Continuum Mech. Thermodyn. (2009) 21:389–399
DOI 10.1007/s00161-009-0112-6

**ORIGINAL ARTICLE**

**R. S. Myong**

# Coupled nonlinear constitutive models for rarefied and microscale gas flows: subtle interplay of kinematics and dissipation effects

Received: 1 March 2009 / Accepted: 19 June 2009 / Published online: 11 July 2009


**Abstract** The constitutive relations of gases in a thermal nonequilibrium (rarefied and microscale) can be derived by applying the moment method to the Boltzmann equation. In this work, a model constitutive relation determined on the basis of the moment method is developed and applied to some challenging problems in which classical hydrodynamic theories including the Navier–Stokes–Fourier theory are shown to predict qualitatively wrong results. Analysis of coupled nonlinear constitutive models enables the fundamentals of gas flows in thermal nonequilibrium to be identified: namely, nonlinear, asymmetric, and coupled relations between stresses and the shear rate; and effect of the bulk viscosity. In addition, the new theory explains the central minimum of the temperature profile in a force-driven Poiseuille gas flow, which is a well-known problem that renders the classical hydrodynamic theory a global failure.

**Keywords** Continuum mechanics · Constitutive relation · Microscale and nanoscale gases · Force-driven Poiseuille flow

**PACS** 47.10.ab Conservation laws and constitutive relations · 47.45.Ab Kinetic theory of gases · 47.61.Cb Non-continuum effects

## 1 Introduction

A constitutive equation represents the relation between the microscopic and macroscopic physics of a specific substance of interest. As the only ingredient that appears in the continuum mechanics intended to bridge two distinctive worlds (macroscopic and microscopic), it plays a critical role in describing the structure of substance. Depending on the type of materials, the constitutive equation can generally take various forms: for example, Hooke's law for pure solid materials which has been studied in previous works [1]. On the other hand, less attention has been directed to the development of the corresponding equations for gases; until recently, virtually all the practical flow and heat transfer problems were dealt in terms of the classical model known as the Navier–Stokes–Fourier model. However, research interests have shifted from the classical problem to the more challenging problem that arises from the micromechanics and nanomechanics of materials related to recent developments in nanotechnology and nanoscience: accordingly, there is a growing need to develop new constitutive equations for rarefied and microscale gas flows [2].

That goal is pursued here by applying the so-called moment method [3,4] to the Boltzmann equation, which is derived from the kinetic viewpoint of gas motion. With the Boltzmann equation as the starting point, a new model of the constitutive relation can be developed and applied to challenging problems, particularly those where the classical hydrodynamic theories including the Navier–Stokes–Fourier theory are shown to

Communicated by M. Torrilhon

R. S. Myong
Department of Mechanical and Aerospace Engineering and Research Center for Aircraft Parts Technology,
Gyeongsang National University, Jinju, Kyeongnam 660-701, South Korea
E-mail: myong@gnu.ac.kr

predict qualitatively wrong results. First, the structure of the constitutive relations in a one-dimensional situation (compression, expansion, and velocity shear flows) of monatomic and diatomic gases is investigated. A special treatment of the dissipative term in the constitutive equation highlights the nonlinearity, asymmetry, and effects of the bulk viscosity associated with the rotational motion of diatomic gases. Attention is then directed to a force-driven Poiseuille gas flow where the classical hydrodynamic theory proves to be a global failure because of its inability to predict the correct flow physics (the so-called central minimum of the temperature profile) even for very small Knudsen numbers. The new theory elegantly explains the central minimum of the temperature profile [5], which was identified as one of three surprising hydrodynamic results discovered by the DSMC method. The approach taken in this study is unique in the sense that the main focus is placed on the subtle interplay of various terms (material derivative, high-order flux, kinematics, and dissipations) in the constitutive equations and on the relation between the constitutive model of gases and equations found in other fields such as rheology [6].

## 2 The moment method and algebraic model constitutive relations

### 2.1 Derivation of constitutive relations by the moment method

The Boltzmann kinetic equation of the distribution of gas particles $f(\mathbf{v};\mathbf{r},t)$ may be written as

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

where the term $C[f]$ represents the collision integral of the interaction among the particles. A constitutive relation for shear stress $\mathbf{\Pi}$ can be obtained by differentiating the statistical definition of tensor $\mathbf{\Pi}$ with time and combining it with the Boltzmann equation [3,4,7–9]:

$$\rho\frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right)+\nabla\cdot\mathbf{\Psi}^{(\mathbf{\Pi})}=\mathbf{Z}^{(\mathbf{\Pi})}+\mathbf{\Lambda}^{(\mathbf{\Pi})} \tag{2}$$

Material Derivative of Shear Stress + High-Order Flux = Kinematic Term + Dissipative Term

where

$$\mathbf{\Pi}=\left\langle m\,[\mathbf{cc}]^{(2)}\,f\right\rangle,\ \mathbf{\Psi}^{(\mathbf{\Pi})}=\left\langle m\,[\mathbf{cc}]^{(2)}\,\mathbf{c}f\right\rangle,$$
$$\mathbf{Z}^{(\mathbf{\Pi})}=\left\langle f\left(\frac{D}{Dt}+\mathbf{c}\cdot\nabla\right)m\,[\mathbf{cc}]^{(2)}\right\rangle,\ \mathbf{\Lambda}^{(\mathbf{\Pi})}=\left\langle m\,[\mathbf{cc}]^{(2)}\,C[f]\right\rangle.$$

