H Theorem, Regularization, and Boundary Conditions for Linearized 13 Moment Equations

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An H theorem for the linearized Grad 13 moment equations leads to regularizing constitutive equations for higher fluxes and to a complete set of boundary conditions. Solutions for Couette and Poiseuille flows show good agreement with direct simulation Monte Carlo calculations. The Knudsen minimum for the relative mass flow rate is reproduced.

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Over the past few years we have developed a set of regularized 13 moment equations ($R13$ equations) for the description of rarefied gas flows in the transition regime (Knudsen numbers $\mathrm{Kn} < 1$) based on Knudsen number expansions of the Boltzmann equation and its system of moment equations [1–5]. The $R13$ equations form a regularization of the well-known 13 moment equations of Grad [6], obtained by adding terms of Super-Burnett order to the balances of pressure deviator and heat flux vector. When expanded in a series in Kn, the system contains the Euler, Navier-Stokes-Fourier, Burnett, and Super-Burnett equations. However, other than the Burnett and Super-Burnett equations [7,8], the $R13$ equations are linearly stable. Dispersion and damping for $R13$ agree better with experimental data than those for Navier-Stokes equations, or the original 13 moments system [1]. They allow the description of Knudsen boundary layers and yield smooth shock structures for large Mach numbers in good agreement with experiments [2]. The textbook [9] provides a comprehensive discussion and derivation of macroscopic models for rarefied gas flows, including the $R13$ equations.

Despite their welcome features, the $R13$ equations have so far defied our attempts to show the existence of an H theorem (entropy inequality). Moreover, the question of how to design boundary conditions for the higher moments is recognized as a major obstacle for any extended continuum model. Gu and Emerson, following ideas outlined in [9], developed a set of boundary conditions for the $R13$ equations [10], but their results show spurious boundary layers, which are probably due to the fact that they prescribe more boundary conditions in their numerical scheme than mathematically required.

In the present Letter we shall tackle both problems for the linearized 13 moment equations. A simple quadratic entropy, similar to the one provided in [11] for the hyperbolic Burnett equations, leads to a proper entropy inequality. The evaluation of the entropy generation rate leads to phenomenological equations [12], which give the regularizing terms. The entropy generation rate due to collisions with a solid wall is computed from the entropy flux and leads to boundary conditions. We consider Couette and Poiseuille flows with heat transfer to show that we obtain just as many boundary conditions as mathematically required, and that they lead to meaningful results. Computation of the mass flow rate in Poiseuille flow reproduces the well-known Knudsen minimum [13].

For greater generality, we base our considerations on the generalized 13 moment equations, which are the proper form of Grad's 13 moment equations for non-Maxwellian molecules [4,9]. The variables are mass density ρ, velocity v_i, temperature θ, deviatoric stress tensor σ_{ij}, and heat flux q_i. The 13 moment equations consist of the conservation laws for mass, momentum, and energy and balance laws for σ_{ij}, q_i. We linearize Eqs. (9.1, 9.17, 9.18) in [9] around a homogeneous and constant equilibrium ground state ρ_0, θ_0, $v_i^0 = \sqrt{R\theta_0} V_i$ (R is the gas constant) and introduce dimensionless quantities to find

$$\frac{D\rho}{Dt} + \frac{\partial v_k}{\partial x_k} = 0, \quad \frac{Dv_i}{Dt} + \frac{\partial \rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = 0, \quad \frac{D\sigma_{ij}}{Dt} + \frac{4}{5}\mathrm{Pr}\frac{\varpi_3}{\varpi_2}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial m_{ijk}}{\partial x_k} = -\frac{2}{\varpi_2}\frac{1}{\mathrm{Kn}}\left[\sigma_{ij} + 2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right],$$
$$\frac{3}{2}\frac{D\theta}{Dt} + \frac{\partial q_k}{\partial x_k} + \frac{\partial v_k}{\partial x_k} = 0, \quad \frac{Dq_i}{Dt} + \frac{5}{4}\frac{1}{\mathrm{Pr}}\frac{\theta_4}{\theta_2}\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{1}{2}\frac{\partial R_{ik}}{\partial x_k} = -\frac{1}{\theta_2}\frac{5}{2}\frac{1}{\mathrm{Pr}}\frac{1}{\mathrm{Kn}}\left[q_i + \frac{5}{2}\frac{1}{\mathrm{Pr}}\frac{\partial \theta}{\partial x_i}\right]. \tag{1}$$

