Revisit to Grad's Closure and Development of Physically Motivated Closure for Phenomenological High-Order Moment Model

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Abstract. The Grad's closure for the high-order moment equation is revisited and, by extending his theory, a physically motivated closure is developed for the one-dimensional velocity shear gas flow. The closure is based on the physical argument of the relative importance of various terms appearing in the moment equation. Also, the closure is derived such that the resulting theory may be inclusive of the well established linear theory (Navier- Stokes-Fourier) as limiting case near local thermal equilibrium.

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INTRODUCTION

The constitutive relations between shear stresses (heat fluxes) and the strain rate (the spatial temperature gradient) play a critical role in describing the motion of gases; in particular, for non-equilibrium regions found in rarefied and microscale flows. It is the only component appearing in the conservation laws in which the microscopic nature of gas molecules is taken into account. It can be derived either based on the purely phenomenological observation or from the viewpoint of the kinetic theory embodied in the Boltzmann transport equation of gas motion. In the latter case, there is non-trivial issue, known as the closure problem in the literature, which basically arises since the resulting constitutive equations are an open system of partial differential equations.

There exist various methods to develop the closure theory for the constitutive equations. The mathematically motivated closure developed in Grad's pioneering work [1] may be considered the most popular and it was applied to several important non-equilibrium gas flows of scientific interests by many researchers. A notable application is the shock wave structure arising in supersonic gas flows and Grad himself studied the problem extensively [2]. However, it was found that, with Grad's closure to the dissipation terms in the moment equations, there exists a critical Mach number for a given order of moments beyond which no continuous shock solution is possible. For this reason, it is generally accepted that there exists no single closure theory founded on a firm theoretical justification [3,4].

In this study, the Grad's closure is revisited and, by extending his idea, a physically motivated closure will be developed for the one-dimensional velocity shear gas flow. The closure is based on the rationale that, in natural science, the difference between theoretical truth and pure mathematical speculation is eventually decided by empirical evidence. In other words, the justification of the theoretical model is a posteriori and will be determined afterward by its ability to describe properties experimentally studied or computationally predicted by more accurate methods, for example, Monte Carlo or molecular dynamic simulation. Specifically, physical observations for *relative* importance of various terms appearing in the constitutive equations will be imposed on the closure. Also, the closure is derived such that the resulting theory may be inclusive of the well established linear theory (Navier-Stokes-Fourier) as limiting case near local thermal equilibrium.

GRAD'S CLOSURE

By applying the so-called Maxwell-Grad moment method, which was first introduced by Maxwell (the so-called equation of change) and later refined by Grad, to the Boltzmann kinetic equation of the distribution of monatomic gas particles $f(\mathbf{v},\mathbf{r},t)$, the following moment equations may be derived (equations (5.13), (5.14) in Grad's paper [1]):

$$\frac{\partial \mathbf{P}}{\partial t}+\nabla\cdot(\mathbf{uP})=-\nabla\cdot\boldsymbol{\psi}^{(P)}-\left[\mathbf{P}\cdot\nabla\mathbf{u}+(\nabla\mathbf{u})^T\cdot\mathbf{P}\right]+\boldsymbol{\Lambda}^{(P)}, \quad (1)$$

$$\frac{\partial \mathbf{S}}{\partial t}+\nabla\cdot(\mathbf{uS})=-\nabla\cdot\boldsymbol{\psi}^{(S)}-\left[\mathbf{S}\cdot\nabla\mathbf{u}+(\nabla\mathbf{u})^T\cdot\mathbf{S}\right]-\mathbf{S}\cdot\nabla\mathbf{u}+\frac{1}{\rho}\left[\mathbf{P}\nabla\cdot\mathbf{P}\right]^{(3)}+\boldsymbol{\Lambda}^{(S)}. \quad (2)$$

