Modeling of Gaseous Expansion in Free Jet and Microchannel Flows Using the Modified Moment Method

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Abstract. With the shock structure problem, gaseous expansion into a near vacuum is regarded as a classical benchmark problem in validating various mathematical models of gas flows with high Knudsen numbers. In the present work, we derive the moment equations for spherically symmetric expanding flows by making use of the Eu's modified moment method to the Boltzmann equation. The general properties of the constitutive equations in spherical geometry are studied. Finally, an experimental result on gaseous expansion along the microchannel with the exit Knudsen number 2.5 is compared with the theoretical prediction in order to validate the theoretical model.

INTRODUCTION

The theoretical modeling of nonlinear gas transport in rarefied or microscale conditions [1,2] remains as a very challenging subject in gas dynamics owing to the complexity of the physical mechanisms. There exist very active research works in solving non-trivial issues such as the formulation of high-order governing equations [3,4] and derivation of models describing the true nature of gas-surface molecular interactions. Among the benchmark problems serving as a test bed for validating new theoretical models, the structure of shock waves is a classical problem. Other interesting cases can be found by considering the shear-driven and rapidly expanding gas flows.

In particular, the free expansion of a gas into near vacuum in the spherical geometry [5,6] has been considered a fundamental problem of rarefied gas dynamics. The studies of this problem were motivated by the practical need of production of high-intensity molecular beams using free jet expansions. This problem, mathematically simple due to the spherical symmetry, can cover a transition from collision-dominated continuum to almost free molecular regimes without the usual complication from the boundary conditions.

In this work, a theoretical model derived by Eu's modified moment method and a slip model based on Langmuir's theory of gas-surface molecular interactions are applied to investigate pressure-driven free jet rarefied gas and micro-channel gas flow. The new constitutive equations in gas flow expanding from a spherical source are analyzed for finding a possible explanation of the freezing mechanism of the parallel temperature reported in the literature [5]. Finally, the theoretical prediction on gaseous expansion along the long microchannel with a high Knudsen number is compared with the experiment.

THEORETICAL MODELS FOR RAREFIED GAS AND MICROFLUIDIC TRANSPORT (EU'S MODIFIED MOMENT METHOD)

The high order hydrodynamic equations can be derived from a kinetic equation such as the Boltzmann equation. The Boltzmann kinetic equation describes the evolution of the singlet distribution function $f(\mathbf{v};\mathbf{r},t)$ of finding a particle at position $\mathbf{r}$ and velocity $\mathbf{v}$ at time t

$$\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right]f(\mathbf{v};\mathbf{r},t)=C[f], \tag{1}$$

where $C[f]$ denotes the Boltzmann collision integral for two-body particle collision. The conservation laws for conserved variables $(\rho,\rho\mathbf{u},\rho E_t)$ can be obtained by differentiating the statistical formula of mass, mean momentum and internal energy density with time and applying the Boltzmann equation and its collisional invariants $I[m,m\mathbf{v},\frac{1}{2}m(v^2-u^2)]^T=0$. The equations of higher moments (stress and heat flux) can also be derived by using similar procedure and, together with the conservation laws, the equations can be written in a compact form [3,7,8]

$$\rho\frac{D}{Dt}\left[\begin{array}{c}\hat{\mathbf{U}}\\ \hat{\mathbf{\Phi}}\end{array}\right]+\nabla\cdot\left[\begin{array}{c}\mathbf{F}\\ \mathbf{\Psi}\end{array}\right]=\left[\begin{array}{c}\mathbf{0}\\ \mathbf{Z}+\mathbf{\Lambda}\end{array}\right] \tag{2}$$

where

$$\hat{\mathbf{U}}=\frac{1}{\rho}\left[1,\rho\mathbf{u},\rho E_t\right]^T,\ \mathbf{F}=\left[\mathbf{u},\mathbf{P},\mathbf{P}\cdot\mathbf{u}+\mathbf{Q}\right],\ \hat{\mathbf{\Phi}}=\frac{1}{\rho}\left[\mathbf{\Pi},\mathbf{Q}\right],\ \mathbf{\Psi}=\left[\psi^{(\Pi)},\psi^{(Q)}\right],$$

$$\mathbf{Z}=\left[\mathbf{Z}^{(\Pi)},\mathbf{Z}^{(Q)}\right],\ \mathbf{\Lambda}=\left[\mathbf{\Lambda}^{(\Pi)},\mathbf{\Lambda}^{(Q)}\right]$$