$\mathrm{Kn} = \frac{\mu}{\rho\sqrt{R\theta_0}L}$ is the Knudsen number (μ is viscosity, L is reference length), $\mathrm{Pr} \simeq \frac{2}{3}$ is the Prandtl number, and ϖ_α, θ_α denote Burnett coefficients [9,14]; for Maxwell molecules $\varpi_2 = 2$, $\varpi_3 = \theta_4 = 3$, $\theta_2 = 45/8$ and for hard sphere molecules $\varpi_2 = 2.028$, $\varpi_3 = \theta_4 = 2.418$, $\theta_2 = 5.822$. Indices in angular brackets denote the symmetric and trace-free part of a tensor. The additional quantities $m_{ijk} = m_{\langle ijk\rangle}$ and $R_{ij} = R_{ji}$ denote higher order fluxes which were not present in the original derivation in [4]. $\frac{D}{Dt} = \frac{\partial}{\partial t} + V_k \frac{\partial}{\partial x_k}$ denotes the convective time derivative which for an observer resting in the equilibrium ground state reduces to the partial derivative $\frac{\partial}{\partial t}$.

We define the convex dimensionless entropy density

$$\eta = \eta_0 - \frac{1}{2}\rho^2 - \frac{1}{2}v_i v_i - \frac{3}{4}\theta^2 - \frac{\varpi_2}{8}\sigma_{ij}\sigma_{ij} - \frac{2\theta_2}{25}\mathrm{Pr}^2 q_i q_i,$$

take its time derivative, and replace the time derivatives of the variables by means of the balance laws (1) to obtain the balance law for entropy—the 2nd law—as

$$\frac{D\eta}{Dt} + \frac{\partial \phi_k}{\partial x_k} = \Sigma$$

with the entropy flux

$$\phi_k = -(\rho + \theta)v_k - v_i\sigma_{ik} - \theta q_k - \frac{\varpi_3}{5}\mathrm{Pr} q_i \sigma_{ik} - \frac{\varpi_2}{4}\sigma_{ij}m_{ijk} - \frac{2\theta_2}{25}\mathrm{Pr}^2 q_i R_{ik}$$

and the bulk entropy generation rate

$$\Sigma = \frac{\sigma_{ij}\sigma_{ij}}{2\mathrm{Kn}} + \frac{2\,\mathrm{Pr}}{5}\frac{q_i q_i}{\mathrm{Kn}} - \frac{\varpi_2}{4}m_{ijk}\frac{\partial\sigma_{ij}}{\partial x_k} - \frac{2\theta_2}{25}\mathrm{Pr}^2 R_{ik}\frac{\partial q_i}{\partial x_k}.$$

The generation rate ought to be non-negative, $\Sigma \geq 0$, for all values of the variables ρ, v_i, θ, σ_{ij}, q_i. This requirement can be fulfilled easily by choosing constitutive equations according to the linear phenomenological laws

$$R_{ij} = -\tau_R\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \frac{\tau_\Delta}{3}\frac{\partial q_k}{\partial x_k}\delta_{ij}, \quad m_{ijk} = -\tau_m\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} \tag{2}$$

with positive coefficients τ_α ($\alpha \in \{R, \Delta, m\}$). For the case of Maxwell molecules the coefficients were derived from kinetic theory in [1,3] as $\tau_R = \frac{24}{5}\mathrm{Kn}$, $\tau_\Delta = 12\mathrm{Kn}$, $\tau_m = 2\mathrm{Kn}$. The regularization of the 13 moment equations (2) arises here quite naturally. The usual Grad closure sets $\tau_\alpha = 0$ and ignores some dissipative contributions.

For a solid wall the dimensionless first law reads $c_v\frac{D\theta_W}{Dt} + \frac{\partial q_k}{\partial x_k} = 0$, where θ_W denotes the temperature of the wall and c_v is its specific heat. A linear second law with entropy $\eta_W = \eta_W^0 - \frac{c_v}{2}\theta_W^2$ gives its entropy flux in the wall rest frame as $\phi_k^W = -\theta_W q_k$. The entropy generation due to interaction between gas and wall must be positive, which requires that the entropy flux out of the gas-wall interface is larger than the entropy flux into the interface. When the normal vector n_k points from the gas to the wall, this condition reads

