat{\Delta} = \frac{1}{8f_b} [(9f_b^2 - 4)\hat{\Pi}_{xx} - 4 + \sqrt{D}]
\]

where

\[
D = (81f_b^4 + 72f_b^2 + 16)\hat{\Pi}_{xx}^2 + (32 - 24f_b^2)\hat{\Pi}_{xx} + 16.
\]

The following constitutive relations for the second solver, which describe the shear flow,

\[
\hat{\Pi}_{xx} q(c \hat{R}) = -2\hat{\Pi}_{xx} \hat{\Pi}_{yy0},
\]

\[
\hat{\Pi}_{xy} q(c \hat{R}) = (1 + \hat{\Pi}_{xx} + f_b \hat{\Delta})\hat{\Pi}_{yy0},
\]

\[
\hat{\Delta} q(c \hat{R}) = 3f_b \hat{\Pi}_{yy} \hat{\Pi}_{yy0},
\]

yield an equation of one variable \( \hat{\Pi}_{xx} \) and an additional equation for \( \hat{\Delta} \).
FIGURE 1. (a) Generalized hydrodynamic constitutive relations (diatomic and monatomic) relative to the Navier-Stokes relations in the \(u_x\)-only problem \((c = 1.0179, f_b = 0.8, \text{no heat flux})\). The horizontal and vertical axes represent the velocity gradient \(\hat{\Pi}_{xx}\), and the relations \(\hat{\Pi}_{xx}\), respectively. The gas is expanding in the range \(\hat{\Pi}_{xx} < 0\), whereas the gas is compressed in the range of \(\hat{\Pi}_{xx} > 0\) (left). (b) Generalized hydrodynamic constitutive relations relative to the Navier-Stokes relations in the \(v_x\)-only problem. The horizontal axis represents the velocity gradient \(\hat{\Pi}_{xy}\). The vertical axis represents the normal \(\hat{\Pi}_{xx}\) and shear \(\hat{\Pi}_{xy}\) stresses (right).

\[
\hat{\Pi}_{xx} q^2(c\hat{R}) = -\frac{2}{3}\{(1 - \frac{9}{2}f_b^2)\hat{\Pi}_{xx} + 1\}\hat{\Pi}_{yy}^2, \quad (20)
\]
\[
\hat{\Delta} = -\frac{9}{2}f_b\hat{\Pi}_{xx}, \quad (21)
\]

where

\[
\hat{R}^2 = 3\hat{\Pi}_{xx}[(1 + \frac{45}{4}f_b^2)\hat{\Pi}_{xx} - 1]
\]

which follows from the stress constraint

\[
\hat{\Pi}_{xy} = \text{sign}(\hat{\Pi}_{xy})\left[-\frac{3}{2}(1 - \frac{9}{2}f_b^2)\hat{\Pi}_{xx} + 1\right]^{1/2}. \quad (22)
\]

The constitutive equations \((14)–(16)\) and \((20)\) for diatomic gases can be solved by extending the method of iteration \([11,13]\) which is originally developed for monatomic gases. All the calculations turned out to provide converged solutions within a few iterations.

The general properties of constitutive relations are shown in Fig. 1. The relations in one-dimensional \(u_x\)-only problem relative to the Navier-Stokes-Fourier theory are depicted in Fig. 1 (a). In this study the heat flux is assumed to be equal to zero for the sake of simplicity. In contrast with the Navier-Stokes-Fourier theory, the asymmetry of the normal stress for rapid expansion and compression of gas is predicted by generalized hydrodynamics. Even though the details are slightly different, the general trend of the stresses for monatomic and diatomic gases remains unchanged. Fig. 1 (b) demonstrates that the shear stresses by generalized hydrodynamics become very small compared to the Navier-Stokes-Fourier theory as the tangential velocity gradient becomes very large. Such an asymptotic behavior indicates that the new relations have a correct free-molecular limit, implying that the velocity-slip phenomenon caused by the non-Newtonian effect can be explained in very simple way. The ultimate origin of this behavior can be traced to the constraint on the normal \(\hat{\Pi}_{xx}\) and shear \(\hat{\Pi}_{xy}\) stresses.
CFD ALGORITHMS

The generalized hydrodynamic equations (1)–(4) must satisfy the following collision-free hyperbolic conservation laws,

\[ \frac{\partial}{\partial t} \int_V U dV + \oint_S \mathbf{F}_T \cdot \mathbf{n} dS = 0, \]

where \( S \) represents the bounding surface of the control volume \( V \). Most of modern CFD schemes based on the hyperbolic conservation laws can be applied to treating these equations. In the present study, the upwind scheme with van Leer’s flux vector splitting solver is used. The one-dimensional discretized form of the hyperbolic conservation laws in the finite volume formulation can be expressed as

\[ U_{i,j}^{n+1} = U_{i,j}^n - \frac{\Delta t}{\Delta x} \left[ F_{i,j}^n - F_{i+1,j}^n \right], \quad (23) \]

where \( U \) is the cell-averaged conserved variables, \( \Delta x \) is the size of \( i \)-cell, \( \Delta t \) is the time step, and \( \mathbf{F}_T \) is the numerical flux function which gives the flux through cell interfaces. Second-order accuracy can be obtained by using the MUSCL-Hancock method.