and

$$\mathbf{Z}^{(\Pi)}=-2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}-2p\left[\nabla\mathbf{u}\right]^{(2)},\ \mathbf{Z}^{(Q)}=-\frac{D\mathbf{u}}{Dt}\cdot\mathbf{\Pi}-\mathbf{P}\cdot\nabla\hat{h}-\psi^{(P)}:\nabla\mathbf{u}-\mathbf{Q}\cdot\nabla\mathbf{u},$$

$$\mathbf{\Lambda}^{(\Pi)}=-\frac{p}{\eta}q(\kappa)\mathbf{\Pi},\ \mathbf{\Lambda}^{(Q)}=-\frac{pC_pT}{\lambda}q(\kappa)\mathbf{Q}\ \text{ where }\ q(\kappa)=\frac{\sinh\kappa}{\kappa},\ \kappa=\frac{(mk_B)^{1/4}}{\sqrt{2}d}\frac{T^{1/4}}{p}\left[\frac{\mathbf{\Pi}:\mathbf{\Pi}}{2\eta}+\frac{\mathbf{Q}\cdot\mathbf{Q}}{\lambda}\right]^{1/2}.$$

With a closure relation, the constitutive equations of kinematic term $\mathbf{Z}$ and dissipative term $\mathbf{\Lambda}$ in the spirit of 13 moments $\mathbf{Z}+\mathbf{\Lambda}=\mathbf{0}$ reduce to, in dimensionless form,

$$0=-2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}-\frac{p/\eta}{N_\delta}\left\{2\eta\left[\nabla\mathbf{u}\right]^{(2)}+q(N_\delta\kappa)\mathbf{\Pi}\right\}, \tag{3}$$

$$0=\mathrm{Ec}\,\mathrm{Pr}\nabla\cdot\left(\frac{1}{N_\delta\mathrm{Re}}p\mathbf{I}+\frac{\mathbf{1}}{\mathrm{Re}}\mathbf{\Pi}\right)\cdot\frac{\mathbf{\Pi}}{\rho}-\mathrm{Pr}\mathbf{\Pi}\cdot\nabla T-\mathbf{Q}\cdot\nabla\mathbf{u}-\mathrm{Pr}\,\frac{pT/\lambda}{N_\delta}\left\{\lambda\nabla\ln T+q(N_\delta\kappa)\mathbf{Q}\right\}, \tag{4}$$

where

$$\kappa=\frac{cN_\delta}{p}\left[\mathbf{\Pi}:\mathbf{\Pi}+\mathbf{Q}\cdot\mathbf{Q}/(T/2\epsilon)\right]^{1/2},\ c^2=\frac{\sqrt{2}}{8}\pi^{3/2}\omega_0(\nu)\text{ and }\omega_0(\nu)=\frac{8\sqrt{2}}{5\pi}A_2(\nu)\Gamma[4-\frac{2}{\nu-1}].$$

The dimensionless numbers N_δ, Eckert (Ec) and ϵ are defined as

$$N_\delta=\frac{\gamma M^2}{\mathrm{Re}},\ \mathrm{Ec}=(\gamma-1)M^2T_r/\triangle T,\ \epsilon=\frac{1}{\mathrm{Ec}\,\mathrm{Pr}}\frac{1}{T_r/\triangle T}.$$

The composite number N_δ measures the magnitude of the viscous stress relative to the hydrostatic pressure, so that it indicates the degree of departure from equilibrium. As N_δ becomes small, the Newtonian law of viscosity and the Fourier law of heat conduction are recovered:

$$\mathbf{\Pi}_0=-2\eta[\nabla\mathbf{u}]^{(2)},\ \mathbf{Q}_0=-\lambda\nabla\ln T. \tag{5}$$

Gaseous expansion in free jet The free jet flow can be found in a continuum gas expansion from a high-pressure source into a low-pressure ambient background. This flow is basically axisymmetric but may be analyzed by the spherically symmetric expanding flow as an approximation. The conservation laws (2) for the purely spherical steady flow of a viscous heat-conducting perfect gas may be written as

$$\frac{d}{dr}\begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho\left(h+\frac{u^2}{2}\right)u \end{bmatrix} + \frac{2}{r}\rho u \begin{bmatrix} 1 \\ u \\ h+\frac{u^2}{2} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{1}{r^3}\frac{d}{dr}\left(r^3\Pi_{rr}\right) \\ \Pi_{rr}\left(\frac{du}{dr}-\frac{u}{r}\right)+\frac{u}{r^3}\frac{d}{dr}\left(r^3\Pi_{rr}\right)+\frac{1}{r^2}\frac{d}{dr}\left(r^2 Q\right) \end{bmatrix} = 0. \tag{6}$$