$$\Sigma_W = (\phi_k^W - \phi_k)n_k \geq 0.$$

For the further evaluation, it is useful to split the variables into their normal and tangential parts as

$$q_k = q_n n_k + \bar{q}_k,$$
$$\sigma_{ij} = \sigma_{nn}(\tfrac{3}{2}n_i n_j - \tfrac{1}{2}\delta_{ij}) + \bar{\sigma}_{ni}n_j + \bar{\sigma}_{nj}n_i + \bar{\sigma}_{ij}$$

with $0 = (v_k - v_k^W)n_k = \bar{q}_k n_k = \bar{\sigma}_{nk}n_k = \bar{\sigma}_{ij}n_i = \bar{\sigma}_{kk}$. The wall moves with the velocity v_i^W with respect to the ground state, and the gas flow normal to the wall must vanish, so that we find the wall entropy generation as

$$\begin{aligned}\Sigma_W = {}& \bar{\sigma}_{ni}\left[v_i - v_i^W + \left(\frac{\varpi_3}{5} - \alpha\right)\mathrm{Pr}\bar{q}_i + \frac{\varpi_2}{2}m_{inn}\right] \\ &+ \bar{q}_i\left[\alpha\,\mathrm{Pr}\bar{\sigma}_{ni} + \frac{2\theta_2}{25}\mathrm{Pr}^2 R_{in}\right] \\ &+ q_n\left[\theta - \theta_W + \left(\frac{\varpi_3}{5}\mathrm{Pr} - \beta\right)\sigma_{nn} + \frac{2\theta_2}{25}\mathrm{Pr}^2 R_{nn}\right] \\ &+ \sigma_{nn}\left[\beta q_n + \frac{3\varpi_2}{8}m_{nnn}\right] + \frac{\varpi_2}{4}\bar{\sigma}_{ij}m_{ijn},\end{aligned}$$

where α and β are arbitrary numbers and all quantities have to be evaluated at the wall. Positive entropy generation can, again, be achieved by phenomenological equations with positive coefficients γ_α which are, indeed, boundary conditions for the variables,

$$\begin{aligned}\bar{\sigma}_{ni} &= \gamma_1\left[v_i - v_i^W + \left(\frac{\varpi_3}{5} - \alpha\right)\mathrm{Pr}\bar{q}_i + \frac{\varpi_2}{2}m_{inn}\right], \\ \bar{q}_i &= \gamma_2\left[\alpha\,\mathrm{Pr}\bar{\sigma}_{ni} + \frac{2\theta_2}{25}\overset{2}{\mathrm{Pr}}R_{ni}\right], \\ \sigma_{nn} &= \gamma_3\left[\beta q_n + \frac{\varpi_2}{4}m_{nnn}\right], \\ q_n &= \gamma_4\left[\theta - \theta_W + \left(\frac{\varpi_3}{5}\mathrm{Pr} - \beta\right)\sigma_{nn} + \frac{2\theta_2}{25}\overset{2}{\mathrm{Pr}}R_{nn}\right], \\ \bar{\sigma}_{ij} &= \gamma_5\left[\frac{\varpi_2}{4}m_{ijn}\right].\end{aligned} \tag{3}$$

Here we have directly linked the unknown boundary values for the moments to their driving forces (the expressions in square brackets); that is, we have ignored the possibility of cross terms (off-diagonal Onsager coefficients [12]). The coefficients α and β reflect some freedom in shifting terms between the driving forces. Equation (3) is the (phenomenological) Maxwell-Smoluchowski jump and slip boundary conditions [9,10].

The coefficients α, β, γ_α must be determined from experiments, or first principles, e.g., from the boundary conditions for the Boltzmann equation with accommodation coefficient χ [9,10]. Comparison of (3) with the slip condition of [10] (Maxwell molecules) allows to identify $\gamma_1 = \frac{\chi}{2-\chi}\sqrt{2/\pi}$, $\alpha = \frac{1}{5}$. Moreover, instead of the factor $\frac{\varpi_2}{2} \simeq 1$ in (3) kinetic theory predicts the factor $\frac{1}{2}$; this value gives better results, and we used it for the Poiseuille flow simulations below. Note that in a higher theory with m_{inn} as variable, part of the expression $\bar{\sigma}_{ni}\frac{\varpi_2}{2}m_{inn}$ would add to the boundary condition for m_{inn}. Similar statements can be made on the other coefficients in (3). A detailed account of kinetic theory based boundary conditions for the fully nonlinear $R13$ equations, and their numerical solutions, will be presented elsewhere.