Here an abbreviation is used for the integration over $\mathbf{v}$ space with angular brackets $\langle\cdots\rangle=\int d\mathbf{v}\cdots$. The symbol $[\,]^{(2)}$ stands for a traceless symmetric part of the tensor; hence, the term $[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)}$, for example, represents the traceless symmetric part of the coupling between the shear stress and the velocity gradient tensor. With the application of the relation

$$\mathbf{Z}^{(\mathbf{\Pi})}=\left\langle f\left(\frac{D}{Dt}+\mathbf{c}\cdot\nabla\right)m\,[\mathbf{cc}]^{(2)}\right\rangle=-2\,[(p\mathbf{I}+\mathbf{\Pi})\cdot\nabla\mathbf{u}]^{(2)},$$

the constitutive equation can be expressed in the following instructive form

$$\rho\frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right)+2\,[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)}+\nabla\cdot\mathbf{\Psi}^{(\mathbf{\Pi})}=-2p\,[\nabla\mathbf{u}]^{(2)}+\mathbf{\Lambda}^{(\mathbf{\Pi})}. \tag{3}$$

The first two terms on the left-hand side describe elastic effects of gases measured by the Weissenberg number *We*, which is well-known in non-Newtonian shear-thinning viscoelastic fluids such as the generalized Oldroyd-B fluids and the quasi-linear upper convective Maxwell model. At this stage, no approximations are made in deriving constitutive Eq. (3). However, Eq. (3) is an open system of partial differential equations; thus, a proper closure must be introduced so that it can be used as a practical constitutive equation. Of the various methods of achieving this goal, the following method is used in this work, primarily due to its simplicity:

$$\rho\frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right)+\nabla\cdot\mathbf{\Psi}^{(\mathbf{\Pi})}=0. \tag{4}$$

This simple method completely circumvents the difficulty associated with additional boundary conditions that are required in other theories retaining non-conserved variables (shear stress and heat flux) in the constitutive equations at the same level of conserved variables (density, velocity and temperature). The model will be applied later to various benchmark flow problems to determine its effectiveness. The constitutive equation is then reduced to

$$2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}+2p\left[\nabla\mathbf{u}\right]^{(2)}=\mathbf{\Lambda}^{(\mathbf{\Pi})}. \tag{5}$$

The only term that requires further refinement is the dissipation term $\mathbf{\Lambda}^{(\mathbf{\Pi})}$ on the right-hand side; this term is directly related to the details of the collision integral in the kinetic equation. In many cases, for mathematical simplicity, a relaxation approximation for the collision integral is often used and the dissipation term is then reduced to

$$\mathbf{\Lambda}^{(\mathbf{\Pi})}=-\frac{\mathbf{\Pi}}{\eta/p}.$$

On the other hand, in the moment method [3,4] the dissipation term may be expressed as

$$\mathbf{\Lambda}^{(\mathbf{\Pi})}=-\frac{\mathbf{\Pi}}{\eta/p}q(\kappa),$$

where

$$q(\kappa)\equiv\frac{\sinh\kappa}{\kappa},\quad \kappa=\frac{(mk_BT)^{1/4}}{\sqrt{2}pd}\left[\frac{\mathbf{\Pi}:\mathbf{\Pi}}{2\eta}+\frac{\mathbf{Q}\cdot\mathbf{Q}}{\lambda}\right]^{1/2}.$$

In this expression, $\kappa$ is the first-order cumulant of the cumulant approximation for dissipation terms; $d$, $m$, and $k_B$ denote the diameter of the molecule, the molecular mass, and the Boltzmann constant, respectively; and $\mathbf{Q}$, $\eta$, and $\lambda$ represent the heat flux, the viscosity and the thermal conductivity, respectively. Finally, constitutive Eq. (5) for shear stress $\mathbf{\Pi}$ becomes the following system of nonlinear *algebraic* equations:

$$-2\left[\frac{\mathbf{\Pi}}{p}\cdot\eta\nabla\mathbf{u}\right]^{(2)}-2\eta\left[\nabla\mathbf{u}\right]^{(2)}=\mathbf{\Pi}q(\kappa). \tag{6}$$

In physical terms, the system represents the constitutive relation for multiaxial states of stress. The first term, which is derived from kinematics, describes the elastic effects of gases, and its magnitude may be measured by the ratio $\mathbf{\Pi}/p$. In mathematical terms, the system becomes a set of coupled nonlinear algebraic equations whose origin can be traced to the presence of the dissipation term $q(\kappa)$ and the kinematic term $[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)}$.

### 2.2 Model constitutive relations with a diatomic case

The Boltzmann–Curtiss kinetic equation for a diatomic molecule with a moment of inertia $I$ and an angular momentum $\mathbf{j}$ can be expressed, under the assumption of no external field, as

$$\left[\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\frac{j}{I}\frac{\partial}{\partial\psi}\right]f(\mathbf{v},\mathbf{r},\mathbf{j},\psi,t)=R\left[f\right]. \tag{7}$$

In this equation $\psi$, $j$ and $R\left[f\right]$ represent the azimuth angle associated with the orientation of the molecule, the magnitude of the angular momentum vector $\mathbf{j}$, and the collision integral, respectively. When the modified moment method described in the previous section is applied, a model constitutive relation of the conserved and nonconserved variables in diatomic gases can be derived as follows (see [9] also):

$$\begin{aligned}\hat{\mathbf{\Pi}}q(c\hat{R})&=\left(1+f_b\hat{\Delta}\right)\hat{\mathbf{\Pi}}_0+\left[\hat{\mathbf{\Pi}}\cdot\nabla\hat{\mathbf{u}}\right]^{(2)},\\ \hat{\Delta}q(c\hat{R})&=\hat{\Delta}_0+\frac{3}{2}f_b\left(\hat{\mathbf{\Pi}}+f_b\hat{\Delta}\mathbf{I}\right):\nabla\hat{\mathbf{u}},\\ \hat{\mathbf{Q}}q(c\hat{R})&=\left(1+f_b\hat{\Delta}\right)\hat{\mathbf{Q}}_0+\hat{\mathbf{\Pi}}\cdot\hat{\mathbf{Q}}_0.\end{aligned} \tag{8}$$