In this expression, ρ and $\mathbf{u}$ denote the density and the average velocity vector, respectively. The $\mathbf{P}$, $\mathbf{S}$, $\boldsymbol{\psi}^{(S)}$ are moments of second, third, fourth order statistically defined by the formulas

$$\mathbf{P}\equiv\langle m\mathbf{cc}f\rangle,\ \mathbf{S}(=\boldsymbol{\psi}^{(P)})\equiv\langle m\mathbf{ccc}f\rangle,\boldsymbol{\psi}^{(S)}\equiv\langle m\mathbf{cccc}f\rangle,$$

respectively, where $m,\mathbf{c}$ denote the molecular mass and the peculiar velocity of the molecule, respectively. An abbreviation is used for the integration over $\mathbf{v}$ space with angular brackets $\langle\cdots\rangle=\int d\mathbf{v}\cdots$. The stress tensor in the case of dilute monatomic gases can be further decomposed into two components; hydrostatic pressure and traceless part , $\mathbf{P}\equiv p\mathbf{I}+\boldsymbol{\Pi}$, where the statistical mechanical formulas for p and $\boldsymbol{\Pi}$ are, respectively,

$$p\equiv\left\langle\frac{1}{3}m\mathrm{Tr}(\mathbf{cc})f\right\rangle,\ \ \boldsymbol{\Pi}\equiv\left\langle m[\mathbf{cc}]^{(2)}f\right\rangle.$$

Here the symbol $[\ ]^{(2)}$ stands for a traceless symmetric part of the tensor. Another symbol $[\ ]^{(2)}$ is used for the equation (2):

$$\left[\mathbf{P}\nabla\cdot\mathbf{P}\right]^{(3)}=P_{ij}\frac{\partial P_{kr}}{\partial x_r}+P_{ik}\frac{\partial P_{jr}}{\partial x_r}+P_{jk}\frac{\partial P_{ir}}{\partial x_r},$$

The dissipation terms $\Lambda^{(P,S)}$, together with the high order terms $\boldsymbol{\psi}^{(P,S)}$, are related directly to the closure and are defined as

$$\boldsymbol{\Lambda}^{(P)}\equiv\langle m\mathbf{cc}C[f]\rangle,\boldsymbol{\Lambda}^{(S)}\equiv\langle m\mathbf{ccc}C[f]\rangle.$$

In addition, the constitutive equation of $\mathbf{P}$ can be expressed in terms of $\boldsymbol{\Pi}$ (equation (5.15) in Grad's paper [1]):

$$\frac{\partial \boldsymbol{\Pi}}{\partial t}+\nabla\cdot(\mathbf{u}\boldsymbol{\Pi})=-\nabla\cdot\boldsymbol{\psi}^{(\Pi)}-2\left[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}-2p\left[\nabla\mathbf{u}\right]^{(2)}+\boldsymbol{\Lambda}^{(\Pi)}, \quad (3)$$

where

$$\boldsymbol{\Lambda}^{(\Pi)}\equiv\left\langle m[\mathbf{cc}]^{(2)}C[f]\right\rangle,\boldsymbol{\psi}^{(\Pi)}\equiv\left\langle m[\mathbf{cc}]^{(2)}\mathbf{c}f\right\rangle=\boldsymbol{\psi}^{(P)}-\frac{1}{3}\mathbf{I}\langle m\mathrm{Tr}(\mathbf{ccc})f\rangle.$$

By using the following third order approximation (equation (5.8) in Grad's paper [1]) (heat flux $\mathbf{Q} = \left\langle mc^2 \mathbf{c} f / 2 \right\rangle$),

$$f = f^{(0)} \left[1 + \frac{1}{2} \hat{\mathbf{\Pi}} : \left[\hat{\mathbf{c}} \hat{\mathbf{c}} \right]^{(2)} - \hat{\mathbf{Q}} \cdot \hat{\mathbf{c}} \left(1 - \frac{1}{5} \hat{c}^2 \right) \right], \tag{4}$$

where $f^{(0)}$ denotes the local equilibrium Maxwell-Boltzmann distribution function and the hat symbol represents non-dimensional quantities, the higher order terms $\boldsymbol{\psi}^{(P,S)}$ may be reduced in terms of lower order moments: for example (equation (5.9) in Grad's paper [1]),

$$\boldsymbol{\psi}_{ijk}^{(P)} = \frac{2}{5} \left(Q_i \delta_{jk} + Q_j \delta_{ik} + Q_k \delta_{ij} \right). \tag{5}$$