In plane Couette flow, two infinite parallel plates at $y = \pm\frac{1}{2}$ move with constant velocities $\pm v_W$ relative to the center into the direction $x = x_1$, and are kept at constant temperatures $\pm\theta_W$. Because of the symmetry of the problem, all variables depend only on the coordinate y which is zero in the middle between the walls. Since the walls are impermeable, the velocity of the gas must point into the x direction, that is $v_i = \{v(y), 0, 0\}_i$ and thus $\frac{\partial v_k}{\partial x_k} = D/Dt = 0$. The setup is independent of the coordinate $z = x_3$, so that neither stress nor heat flux is associated with that direction, and $\sigma_{13} = \sigma_{23} = q_3 = 0$, $\sigma_{33} = -\sigma_{11}(y) - \sigma_{22}(y)$; all other components depend solely on y.

The equations (1) with the regularization (2) split into three independent subsets, each with its own wall entropy generation rate. For Maxwell molecules we obtain (a) velocity problem

$$\begin{gathered}
v = A_1 - \sigma_{12}\frac{y}{\mathrm{Kn}} - \frac{2}{5}q_1, \quad \sigma_{12} = \sigma_{12}^0, \\
q_1 = A_2 \sinh\left[\sqrt{\frac{5}{9}}\frac{y}{\mathrm{Kn}}\right] + A_3 \cosh\left[\sqrt{\frac{5}{9}}\frac{y}{\mathrm{Kn}}\right], \\
R_{12} = -\frac{4}{\sqrt{5}}A_2 \cosh\left[\sqrt{\frac{5}{9}}\frac{y}{\mathrm{Kn}}\right] - \frac{4}{\sqrt{5}}A_3 \sinh\left[\sqrt{\frac{5}{9}}\frac{y}{\mathrm{Kn}}\right], \\
\Sigma_W^v = \pm\sigma_{12}\left[v \mp v_W + \left(\frac{2}{5} - \alpha\right)q_1\right] \pm q_1\left(\alpha\sigma_{12} + \frac{1}{5}R_{12}\right),
\end{gathered} \tag{4}$$

(b) temperature problem

$$\begin{gathered}
\theta = B_1 - \frac{4}{15}q_2\frac{y}{\mathrm{Kn}} - \frac{2}{5}\sigma_{22}, \quad q_2 = q_2^0, \\
\sigma_{22} = B_2 \sinh\left[\sqrt{\frac{5}{6}}\frac{y}{\mathrm{Kn}}\right] + B_3 \cosh\left[\sqrt{\frac{5}{6}}\frac{y}{\mathrm{Kn}}\right], \\
m_{222} = -\sqrt{\frac{6}{5}}B_2 \cosh\left[\sqrt{\frac{5}{6}}\frac{y}{\mathrm{Kn}}\right] - \sqrt{\frac{6}{5}}B_3 \sinh\left[\sqrt{\frac{5}{6}}\frac{y}{\mathrm{Kn}}\right], \\
\Sigma_W^T = \pm q_2\left[\theta \mp \theta_W + \left(\frac{2}{5} - \beta\right)\sigma_{22}\right] \pm \sigma_{22}\left(\beta q_2 + \frac{3}{4}m_{222}\right),
\end{gathered} \tag{5}$$

(c) the rest

$$\begin{gathered}
\sigma_{11} + \frac{1}{2}\sigma_{22} = C_1 \sinh\left[\sqrt{\frac{3}{2}}\frac{y}{\mathrm{Kn}}\right] + C_2 \cosh\left[\sqrt{\frac{3}{2}}\frac{y}{\mathrm{Kn}}\right], \\
m_{112} + \frac{1}{2}m_{222} = -\frac{2}{3}\mathrm{Kn}\frac{\partial}{\partial y}\left(\sigma_{11} + \frac{1}{2}\sigma_{22}\right), \\
\Sigma_W^\sigma = \pm\left(\sigma_{11} + \frac{1}{2}\sigma_{22}\right)\left(m_{112} + \frac{1}{2}m_{222}\right).
\end{gathered} \tag{6}$$

Moreover, we have an equation for the mass density, $\rho + \theta + \sigma_{22} = P_0$. In the expressions for wall entropy generation the upper sign is for the right wall; the lower sign for the left wall. The general solution includes 11 constants of integration, σ_{12}^0, q_2^0, A_1, A_2, A_3, B_1, B_2, B_3, P_0, C_1, C_2; these must be determined from the boundary conditions.