Here the variable $\hat{\Delta}$ denotes the excess normal stress and the caret ˆ over a symbol represents a quantity with the dimension of the ratio of the stress to the pressure. The values $\hat{\mathbf{\Pi}}_0$, $\hat{\Delta}_0$, and $\hat{\mathbf{Q}}_0$ are determined as follows by the Newtonian law of shear (shear stress) and bulk viscosity (excess normal stress) and the Fourier law of heat conduction (heat flux), respectively:

$$\mathbf{\Pi}_0 = -2\eta\,[\nabla\mathbf{u}]^{(2)}\,,\ \Delta_0 = -\eta_b\nabla\cdot\mathbf{u},\ \mathbf{Q}_0 = -\lambda\nabla\ln T. \tag{9}$$

Here $\eta_b$ and $f_b$ denote the bulk viscosity and the ratio of the bulk viscosity to the shear viscosity, respectively. Note also that the second coefficient of viscosity in Stokes' hypothesis is equivalent to $\eta_b - \frac{2}{3}\eta$. All the variables in the aforementioned Eqs. (8) and (9) are made dimensionless by introducing the proper dimensionless variables and parameters. The other variables are defined as

$$\hat{\mathbf{\Pi}} \equiv \frac{N_\delta}{p}\mathbf{\Pi},\ \hat{\Delta} \equiv \frac{N_\delta}{p}\Delta,\ \hat{\mathbf{Q}} \equiv \frac{N_\delta}{p}\frac{\mathbf{Q}}{\sqrt{T/(2\varepsilon)}},\ \nabla\hat{\mathbf{u}} \equiv -2\eta\frac{N_\delta}{p}\nabla\mathbf{u},\ \varepsilon \equiv \frac{1}{EcPr}\frac{1}{T_r/\Delta T} \tag{10}$$

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

$$q(c\hat{R}) = \frac{\sinh(c\hat{R})}{c\hat{R}},\ \hat{R}^2 = \hat{\mathbf{\Pi}}:\hat{\mathbf{\Pi}} + \frac{4}{5f_b}\hat{\Delta}^2 + \hat{\mathbf{Q}}\cdot\hat{\mathbf{Q}},\ c^2 = \frac{8\sqrt{2}}{5\pi}A_2(\nu)\Gamma\left[4 - \frac{2}{\nu-1}\right], \tag{11}$$

where $M$, $Re$, $Ec$, and $Pr$ are the dimensionless fluid dynamic numbers for the Mach, Reynolds, Eckert, and Prandtl numbers, respectively. The value of $f_b$ is 0.8 for nitrogen according to the experimental data. The subscript $r$ stands for the reference state, which is the state of the inflow condition. The parameter $\nu$ is the exponent of the inverse power law for the gas particle interaction potential, and the tabulated values of $A_2(\nu)$ are available in the literature. A composite number defined by

$$N_\delta \equiv \frac{\Pi}{p} = \frac{\eta_r u_r/L}{p_r} \approx \frac{M^2}{Re} \approx \mathrm{Kn}M \tag{12}$$

measures the magnitude of the viscous stress relative to the hydrostatic pressure; hence, it indicates the degree of departure from equilibrium in bulk flow region. As $N_\delta$ becomes small, the Newtonian law and the Fourier law are recovered from the constitutive relations of (8) as follows:

$$\mathbf{\Pi} = \mathbf{\Pi}_0,\ \Delta = \Delta_0,\ \mathbf{Q} = \mathbf{Q}_0. \tag{13}$$

## 3 Analysis of constitutive equation in a one-dimensional problem

### 3.1 Compression and expansion flow

In the case of a one-dimensional problem that describes the compression and expansion of gas, the stress and heat flux components $(\Pi_{xx}, \Delta, Q_x)$ induced by the thermodynamic forces $u_x \equiv \partial u/\partial x$ and $T_x \equiv \partial T/\partial x$ can be given by

$$\begin{aligned}
\hat{\Pi}_{xx}q(c\hat{R}) &= \left(1 + f_b\hat{\Delta} + \hat{\Pi}_{xx}\right)\hat{\Pi}_{xx_0},\\
\hat{\Delta}q(c\hat{R}) &= \left[1 + 3\left(f_b\hat{\Delta} + \hat{\Pi}_{xx}\right)\right]\hat{\Delta}_0,\\
\hat{Q}_x q(c\hat{R}) &= \left(1 + f_b\hat{\Delta} + \hat{\Pi}_{xx}\right)\hat{Q}_{x_0},
\end{aligned} \tag{14}$$

where

$$\hat{R}^2 = \frac{3}{2}\hat{\Pi}_{xx}^2 + \frac{4}{5f_b}\hat{\Delta}^2 + \hat{Q}_x^2,\ \hat{\Delta}_0 = \frac{3}{4}f_b\hat{\Pi}_{xx_0}.$$

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

$$\hat{\Delta} = \frac{1}{8f_b}\left\{\left(9f_b^2 - 4\right)\hat{\Pi}_{xx} - 4 + \sqrt{\left(81f_b^4 + 72f_b^2 + 16\right)\hat{\Pi}_{xx}^2 + \left(32 - 24f_b^2\right)\hat{\Pi}_{xx} + 16}\right\}.$$