With this closure, the constitutive equation of $\mathbf{\Pi}$ is reduced to

$$\frac{\partial \mathbf{\Pi}}{\partial t} + \nabla \cdot \left(\mathbf{u} \mathbf{\Pi} \right) = -\frac{2}{5} \left[\nabla \mathbf{Q} \right]^{(2)} - 2 \left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]^{(2)} - 2 p \left[\nabla \mathbf{u} \right]^{(2)} + \mathbf{\Lambda}^{(\Pi)}. \tag{6}$$

The Grad theory represented by the equations (4)-(6) may be considered the most extensively studied closure and was applied to important non-equilibrium gas flows such as the shock wave structure by many researchers. It has been, however, reported that it can suffer erroneous behavior for high Mach number shock wave structure. For example, when Grad's closure (4) is applied to the dissipation term $\Lambda^{(\Pi)} = \left\langle m \left[\mathbf{cc} \right]^{(2)} C[f] \right\rangle$ in the moment equation, it was found that there exists a critical Mach number beyond which no continuous shock solution is possible. Such breakdown may be related to the fact that the polynomial expansion (4) can not satisfy the non-negativity of the distribution function in rigorous way. Also, it can be noticed that the normalization factor (defined as the integral of the distribution function in the velocity space) in the case of the distribution functional form (4) may not exist in non-equilibrium since the integral consists of a cubic polynomial of $\mathbf{c}$ and thus becomes divergent [5]. In addition, it has been argued that the chemical potential of the gas, which is a measure of how much the free energy changes if a number particles are added (or removed) while keeping the temperature and the pressure constant, when the polynomial expansion (4) is used, is simply the same as the equilibrium chemical potential, which is unrealistic [4].

However, the main factor limiting widespread use of the Grad closure in gas flow problems of technical interests is its inherent difficulty in handling the boundary condition at the solid wall. This point can be best explained by examining the equation (6). Owing to the closure (5), the constitutive equation of the shear stress (6) now contains a term associated with $\nabla \mathbf{Q}$, which is the *spatial derivative of the heat flux*. Since the heat flux is dependent variable in the constitutive equations, just like the shear stress $\mathbf{\Pi}$, the constitutive equations are now partial differential equations, in stark contrast with algebraic equations of Navier-Stokes-Fourier theory. This in turn means that, in order to make the flow problem well-posed, integration constants (that is, information of dependent variables $\mathbf{\Pi}$ and $\mathbf{Q}$ at the solid wall) are necessary. Consequently the situation becomes drastically different from the classical Navier-Stokes-Fourier case, where variables $\mathbf{\Pi}$ and $\mathbf{Q}$ at the solid wall remain strictly to-be-determined quantities, not something to-be-prescribed.

PHYSICALLY MOTIVATED CLOSURE FOR THE VELOCITY SHEAR FLOW

The primary role of the constitutive equations is to provide information for the shear stress and the heat flux, which are fundamental variable appearing in the conservation laws [6-9]. Therefore, the requirement for any closure theory to be consistent is no implication of vanishing the shear stress and the heat flux in the theory. With this in mind, a physically motivated closure will be developed for the velocity shear flow. A method called the modified moment method developed by Eu [3] is adopted in the present study. This method starts with differentiating the statistical definition of variable in question and later combining with the Boltzmann equation, in contrast with taking first the velocity moments of the Boltzmann equation in the conventional Maxwell-Grad method. In this way, one can keep track on how various terms in constitutive equations are derived from the original Boltzmann equation. For the shear stress $\mathbf{P}$, it yields