The constant P_0 follows from the requirement that mass is conserved in the process, $\int_{-1/2}^{1/2} \rho dy = \int_{-1/2}^{1/2} \rho_0 dy = 1$. The entropy generation rate Σ_W^σ (6) can only be nonnegative at $y = \pm\frac{1}{2}$ if $C_1 = C_2 = 0$. Since velocity and temperature are prescribed symmetric to the center, their curves must be point symmetric to the center, so that $A_1 = A_3 = B_1 = B_3 = 0$. All remaining constants can be determined from boundary conditions at the right wall.

The velocity and temperature problems have the same structure, and we consider only the velocity problem, for which we need to find σ_{12}^0 and A_2. The wall entropy generation suggests phenomenological equations for the boundary conditions as (at $y = \frac{1}{2}$)

$$\begin{aligned}
\sigma_{12} &= \gamma_1[v - v_W + (\tfrac{2}{5} - \alpha)q_1 + \tfrac{1}{2}m_{122}], \\
q_1 &= \gamma_2[\alpha\sigma_{12} + \tfrac{1}{5}R_{12}].
\end{aligned} \tag{7}$$

with $m_{122} = 0$. Insertion of (4) leads to an algebraic system for σ_{12}^0 and A_2 with the solution

$$\sigma_{12}^0 = -\frac{v_W}{(\frac{1}{\gamma_1} + \frac{1}{2\mathrm{Kn}}) + \frac{\alpha^2\gamma_2}{1 + \frac{4\gamma_2}{5\sqrt{5}}\coth\frac{\sqrt{5}}{6\mathrm{Kn}}}},$$

$$A_2 = \frac{\alpha\gamma_2}{1 + \frac{4\gamma_2}{5\sqrt{5}}\coth\frac{\sqrt{5}}{6\mathrm{Kn}}}\frac{\sigma_{12}^0}{\sinh\frac{\sqrt{5}}{6\mathrm{Kn}}}.$$

Figure 1 shows the $R13$ profiles for velocity and heat flux parallel to the wall compared to DSMC simulations in argon at Kn = 0.05, 0.1, 0.5 with plate velocities $\pm 100\,\frac{m}{s}$ at 273 K so that $v_W = 0.419\,543$. The DSMC simulations were performed for Maxwell molecules with fully diffusive boundary conditions ($\chi = 1$). We use the kinetic theory values $\gamma_1 = \sqrt{2/\pi}$, $\alpha = \frac{1}{5}$ while $\gamma_2 = 3$ was chosen to obtain reasonable results. The agreement between DSMC and $R13$ is fairly good. The DSMC simulations are slightly affected by nonlinear effects which can be described by the nonlinear bulk solution [9].

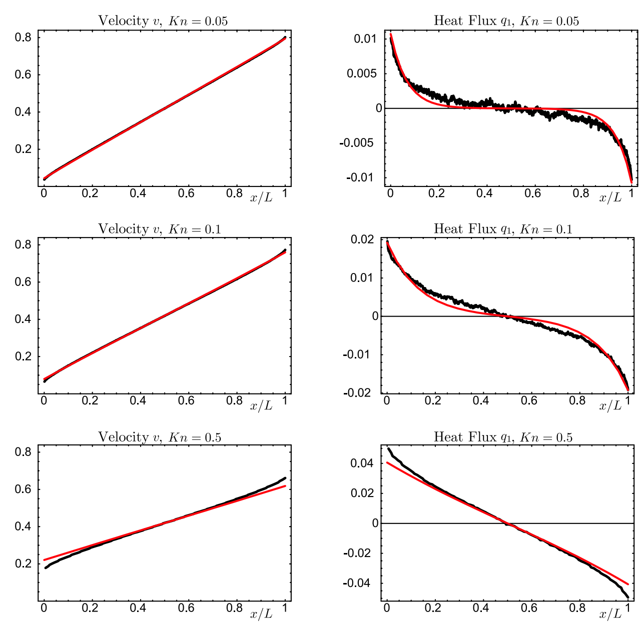

FIG. 1 (color online). Dimensionless velocity and heat flux parallel to the wall for Couette flow computed from the $R13$ equations (red) and DSMC (black).