## 3.2 Velocity shear flow

In the case of the shear flow, the stresses ($\Pi_{xx}$, $\Pi_{xy}$, $\Delta$) induced by the thermodynamic forces of $v_x \equiv \partial v/\partial x$ can be given by

$$\begin{aligned}\hat{\Pi}_{xx} q(c\hat{R}) &= -\frac{2}{3}\hat{\Pi}_{xy}\hat{\Pi}_{xy_0},\\ \hat{\Pi}_{xy} q(c\hat{R}) &= \left(1 + f_b\hat{\Delta} + \hat{\Pi}_{xx}\right)\hat{\Pi}_{xy_0},\\ \hat{\Delta} q(c\hat{R}) &= 3 f_b\hat{\Pi}_{xy}\hat{\Pi}_{xy_0},\end{aligned} \tag{15}$$

and yield the following equation of one variable, $\hat{\Pi}_{xx}$, and an additional equation for $\hat{\Delta}$:

$$\hat{\Pi}_{xx} q^2(c\hat{R}) = -\frac{2}{3}\left[\left(1 - \frac{9}{2}f_b^2\right)\hat{\Pi}_{xx} + 1\right]\hat{\Pi}_{xy_0}^2,\; \hat{\Delta} = -\frac{9}{2}f_b\hat{\Pi}_{xx}, \tag{16}$$

where

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

which follows from the stress constraint

$$\hat{\Pi}_{xy} = \mathrm{sign}\left(\hat{\Pi}_{xy_0}\right)\left\{-\frac{3}{2}\left[\left(1 - \frac{9}{2}f_b^2\right)\hat{\Pi}_{xx} + 1\right]\hat{\Pi}_{xx}\right\}^{1/2}. \tag{17}$$

The constitutive equations for diatomic gases can be solved numerically by the method of iteration [7–9].

## 3.3 General properties of algebraic model constitutive equations

### *3.3.1 Degree of thermal nonequilibrium*

The general properties of the model constitutive equation are shown in Figs. 1 and 2. The relations in one-dimensional $u_x$-only and $v_x$-only problems relative to the Navier–Stokes–Fourier and other theories are depicted in Figs. 1 and 2, respectively. The heat flux is assumed to be zero for the sake of simplicity, but inclusion of the heat flux does not change the essence of the results. In these figures, note that the relations are expressed in terms of the composite number $N_\delta$, which is defined in (12). The reason this parameter, not the Knudsen number alone, can best represent the degree of thermal nonequilibrium in bulk flow region in macroscopic thermodynamic space is because the viscous force is a direct consequence of the nonequilibrium effect.

### *3.3.2 Nonlinearity and asymmetry*

From the Figs. 1 and 2, it also becomes obvious that the relations away from the origin—that is, thermal equilibrium—are generally nonlinear and asymmetric in the case of the compression and expansion flow, though these relations are in sharp contrast with those of the Navier–Stokes–Fourier theory. For comparison, the relation $\left(-3 + 2\hat{\Pi}_{xx0} + 3\sqrt{1 - 4\hat{\Pi}_{xx0}/3 + 4\hat{\Pi}_{xx0}^2}\right)\left(4\hat{\Pi}_{xx0}\right)^{-1}$, which was derived independently by Karlin [10] on the basis of a resummation technique, is also plotted. The ultimate origin of nonlinearity and asymmetry can be traced to the dissipation term $q(\kappa)$ and the kinematic term $[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)}$ in the constitutive equations. Moreover, even though the details are slightly different, the general trend of the stresses for monatomic and diatomic gases remains unchanged.

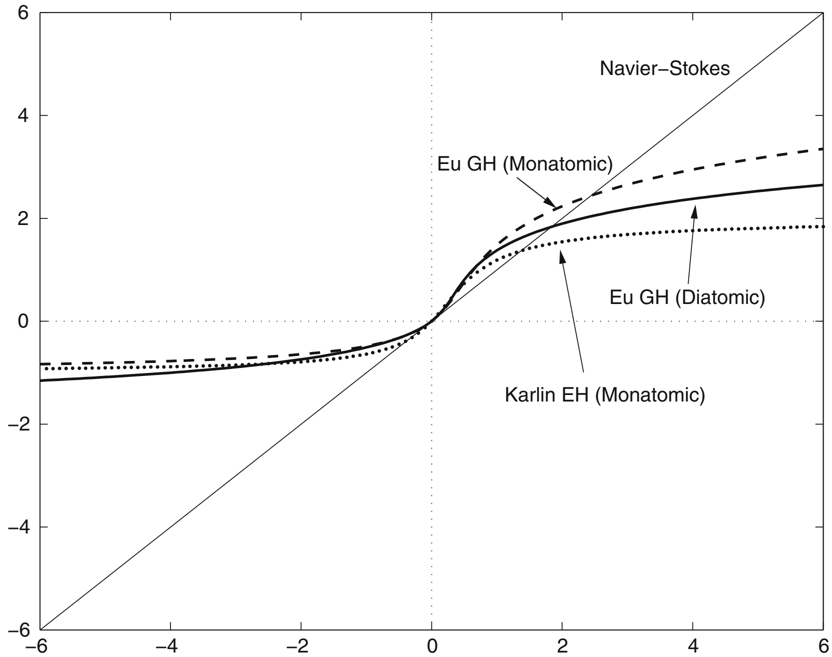


**Fig. 1** Nonlinear asymmetric constitutive relations relative to the Navier–Stokes relations in the $u_x$-only problem ($c = 1.0179$, $f_b = \sqrt{2}/3$). NS and GH represent the Navier–Stokes theory and the generalized hydrodynamic theory developed in the present work, respectively. The *horizontal* and *vertical axes* represent the Navier–Stokes relation $\hat{\Pi}_{xx_0}$ and the normal stress $\hat{\Pi}_{xx}$, respectively. The gas is expanding in the range $\hat{\Pi}_{xx_0} < 0$, whereas the gas is compressed in the range of $\hat{\Pi}_{xx_0} > 0$