The constitutive equations of shear stress and heat flux reduce to

$$\Pi_{rr} q(\kappa) = \Pi_{rr_0}\left[1+\frac{\Pi_{rr}}{p}\left(1+\frac{3}{2}\frac{\frac{u}{r}}{\frac{du}{dr}-\frac{u}{r}}\right)\right], \tag{7}$$

$$Q q(\kappa) = Q_0\left[1+\frac{\Pi_{rr}}{p}\right], \tag{8}$$

where

$$\kappa = \frac{(mk_B)^{1/4}}{\sqrt{2}d}\frac{T^{1/4}}{p}\left[\frac{\mathbf{3/2}\Pi_{rr}^2}{2\eta}+\frac{Q^2}{\lambda}\right]^{1/2},$$

and

$$\Pi_{rr_0} = -\frac{4}{3}\eta r\frac{d}{dr}\left(\frac{u}{r}\right) = -\frac{4}{3}\eta\left(\frac{du}{dr}-\frac{u}{r}\right),\ Q_0 = -\lambda\frac{d}{dr}\left(\ln T\right).$$

Only the primary kinematic term $\mathbf{\Pi}\cdot\nabla T$ has been retained in the equation of heat flux for the simplicity. It should also be noted that the following relations hold for the spherically symmetric case

$$-\frac{1}{2}\Pi_{rr} = \Pi_{\theta\theta} = \Pi_{\phi\phi} \text{ and } -\frac{1}{2}\Pi_{rr_0} = \Pi_{\theta\theta_0} = \Pi_{\phi\phi_0}.$$

The general properties of the new constitutive equations in the spherically symmetric flow can be found by analyzing the equations (7) and (8). If the role of heat flux is assumed to be negligible in this case, the behavior of the stress should be explained by the following model equation

$$\Pi_{rr} q\left(\frac{\Pi_{rr}}{p}\right) = \Pi_{rr_0}\left[1+\frac{\Pi_{rr}}{p}\left(1+\frac{3}{2}\frac{\frac{u}{r}}{\frac{du}{dr}-\frac{u}{r}}\right)\right]. \tag{9}$$

Furthermore, if the stress remains a negative constant in the radial direction, the velocity profile can be written as (positive constant C)

$$u = r\left(1+C\ln r\right),$$

and the model constitutive equation of Π_{rr}/p can be written as

$$\frac{\Pi_{rr}}{p} q\left(\frac{\Pi_{rr}}{p}\right) = \frac{\Pi_{rr_0}}{p}\left\{1+\frac{\Pi_{rr}}{p}\left[1+\frac{3}{2}\left(\ln r+\frac{1}{C}\right)\right]\right\}. \tag{10}$$

The new constitutive relations in one-dimensional $u(r)$-only problem for different values of a factor of stress components, $\frac{3}{2}\left(\ln r+\frac{1}{C}\right)$, are depicted in comparison with the Navier-Stokes theory in Fig. 1. It can be shown in the expansion regime that the absolute value of $\frac{\Pi_{rr}}{p}$ decreases as the factor increases. This may provide a