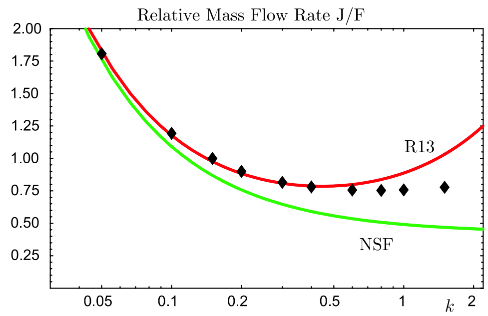

FIG. 2 (color online). Relative mass flow rate for Poiseuille flow as function of $k = \frac{4\sqrt{2}}{5}\mathrm{Kn}$ from Boltzmann equation (symbols) [13] in comparison with $R13$ equations and Navier-Stokes.

Similar agreement was obtained in [15] from an analytical solution of a Lattice Boltzmann model, which gives the same final equation for velocity with only small differences in the numerical factors.

Finally we consider the velocity problem for force-driven Poiseuille flow where the dimensionless pressure gradient $\frac{\partial \rho + \theta}{\partial x}$ is replaced by the constant force $(-F)$. The solution of the relevant moment equations must be axisymmetric to the center,

$$\sigma_{12} = Fy, \qquad v = A_1 - \frac{F}{2\mathrm{Kn}} y^2 - \frac{2}{5} q_1 - m_{122},$$

$$q_1 = -\frac{3}{2} F\mathrm{Kn} + A_2 \cosh\left[\sqrt{\frac{5}{9}} \frac{y}{\mathrm{Kn}}\right],$$

$$m_{122} = -\frac{16}{15}\mathrm{Kn}F, \qquad R_{12} = -\frac{4}{\sqrt{5}} A_2 \frac{\partial q_1}{\partial y},$$

with the entropy generation at the right wall

$$\Sigma_W^v = \sigma_{12}[v - v_W + (\tfrac{2}{5} - \alpha) q_1 + \tfrac{1}{2} m_{122}] + q_1(\alpha \sigma_{12} + \tfrac{1}{5} R_{12}).$$

We use the same coefficients as before and compute the total mass flow rate $J = \int_{-1/2}^{1/2} v dy$ as

$$J = \frac{F}{2}\left[\frac{3}{25} + \sqrt{\frac{\pi}{2}} + \frac{1}{6\mathrm{Kn}} + \frac{34}{15}\mathrm{Kn} - \frac{3(1+5\mathrm{Kn})^2}{25(1 + \frac{5}{12}\sqrt{5}\coth\frac{\sqrt{5}}{6\mathrm{Kn}})}\right].$$

It is well known that the relative mass flow rate J/F as function of the Knudsen number exhibits the *Knudsen minimum* around $\mathrm{Kn} = 1$ [13,16] and our result indeed has a distinct minimum at $\mathrm{Kn} \approx 0.5$. Figure 2 compares values for $J/(\sqrt{2}F)$ as function of $k = \frac{4\sqrt{2}}{5}\mathrm{Kn}$ obtained from numerical solutions of the Boltzmann equation [13] to the predictions of the $R13$ equations, and the Navier-Stokes equations (with slip). The $R13$ equations match the data very well. The deviation of the $R13$ results from kinetic theory for large Knudsen numbers shows that Knudsen numbers above unity are outside the range of application of $R13$.

While the Navier-Stokes equations can describe the Knudsen minimum when second order boundary conditions are employed [17], they cannot describe rarefaction effects like parallel heat flux q_1, or the temperature dip in the center of the channel [18]. In future papers we shall show that the nonlinear $R13$ equations can describe these effects in good agreement to DSMC simulations.

We have given an H theorem for the regularized 13 moment equations in the linear case. The non-negativity of the entropy generation rate in the bulk is guaranteed by the constitutive equations for the higher fluxes, which just lead to the regularization. The requirement of non-negative wall entropy generation leads to boundary conditions. Computations for Couette and Poiseuille flows show good agreement with solutions of the Boltzmann equation including the Knudsen minimum. Our findings add to the positive properties of the $R13$ equations shown earlier [1,2,9]. Further fine-tuning of the coefficients in the boundary conditions will render the $R13$ equations into a successful mathematical model for microscopic gas flows of third order accuracy in the Knudsen number.

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