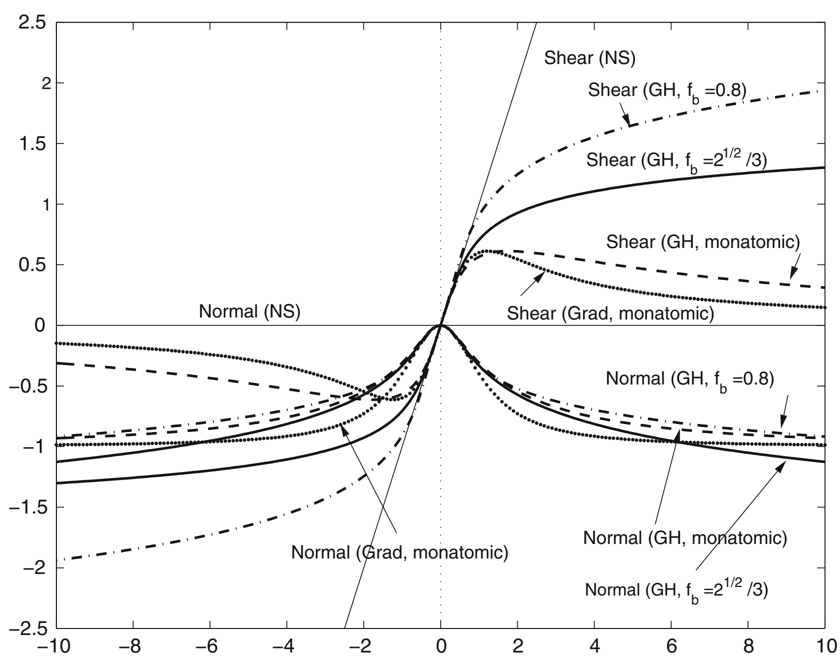


**Fig. 2** Nonlinear coupled constitutive relations relative to the Navier–Stokes relations in the $v_x$-only problem ($c = 1.0179$, $f_b = 0.0, \sqrt{2}/3, 0.8$). *NS* and *GH* represent the Navier–Stokes theory and the generalized hydrodynamic theory developed in the present work, respectively. The *horizontal axis* represents the Navier–Stokes relation $\hat{\Pi}_{xy_0}$. The *vertical axis* represents the normal ($\hat{\Pi}_{xx}$) and shear ($\hat{\Pi}_{xy}$) stresses

### *3.3.3 Coupling between stresses*

The one-dimensional velocity shear flow, which is shown in Fig. 2, reveals that the gases far from thermal equilibrium experience shear thinning behavior [6]; that is, the actual value of the shear stress is smaller than the value predicted by the classical Navier law. This behavior coincides with the finding reported in [11] where the rheological properties of a gas of Maxwell molecules are investigated by moment equations. Note also that the normal stresses, $\Pi_{xx}$, are induced by the shear velocity gradient, $\Pi_{xy_0}$, as the flow regime deviates from thermal equilibrium, resulting in the coupling of the stress components. Furthermore, as observed in the behavior of normal stresses near the origin, the coupling is not limited to a large deviation from thermal equilibrium. Another interesting finding is that the role of the dissipation term $q(\kappa)$ becomes less important in the shear flow situation because the constitutive relations of Eu and Grad are almost the same. Moreover, as demonstrated below in the section of the force-driven Poiseuille gas flow, this property can drastically decrease the mathematical complexity of solving rarefied and microscale gas flows. The Grad's relation can be obtained by assuming $q(\kappa) = 1$ in Eq. (15); that is, $\hat{\Pi}_{xx} = -\frac{2}{3}\left(\hat{\Pi}_{xx} + 1\right)\hat{\Pi}^2_{xy_0}$ or $\hat{\Pi}_{xx} = -2\hat{\Pi}^2_{xy_0}\Big/\left(3 + 2\hat{\Pi}^2_{xy_0}\right)$ for monatomic gas [12].

### *3.3.4 Bulk viscosity*

Bulk viscosity has been studied by Emanuel [13] for a better understanding of its role in hypersonic rarefied gas flows. In the present work, the derivation of its exact form is determined by starting with the Boltzmann–Curtiss kinetic equation for a diatomic molecule. Figure 2 clearly shows that it plays a non-negligible role in constitutive relations. For example, the asymptotic behaviors of shear and normal stresses differ from a monatomic case with a zero bulk viscosity. Interestingly, the stress constraint of (16) and (17) is an elliptic type for a small bulk viscosity but it changes into a hyperbolic type beyond a threshold value of $\sqrt{2}/3$.

## 4 Force-driven Poiseuille gas flow: subtle interplay of kinematic and dissipative terms

The treatment of the kinematic and dissipative terms that appear in the moment equations is an essential element of the theoretical investigation of gas flows that are far from thermal equilibrium. The treatment may seem straightforward at first glance but it turns out to be extremely difficult even in a simple problem such as a pure one-dimensional situation because of the complexity involved with the coupled and nonlinear mathematical structure of those terms. Such difficulty may be best demonstrated in a simple but very tricky problem known in the literature as the force-driven Poiseuille gas flow. This type of flow is defined as a stationary flow in a slab under the action of a constant external force parallel to the walls [5,14]. The classical Navier–Stokes–Fourier theory has been shown to be inadequate for predicting the correct flow physics even for a flow with very small Knudsen numbers. For example, the classical theory is unable to predict the nonuniform pressure distribution and the nonmonotonic temperature distribution across a channel. Efforts to solve this dilemma have led to the development of various high-order methods including the Burnett equations [15] and the regularized 13 moment equations [16]. In this work, the problem is revisited and abnormal properties in qualitative aspect are explained by focusing on the subtle interplay of kinematic and dissipative terms in the constitutive equations.