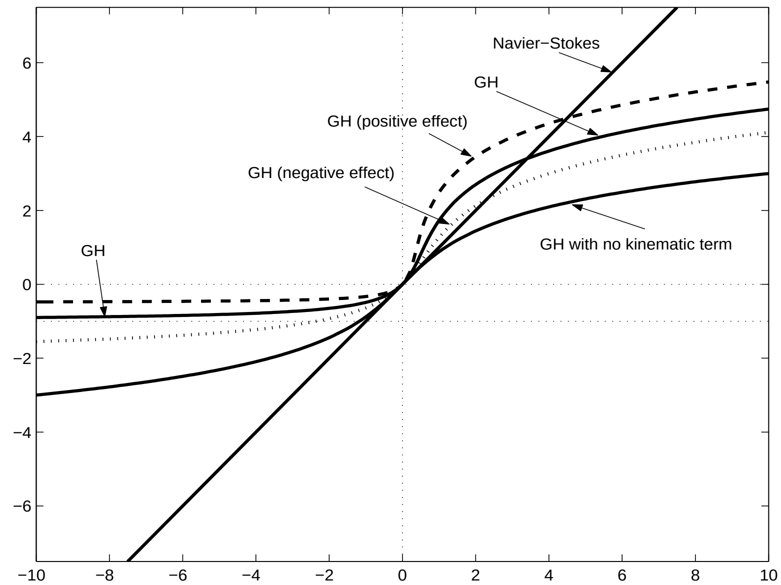

FIGURE 1. Generalized hydrodynamic constitutive relations relative to the Navier–Stokes relations in the u_r-only problem. The horizontal and vertical axes represent the Navier–Stokes relations Π_{rr0}/p, and the relations Π_{rr}/p, respectively. The gas is expanding in the range $\Pi_{rr0} < 0$, whereas the gas is compressed in the range of $\Pi_{rr0} > 0$.

clue in explaining the so-called freezing of the parallel temperature in the expansion from a spherical source reported in the literature [5].

Gaseous expansion in micro-channel The pressure-driven isothermal gas flows in a very long micro-channel of high aspect ratio(ϵ) is considered [9]. For low Mach number flow, the compressible Navier-Stokes equations, at the zeroth order of ϵ, may be valid [10]

$$\epsilon\frac{\partial(pu)}{\partial x}+\frac{\partial(pv)}{\partial y}=0,\ \frac{24}{\delta}\frac{dp}{dx}=-\frac{\partial\Pi_{xy}}{\partial y},\ \ q\left(CN_\delta\frac{|\Pi_{xy}|}{p}\right)\Pi_{xy}=-\frac{\partial u}{\partial y}\ \text{ where } \delta=24\frac{N_\delta}{\epsilon}\ \text{ and }\ C=\sqrt{2}c. \quad (11)$$

In this expression the streamwise coordinate x and the coordinate y normal to the wall are non-dimensionalized by the length and height of the channel. The reference state is chosen as the exit conditions ($x = 1$). The geometry of the channel is represented by $0 \le x \le 1$ and $-1/2 \le y \le 1/2$.

For the microscale gas flows with non-negligible Knudsen number, a model of the interaction between gas particles and surface wall atoms should be developed. In the present study, a model based on the Langmuir's theory of adsorption is used and in this model the fraction of the surface covered by adsorbed atoms at thermal equilibrium, α, is expressed as:

$$\alpha=(1-\alpha)\beta p \text{ or } \alpha=\frac{\beta p}{1+\beta p} \text{ where } \beta=\frac{K}{k_BT_w} \text{ and } K=\frac{C_c}{C_mC_s}. \quad (12)$$

The fraction α is a function of the pressure, p, and the equilibrium constant, K, which are functions of the concentrations $C_{m,s,c}$, and the surface temperature, T_w. The m, s, c, denote the gas molecule, the site, and the complex, respectively. The velocity slip can be expressed, in dimensional form, as

$$u=\alpha u_w+(1-\alpha)u_g, \quad (13)$$

where subscript g denotes a local value adjacent to the wall. The only parameter requiring further investigation is β (or the equilibrium constant K). A previous study [11] showed that the parameter β takes the form

$$\beta=\frac{1}{4\omega\mathrm{Kn}}\frac{1}{p_r}, \quad (14)$$

where

$$\omega = \omega_0(\nu)\left(\frac{T_w}{T_r}\right)^{1+2/(\nu-1)} \exp\left(-\frac{D_e}{k_B T_w}\right). \tag{15}$$

Finally the equation of the fraction α reduces to (in dimensionless form),

$$\alpha = \frac{\bar{\beta}p}{1+\bar{\beta}p} \text{ where } \bar{\beta} = \frac{1}{4\omega \mathrm{Kn}}. \tag{16}$$

With the Langmuir slip model of a monatomic gas,

$$u(x, y = \pm\frac{1}{2}) = \frac{u(x, y=0)}{1+\bar{\beta}p},$$

the following exact solutions–the dimensionless streamwise velocity and the dimensional mass flow rate–can be obtained:

$$\frac{u(x,y)}{u(x,y=0)} = 1 - \alpha\left[\frac{1-\cosh(\Phi y)}{1-\cosh(\Phi/2)}\right], \tag{17}$$

$$\dot{m} = \frac{H^3 W p_{\text{out}}^2}{24\eta LRT}\delta, \tag{18}$$

where

$$\delta = (p_{\text{in}}^2 - 1)\left[\frac{\cosh\Phi - q(\Phi)}{\Phi^2/3}\right] + \frac{6}{\bar{\beta}}(p_{\text{in}} - 1)\left[\frac{\cosh\Phi - 1}{\Phi^2}\right] \quad \text{where } \Phi = -C\epsilon\frac{d(\ln p)}{dx}.$$