$$\frac{\partial \mathbf{P}}{\partial t} + \nabla \cdot \left\langle \mathbf{u} m \mathbf{c}\mathbf{c} f \right\rangle = -\nabla \cdot \left\langle m \mathbf{c}\mathbf{c}\mathbf{c} f \right\rangle + \left\langle f \left(\frac{D}{Dt} + \mathbf{c} \cdot \nabla + \mathbf{a} \cdot \nabla_{\mathbf{v}} \right) m \mathbf{c}\mathbf{c} \right\rangle + \boldsymbol{\Lambda}^{(P)}, \tag{7}$$

where $\mathbf{a}$ represents the external force. When the second term on the right-hand side is expanded further, the equation (7) is reduced to (1). When the nonequilibrium part of the stress $\boldsymbol{\Pi}$ instead of the stress tensor $\mathbf{P}$ is considered, through subtracting the trace part of the tensor $\mathbf{P}$, the equation (7) is reduced to

$$\frac{\partial \boldsymbol{\Pi}}{\partial t} + \nabla \cdot \left(\mathbf{u} \boldsymbol{\Pi} \right) = -\nabla \cdot \boldsymbol{\psi}^{(\Pi)} - 2\left[\boldsymbol{\Pi} \cdot \nabla \mathbf{u} \right]^{(2)} - 2p\left[\nabla \mathbf{u} \right]^{(2)} + \boldsymbol{\Lambda}^{(\Pi)}, \tag{8}$$

which is exactly the same as the result by the Maxwell-Grad moment method. Similarly, the constitutive equation of the heat flux $\mathbf{Q}$ can be derived:

$$\frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \left(\mathbf{u} \mathbf{Q} \right) = -\nabla \cdot \boldsymbol{\psi}^{(Q)} - \boldsymbol{\psi}^{(P)} : \nabla \mathbf{u} - C_p \boldsymbol{\Pi} \cdot \nabla T - \mathbf{Q} \cdot \nabla \mathbf{u} - \left(\frac{D\mathbf{u}}{Dt} - \mathbf{a} \right) \cdot \boldsymbol{\Pi} - C_p p \nabla T + \boldsymbol{\Lambda}^{(Q)}, \tag{9}$$

where the C_p is the heat capacity per mass at constant pressure and

$$\boldsymbol{\Lambda}^{(Q)} \equiv \left\langle \frac{1}{2} m c^2 \mathbf{c} C[f] \right\rangle, \boldsymbol{\psi}^{(Q)} \equiv \left\langle \frac{1}{2} m c^2 \mathbf{c}\mathbf{c} f \right\rangle.$$

Up to now, no approximations are made in the process and therefore the constitutive equations (8) and (9) are a direct consequence of the Boltzmann equation. Since it is generally accepted that there exists no single closure theory founded on a firm theoretical justification, a physically motivated closure based on phenomenological observations for *relative* importance of various terms appearing in the constitutive equations will be developed. If we confine our interest to the steady-state and pure one-dimensional velocity shear flow, that is, all variables depending on the coordinate y only, the substantial derivative of shear stress and heat flux will vanish since the convective derivatives $\mathbf{u} \cdot \nabla$ are zero by definition ($v = \partial / \partial x = 0$). Also, the terms associated with $\boldsymbol{\psi}^{(\Pi),(P)}, \boldsymbol{\psi}^{(Q)}$ in (8) and (9), which are one order higher than the dependent variables $\boldsymbol{\Pi}$ and $\mathbf{Q}$, respectively, may be assumed small; that is,

$$\nabla \cdot \boldsymbol{\psi}^{(\Pi)} \approx 0, \nabla \cdot \boldsymbol{\psi}^{(Q)} + \boldsymbol{\psi}^{(P)} : \nabla \mathbf{u} \approx 0. \tag{10}$$