### 4.1 Derivation of governing equations

When the acceleration force, **a**, is added to the Boltzmann equation, the kinetic equation may be written as

$$\left[\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla + \mathbf{a}\cdot\nabla_{\mathbf{v}}\right] f(\mathbf{v},\mathbf{r},t) = C[f]. \tag{18}$$

Furthermore, when the same procedure of deriving the moment equations from the kinetic equation described in Sect. 2 is followed, the conservation laws and the constitutive equations can be derived as follows:

$$\rho\frac{D}{Dt}\begin{bmatrix}[1,\rho\mathbf{u},\rho E_t]^T/\rho\\ \boldsymbol{\Pi}/\rho\\ \mathbf{Q}/\rho\end{bmatrix} + \nabla\cdot\begin{bmatrix}[\mathbf{u},p\mathbf{I}+\boldsymbol{\Pi},(p\mathbf{I}+\boldsymbol{\Pi})\cdot\mathbf{u}+\mathbf{Q}]^T\\ \boldsymbol{\Psi}^{(\boldsymbol{\Pi})}\\ \boldsymbol{\Psi}^{(\mathbf{Q})}\end{bmatrix} = \begin{bmatrix}[0,\rho\mathbf{a},\rho\mathbf{a}\cdot\mathbf{u}]^T\\ \mathbf{Z}^{(\boldsymbol{\Pi})}+\boldsymbol{\Lambda}^{(\boldsymbol{\Pi})}\\ \mathbf{Z}^{(\mathbf{Q})}+\boldsymbol{\Lambda}^{(\mathbf{Q})}\end{bmatrix}. \tag{19}$$

The inclusion of the acceleration force does not change the dissipation terms; however, it does affect the momentum equation in the conservation laws and the kinematic terms in the constitutive equation of the heat flux. In the case of gravitational force, the effect of the acceleration force can be represented by the Rayleigh dimensionless number. When the closure relation of (4) and $q(\kappa) \cong 1$ are applied, the governing equation is reduced to

$$\nabla \cdot \begin{bmatrix} [\mathbf{u}, p\mathbf{I} + \mathbf{\Pi}, (p\mathbf{I} + \mathbf{\Pi}) \cdot \mathbf{u} + \mathbf{Q}]^T \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} [0, \rho\mathbf{a}, \rho\mathbf{a} \cdot \mathbf{u}]^T \\ \mathbf{Z}^{(\mathbf{\Pi})} - \frac{\mathbf{\Pi}}{\eta/p} \\ \mathbf{Z}^{(\mathbf{Q})} - \frac{\mathbf{Q}}{\lambda/pC_pT} \end{bmatrix}, \tag{20}$$

where the kinematic terms are defined as

$$\mathbf{Z}^{(\mathbf{\Pi})} = -2p\,[\nabla\mathbf{u}]^{(2)} - 2\,[\mathbf{\Pi} \cdot \nabla\mathbf{u}]^{(2)}, \mathbf{Z}^{(\mathbf{Q})} = \left(\mathbf{I} + \frac{\mathbf{\Pi}}{p}\right) \cdot \frac{\mathbf{Q}_0}{\lambda/pC_pT} + \mathbf{a} \cdot \mathbf{\Pi}.$$

Furthermore, through the one-dimensional assumption of $\partial/\partial x = 0$, the governing equation is reduced to the following system of ordinary differential equations comprised of the conservation laws and constitutive equations of the shear and normal stresses and the heat flux

$$\frac{\mathrm{d}}{\mathrm{d}y}\begin{bmatrix} \Pi_{xy} \\ p + \Pi_{yy} \\ \Pi_{xy}u + Q_y \end{bmatrix} = \begin{bmatrix} \rho a \\ 0 \\ \rho a u \end{bmatrix}, \frac{\mathrm{d}}{\mathrm{d}y}\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{3p\Pi_{xy_0}/\eta}{3+2\left(\Pi_{xy_0}/p\right)^2} - \frac{\Pi_{xy}}{\eta/p} \\ -\frac{2\Pi_{xy_0}^2/\eta}{3+2\left(\Pi_{xy_0}/p\right)^2} - \frac{\Pi_{yy}}{\eta/p} \\ \left(1 + \frac{\Pi_{yy}}{p}\right)\frac{Q_{y_0}}{\lambda/pC_pT} + a\Pi_{xy} - \frac{Q_y}{\lambda/pC_pT} \end{bmatrix}. \tag{21}$$

## 4.2 Analytical solution by new algebraic constitutive relations

The system of ordinary differential equations with dependent variables, $u$, $p$, $T$, $\Pi_{xy}$, $\Pi_{yy}$, and $Q_y$ is solved by first considering the $y$-momentum equation in the conservation laws. When it is integrated once with respect to $y$, the solution can be written as

$$p + \Pi_{yy} = p(y = 0).$$

Furthermore, when the constitutive equations of $\Pi_{yy}$ and $\Pi_{xy}$ are combined, the following equations can be derived ($0 \le y \le h/2$);

$$\frac{\Pi_{xy}}{\Pi_{xy_0}} = \frac{p(y = 0)}{p},$$

$$\frac{\Pi_{xy}}{p(y = 0)} = \sqrt{\frac{3}{2}\left(\frac{p}{p(y = 0)} - 1\right)}.$$

The $x$-momentum equation together with the equation of state, $p = \rho RT$, is then reduced as follows to an ordinary differential equation of the pressure, $p$:

$$\frac{p(y = 0)}{p}\mathrm{d}\left(\sqrt{\frac{3}{2}\left(\frac{p}{p(y = 0)} - 1\right)}\right) = \frac{a}{RT}\mathrm{d}y.$$