The numerical flux through the interface in the equation (23) in general non-Cartesian domains can be determined by exploiting the rotational invariance of the conservation laws (1). Let us consider the \( l \)-th intercell boundary \( \Delta L_l \) of finite area \( A_{i,j} \) in two-dimensional \((x,y)\) space. Let \((\mathbf{n}, \mathbf{s})\) be the outward unit vector normal to the \( l \)-th boundary, and the unit vector tangent to the \( l \)-th boundary with the convention that the interior of the volume always lies on the left hand side of the boundary. If \( \theta_l \) is defined as the angle formed by the \( x \)-direction and the normal vector \( \mathbf{n}_l \), it can be shown that the equation (23) becomes

\[ U_{i,j}^{n+1} = U_{i,j}^n - \frac{\Delta t}{A_{i,j}} \sum_{l=1}^{N} R_l^{-1} F_{i,l} \Delta L_l, \quad (24) \]

where

\[ U_{i,j} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{pmatrix}_{i,j}, \quad F_l = \begin{pmatrix} \rho S_{i,j}^n + \frac{1}{2} \mathbf{u}_i^2 \rho \\ \rho S_{i,j}^n u_i + \frac{1}{2} \mathbf{u}_i \mathbf{u}_j \rho \\ \rho S_{i,j}^n u_j + \frac{1}{2} \mathbf{u}_i \mathbf{u}_j \rho \\ \rho S_{i,j}^n \mathbf{u}_j \end{pmatrix} I, \quad F_{v_i} = \frac{1}{Re} \begin{pmatrix} 0 \\ \Pi_{nn} + f_h \Delta \\ \Pi_{ns} \\ (\Pi_{nn} + f_h \Delta) \mathbf{u}_n + \Pi_{ns} \mathbf{u}_s + \frac{1}{EcPr} Q_n \end{pmatrix}_I. \]

Here \( N, R_l \) represent the number of interfaces in a cell and the rotation matrix.

For given \( T_w, T_r, u_w, u_r \), and \( p_r \), the boundary conditions and the mechanical balance condition (zero normal gradient of pressure) yield the boundary values of temperature, tangential velocity, and pressure. From these values the boundary value of the density can be determined by the perfect gas relation. The velocity normal to the surface can be assumed to be zero. For artificial boundaries, inflow and outflow conditions based on the number of Euler characteristics can be employed.

NUMERICAL EXPERIMENT

The capability of the new equations can be demonstrated by solving two problems: shock structure and two-dimensional blunt body flow. The gas is assumed as nitrogen \((s = 0.78 \text{ in the coefficient of viscosity, } c = 1.0179, f_b = 0.8)\). In general, the initial data necessary to define a well-posed problem consist of dimensionless parameters \((M, Kn \text{ or } Re)\), thermodynamic values \((T_w, T_\infty)\), gas properties \((s \text{ or } \nu, d_{STP})\), and gas-surface molecular interaction parameters \((D_c, A)\).

**Shock Structure Problem** The shock structure is computed for various Mach numbers with a grid of 500 points. The results of the inverse density thickness are summarized in Fig. 2 (a). The second-order accuracy was maintained in this computation. The general configuration of the shock structure of the present solutions was shown to be in good agreement with the experiment. The Navier-Stokes-Fourier theory, however, yields the inverse widths much large compared with experimental data. The Navier-Stokes-Fourier theory with
Stokes’ hypothesis, which is the foundation of computational aerodynamics, gives the worst prediction. This can be highlighted in Fig. 2 (b) where shock profiles for excess normal stress are compared.

Two-Dimensional Blunt Body Flow The second problem is the hypersonic rarefied blunt body flow. In Fig. 3, the hypersonic rarefied blunt body flows ($M = 10$, $Kn = 0.1$, $T_w = 4.8T_{\infty}$, $T_{\infty} = 208.4K$) are described. The computational domain is defined by a patch with a grid of $40 \times 60$ points. A gas-surface ($N_2$–Al) molecular interaction model is used that depends on the pressure and temperature and provides the boundary values of temperature and velocity. The free-stream mean free path is taken as a mean collision distance. The boundary condition at the outflow was specified by extrapolation. The slip condition on the wall was applied by defining the dual ghost cells, one for the inviscid part where the boundary values of velocity and temperature are specified, and another for the viscous part where the values at the wall are used. The first-order accuracy was maintained throughout the computational domain including the boundaries for simplicity. Exactly the same conditions, including the slip boundary condition, are applied to both Navier-Stokes-Fourier and generalized hydrodynamics codes.

The temperature contours around the body are depicted in Fig. 3 (a). The comparison of temperature change along the stagnation streamline is shown in Fig. 3 (b). As noted in the results of the inverse shock density thickness, there are noticeable differences among the Navier-Stokes-Fourier, the Navier-Stokes-Fourier with Stokes’ hypothesis, and the generalized hydrodynamics solutions.

SUMMARY

The new equations (1)-(22) represent a complete set of the generalized hydrodynamic computational model for nonequilibrium diatomic gas flows. The general properties of the constitutive equations are obtained through a simple mathematical analysis. With an iterative computational algorithm of the constitutive equations, numerical solutions for the multi-dimensional problem are obtained. Numerical results of the shock structure and the rarefied hypersonic flow over a blunt body are presented. An excellent agreement with experiment is observed for the inverse shock density thickness.
FIGURE 3. (a) Temperature contours around the two-dimensional blunt body at $M = 10$ and $Kn = 0.1$ (nitrogen, $s = 0.78$, $f_b = 0.8$). The result by the generalized hydrodynamic theory. Selected minimum and maximum contour levels are: 1; 1.85, and 15; 13.7. $L$ is the characteristic length of the blunt body, in this case, the radius of a circular cylinder ($L = 10l_\infty$) (left). (b) Temperature distribution along stagnation streamline of the two-dimensional blunt body. The same meanings for the symbols as in Fig. 2 (right).

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REFERENCES