It is interesting to note that the new closure is based mainly on $\boldsymbol{\Pi}$ (or $\boldsymbol{\psi}^{(\Pi)}$) and $\mathbf{Q}$ (or $\boldsymbol{\psi}^{(Q)}$), while the Grad closure is based on $\mathbf{P}$ (or $\boldsymbol{\psi}^{(P)}$) and $\mathbf{S}$ (or $\boldsymbol{\psi}^{(S)}$). The relative importance of $\nabla \cdot \boldsymbol{\psi}^{(\Pi)}$ and $2\left[\boldsymbol{\Pi} \cdot \nabla \mathbf{u} \right]^{(2)}$ can be checked by comparing their original expressions in the velocity shear flow. For example, xy-component of these terms are $d\left\langle m c_x c_y^2 f \right\rangle / dy$ and $(-) du/dy \left\langle m c_y^2 f \right\rangle$, respectively, and, by combining with the third order distribution function (4), it can be shown that the former is smaller than the latter. Thus,

$$\left| \nabla \cdot \boldsymbol{\psi}^{(\Pi)} \right| < \left| \left[\boldsymbol{\Pi} \cdot \nabla \mathbf{u} \right]^{(2)} \right| < \left| p \left[\nabla \mathbf{u} \right]^{(2)} \right|. \tag{11}$$

In fact, the closure (10) is not unprecedented since a similar practice was used in the past when the (inviscid) Euler equation is derived from the (viscous) Navier-Stokes-Fourier equation. In such a case, the $\nabla \cdot \mathbf{\Pi}$ appearing in the conservation law of momentum, which is the divergence of shear stress tensor $\mathbf{\Pi}$, one order higher than the dependent variable $\mathbf{u}$, was assumed small.

The closure (10) is derived based on the physical argument that some terms appearing in the constitutive equations are small in comparison with other terms. The resulting equations now become the algebraic type, for example, in the case of shear stress, $\mathbf{\Lambda}^{(\Pi)} = 2\left[\mathbf{\Pi} \cdot \nabla \mathbf{u}\right]^{(2)} + 2p\left[\nabla \mathbf{u}\right]^{(2)}$ and consequently the theory is mathematically far simpler than the Grad theory. It will be shown that this constitutive model (called NCCR hereafter) based on the aforementioned approximations is suitable for fully analytical treatment due to its algebraic nature and is just enough to describe most of qualitative properties of the velocity shear gas flow observed by DSMC.

APPLICATION TO FORCE-DRIVEN COMPRESSIBLE POISEUILLE FLOW

The force-driven compressible Poiseuille flow is defined as a stationary flow in a channel under the action of a constant external force parallel to the walls. It is a simple, albeit very instructive, problem in the sense that it is purely one-dimensional but brings out the essence of the closure theory. The conservation laws in the velocity shear dominated Poiseuille flow can be written as

$$\frac{d}{dy}\left[\Pi_{xy}, p+\Pi_{yy}, \Pi_{yz}, \Pi_{xy}u + Q_y\right]^T = \left[\rho a, 0, 0, \rho a u\right]^T . \tag{12}$$

The constitutive equation of the shear stress $\mathbf{\Pi}$ derived by the new closure is written as

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\eta}\begin{bmatrix} (4/3)\left[\Pi_{xy}\right]_0\left[\Pi_{xy_0}\right]_0 \\ -(2/3)\left[\Pi_{xy}\right]_0\left[\Pi_{xy_0}\right]_0 \\ \left(p+\left[\Pi_{yy}\right]_0\right)\left[\Pi_{xy_0}\right]_0 \end{bmatrix} - \frac{p}{\eta}\begin{bmatrix} \left[\Pi_{xx}\right]_0 \\ \left[\Pi_{yy}\right]_0 \\ \left[\Pi_{xy}\right]_0 \end{bmatrix} F(p, T, \mathbf{\Pi}, \mathbf{Q}, \cdots), \tag{13}$$