The integration of the differential equation with the introduction of the assumption $\int 1/T\mathrm{d}y \approx y/T(y = 0)$ defined at the centerline temperature in the system yields the following analytical solution for the pressure and shear stress distribution in the $y$-direction

$$\frac{p(y)}{p(y = 0)} = 1 + \tan^2\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{y}{h}\right), \frac{\Pi_{xy}(y)}{p(y = 0)} = \sqrt{\frac{3}{2}}\tan\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{y}{h}\right). \tag{22}$$

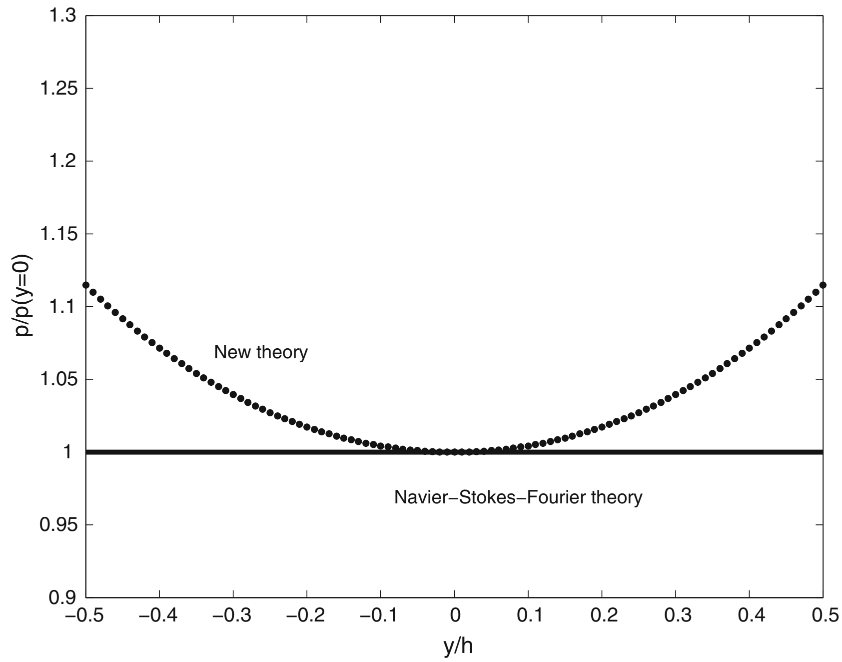


**Fig. 3** Nonuniform pressure distribution across the channel in a force-driven Poiseuille gas flows ($\varepsilon_h = 0.6, T(y = h/2) = 0.9T(y = 0)$). The *symbols* represent the value by the new theory, while the *solid line* represents the result by the Navier–Stokes–Fourier theory

When the constitutive equations of the stresses $\Pi_{yy}$ and $\Pi_{xy}$ and the stick boundary condition and the assumption of Maxwell molecules are applied, the velocity profile can then be determined as follows:

$$\frac{u(y)}{u(y=0)} = \operatorname{cosec}^2\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{0.5}{h}\right) - \cot^2\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{0.5}{h}\right)\sec^2\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{y}{h}\right). \tag{23}$$

Note that the stick boundary condition is used for mathematical simplicity instead of the slip boundary condition. It is well known that the slip boundary condition does not affect the qualitative aspect of pressure and temperature distributions in the central region of the force-driven Poiseuille gas flow [17]. Finally, when the constitutive equation of the heat flux $Q_y$ with the coupling term of viscous shear stress and acceleration force $a\Pi_{xy}$ is applied, a compact form of the analytical solution for the temperature distribution across the channel in the force-driven Poiseuille gas flow is obtained as follows:

$$\frac{T(y)}{T(y=0)} = \sec^e\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{y}{h}\right)\left\{1 - \left[1 - \frac{T(y=h/2)}{T(y=0)}\sec^{-e}\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{0.5}{h}\right)\right]\frac{F\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{y}{h}\right)}{F\left(\sqrt{\frac{2}{3}}\varepsilon_h\frac{0.5}{h}\right)}\right\}$$
$$F(y) = \frac{\sin^2(y)}{\cos^{4-e}(y)} + \frac{2}{2-e}\left(1 - \frac{1}{\cos^{2-e}(y)}\right), e = \frac{3(\gamma-1)}{2\gamma}, \varepsilon_h = \frac{ah}{RT(y=0)} \tag{24}$$

Here the parameter $\gamma$ denotes the specific heat ratio. Note that the dimensionless number $\varepsilon_h$ is the primary parameter in solutions (22) to (24). Thus the exact solutions are highly dependent on the exact value of $\varepsilon_h$. The validity of the new solutions is assessed from the pressure distribution and the temperature profile across the channel. In Fig. 3, the nonuniform pressure distribution in the $y$-direction is convincingly demonstrated by the new theory. Furthermore, as illustrated in Fig. 4, the existence of the central minimum of the temperature distribution near the centerline is predicted by the new theory. In summary, the origin of the nonuniform pressure distribution may be traced to the nonzero normal stress effect in the coupled nonlinear constitutive relation of stresses. In the case of the central minimum of the temperature distribution, the extra coupling term of viscous shear stress and acceleration force $a\Pi_{xy}$ appearing in the constitutive relation of the heat flux (21) is the main source of such abnormal behavior.