By using the continuity equation and further applying the vanishing normal velocity at the wall, a solvability condition of the pressure distribution can be derived;

$$p'' = \frac{p'^2}{p}\left\{\left[2 + \frac{\Phi^2}{8}\left(1 + \frac{1}{\bar{\beta}p}\right)\right] q\left(\frac{\Phi}{2}\right) - 2\cosh\frac{\Phi}{2} + \frac{1}{\bar{\beta}p}\left(1 - \cosh\frac{\Phi}{2}\right)\right\}$$

$$\left\{\left[1 + \frac{\Phi^2}{8}\left(1 + \frac{1}{\bar{\beta}p}\right)\right] q\left(\frac{\Phi}{2}\right) - \cosh\frac{\Phi}{2} + \frac{1}{2\bar{\beta}p}\left(1 - \cosh\frac{\Phi}{2}\right)\right\}^{-1}.$$

With these results, comparison with experimental data is performed for helium gas in Fig. 2. An experimental work on gas flows in uniform microchannels by Arkilic [12] is utilized. The dimensions of the microchannel are as follows:

$$H = 1.33\,\mu\text{m},\ L = 7490\,\mu\text{m},\ w = 52.3\,\mu\text{m}.$$

Other important conditions concerning the experimental setup and the physical properties of helium gas are:

$$T = 293\,^\circ\text{K},\ p_{\text{out}} = 6500\,\text{Pa},\ R = 2077\,\text{J/kg}^\circ\text{K},\quad \eta = 1.97\cdot 10^{-5}\,\text{Ns/m}^2,\ \nu = 14,\ c = 1.046.$$

The Knudsen number based on the density at the exit and the channel height is 2.5. By following the same spirit as found in other studies, the values for the adjustable parameter ω are taken so as to best fit the experimental data. The adsorption coefficient $\omega = 1.42$ in the Langmuir slip model was chosen in the present work. In Fig. 2, dimensional mass flow rates per pressure drop $(p_{\text{in}} - p_{\text{out}})$ are depicted as a function of mean pressure. Using the values assigned to the adsorption coefficients, the model seems to predict the experimental values very closely.

CONCLUDING REMARK

In this work a theoretical model within the framework of Eu's generalized hydrodynamics and a slip model based on Langmuir's theory of gas-surface molecular interactions are applied to investigate pressure-driven free jet in rarefied gas and micro-channel gas flow. In particular, the general properties of constitutive equations in gas flow expanding from a spherical source are analyzed for finding a possible explanation of the freezing mechanism of the parallel temperature reported in the literature. The kinematic term in the constitutive equation associated with the ratio of radial stress components in spherical geometry seems to be responsible for such unusual behavior. The full studies of this problem will be reported in the future work.

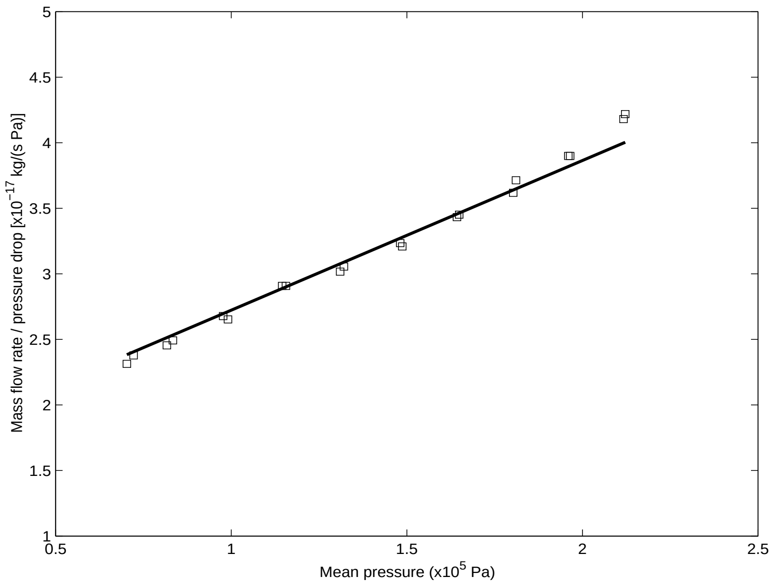

FIGURE 2. Mass flow rate of helium gas exhausting to an exit pressure of 6.5 kPa (Kn = 2.5). The square represents the experimental data.

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