Here the dissipation terms are approximated as shear stress and heat flux multiplied by a general function of conserved and non-conserved variables. Also, the constitutive equations are expressed in terms of non-conserved variables measured from its value at the center ($\left[A\right]_0 \equiv A - A(0)$ where $A(y=0)$). When the constitutive equations of Π_{xy} and Π_{yy} are combined, there exists a constraint on the shear and normal stresses, implying their inter-dependence,

$$\left(\frac{\left[\Pi_{xy}\right]_0}{p}\right)^2 = -\frac{3}{2}\left(\frac{\left[\Pi_{yy}\right]_0}{p} + 1\right)\frac{\left[\Pi_{yy}\right]_0}{p} . \tag{14}$$

A qualitative comparison with DSMC data on the stress constraint (14) for the purpose of validating the closure theory was conducted in the previous works. It was observed that the new theory is in qualitative agreement with the DSMC prediction [10].

Finally, an interesting observation can be found for the values of non-conserved variables at the center. The properties of conserved variables near the centerline must satisfy the continuous symmetric condition arising from the flow geometry in the present problem. In order that the conserved variables may be continuous, symmetric, and differentiable at the center, their first derivatives must vanish. This condition is equivalent to a physical requirement that all components of the thermodynamic driving forces vanish as well, since spatial gradient of all the conserved variables near the centerline are zero and the force field exerted on gas molecules is uniform in space. However, owing to the presence of $\nabla\mathbf{Q}$ term in the constitutive equation (6) in the case of Grad's closure, the shear stress at the center does not vanish even when all the first derivatives of conserved variables are zero (denoted by NCCR-B in Fig. 1 (b)), since their *second* derivatives may not be strictly zero. This in turn implies that the Grad's closure changes the mathematical structure at the center, since the original constitutive equation (3) or (8) does not possess the second derivatives. Non-zero stress for zero strain rate is very similar to the phenomenon observed in a special fluid known as Bingham (plastic) fluids in the literature [11]. A Bingham fluid is a visco-plastic material that behaves as a rigid body at low stresses but flows as a viscous fluid at high stress. The physical reason for this behavior is that the liquid contains particles (e.g. clay) or large molecules (e.g. polymers) with a weak solid structure and a certain amount of stress is required to break this structure. Since gases do not possess such structure, non-zero stress for zero strain rate seems to be numerical artifact rather than physical phenomenon.

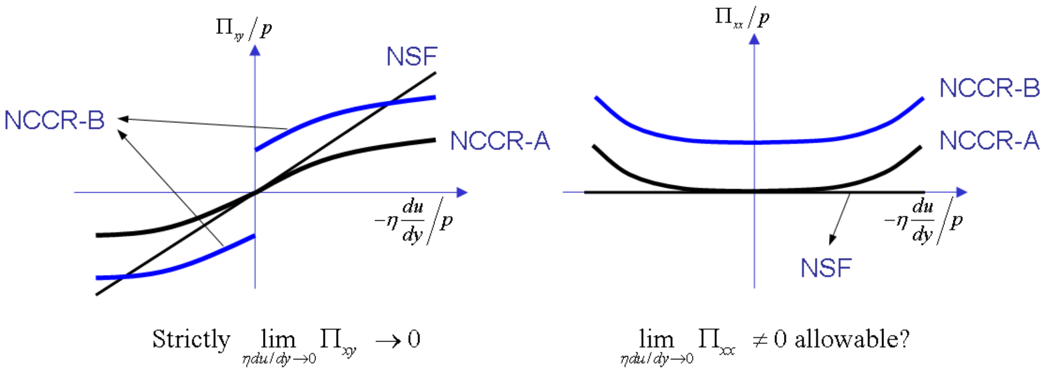

FIGURE 1. Examples of constitutive relation in the velocity shear flow. (a) shear stress (left). (b) normal stress (right).

CONCLUSIONS

In this study, the Grad's closure is revisited and, by extending his theory, a physically motivated closure is developed for the one-dimensional velocity shear gas flow. The closure is based on the physical argument of the relative importance of various terms appearing in the constitutive equations. An algebraic constitutive relation model is developed and, as a validation study, it is applied to the force-driven compressible Poiseuille gas flow.

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