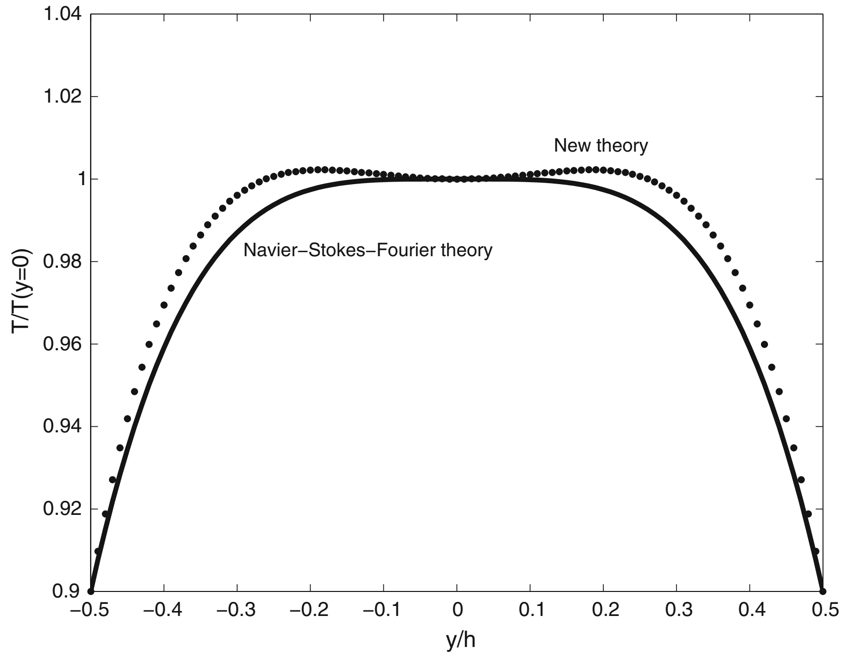


**Fig. 4** Nonmonotonic temperature distribution across the channel in a force-driven Poiseuille gas flow ($\varepsilon_h = 0.6, T(y = h/2) = 0.9T(y = 0)$). Notice the existence of the central minimum of the temperature distribution near the centerline. The *symbols* represent the value by the new theory, while the *solid line* represents the result by the Navier–Stokes–Fourier theory

## 5 Concluding remarks

A model constitutive relation derived from the moment method is studied for the purpose of understanding the fundamentals of gas flows in thermal nonequilibrium. For a one-dimensional problem, Eqs. (8) and (14) to (17) represent a complete set of constitutive equations for nonequilibrium gas flows. The constitutive relation of shear stress in the domain divided by the hydrodynamic pressure is generally nonlinear, asymmetric, and coupled between stresses and the shear rate. Interestingly, the nonlinearity is very similar to the generalized Newtonian fluids (cross-fluid) in which the shear stress depends on the normal and shear strain rates but not on the history of deformation. The difference is that the shear stress of gases depends on the pressure applied to it as well. This similarity may imply that the same numerical scheme developed for generalized Newtonian fluids, which is the finite element method in most cases, is suitable for microscale gas flows. In addition, the same method of deriving the nonuniform pressure distribution across the channel of a force-driven Poiseuille gas flow may be applicable for the analysis of a pressure-driven Poiseuille gas flow in a microchannel. These lines of investigation will be reported in a future work.

**Acknowledgments** This work was supported by a grant from Korea Research Foundation (grant no. KRF-2008-005-J01002) through Research Center for Aircraft Parts Technology.

## References

1. Truesdell, C., Noll, W.: The Non-Linear Field Theories of Mechanics. Springer, Heidelberg (2003)
2. Reese, J.M., Gallis, M.A., Lockerby, D.A.: New directions in fluid dynamics: non-equilibrium aerodynamic and microsystem flows. Phil. Trans. Roy. Soc. Lond. A **361**, 2967–2988 (2003)
3. Eu, B.C.: Kinetic Theory and Irreversible Thermodynamics. Wiley, New York (1992)
4. Eu, B.C.: Generalized Thermodynamics: The Thermodynamics of Irreversible Processes and Generalized Hydrodynamics. Kluwer Academic Publishers, Dordrecht (2002)
5. Tij, M., Santos, A.: Perturbation analysis of a stationary nonequilibrium flow generated by an external force. J. Stat. Phys. **76**, 1399–1414 (1994)
6. Huang, P.Y., Joseph, D.D.: Effects of shear thinning on migration of neutrally buoyant particles in pressure driven flow of Newtonian and viscoelastic fluids. J. Non-Newton. Fluid Mech. **90**(2–3), 159–185 (2000)

7. Myong, R.S.: Thermodynamically consistent hydrodynamic computational models for high-Knudsen-number gas flows. Phys. Fluids **11**(9), 2788–2802 (1999)
8. Myong, R.S.: A computational method for Eu's generalized hydrodynamic equations of rarefied and microscale gasdynamics. J. Comput. Phys. **168**, 47–72 (2001)
9. Myong, R.S.: A generalized hydrodynamic computational model for rarefied and microscale diatomic gas flows. J. Comput. Phys. **195**, 655–676 (2004)
10. Karlin, I.V., Dukek, G., Nonnenmacher, T.F.: Invariance principle for extension of hydrodynamics: nonlinear viscosity. Phys. Rev. E **55**(2), 1573–1576 (1997)
11. Garzo, V., Santos, A.: Kinetic Theory of Gases in Shear Flows: Nonlinear Transport. Kluwer Academic Publishers, Boston (2003)
12. Myong, R.S.: Gaseous slip model based on the Langmuir adsorption isotherm. Phys. Fluids **16**(1), 104–117 (2004)
13. Emanuel, G.: Effect of bulk viscosity on a hypersonic boundary layer. Phys. Fluids A **4**(3), 491–495 (1992)
14. Mansour, M.M., Baras, F., Garcia, A.L.: On the validity of hydrodynamics in plane Poiseuille flows. Physica A **240**, 255–267 (1997)
15. Xu, K.: Super-Burnett solutions for Poiseuille flow. Phys. Fluids **15**(7), 2077–2080 (2003)
16. Torrilhon, M., Struchtrup, H.: Boundary conditions for regularized 13-moment-equations for micro-channel flows. J. Comput. Phys. **227**, 1982–2011 (2008)
17. Ansumali, S.: Minimal kinetic modeling of hydrodynamics, Doctor of Technical Sciences Dissertation. Swiss Federal Institute of Technology Zurich (2004)