The Subtle Interplay of Kinematics and Dissipation Terms in the Constitutive Equations of Rarefied and Microscale Gases

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Theoretical modeling for gas flows in thermal nonequilibrium

- Hydrodynamic theories in thermodynamic space:
  **Linear:** Navier-Stokes-Fourier (suitable for preliminary calculation; very efficient and powerful; question of applicability)
  **High order:** Chapman-Enskog method (Burnett etc.), Grad’s and Eu’s modified moment methods, (rational) extended irreversible thermodynamics, information entropy maximization method, resummation technique (Karlin) etc  
  => Achieving economy of thoughts and description (**constitutive relations** between microscopic and macroscopic physics specific to a substance); computational issues

- Molecular description in phase space: Boltzmann equation, DSMC, MD, etc
  Valid for whole flow regimes; non-trivial issue in computational efficiency
Modelling of nonequilibrium gas system (I)

Molecular (Deterministic)
Equation of Motion
(Molecular Dynamics)

Molecular (Probabilistic)
Liouville Equation
(Monte Carlo)

Molecular (Probabilistic)
(Generalized) Boltzmann Eq.
(Direct CFD, DSMC)

Molecular Chaos
Modelling of nonequilibrium gas system (II)

Molecular (Probabilistic) \[ f(t,r;v) \]

Phase Space \[ \left( \frac{\partial}{\partial t} + v \cdot \nabla \right)f(t,r;v) = C[f,f_2] \]

Boltzmann \[ \rho = \langle mf(t,r;v) \rangle \]
\[ \rho u = \langle mvf(t,r;v) \rangle \]
\[ \langle \cdots \rangle = \iiint \cdots dv_x dv_y dv_z \]

Continuum (Hydrodynamic) \[ \left( \rho, u, T, \Pi, Q, \cdots \right)(t,r) \]

Thermodynamic Space \[ \rho \frac{Du}{Dt} + \nabla \cdot \left( p I + \Pi \right) = 0 \]

Thermodynamics (Reduction of Information) \[ \beta = \frac{1}{k_B T} \]

Not far from LTE \[ \text{Navier-Stokes-Fourier} \]
Modelling of nonequilibrium gas system (III):

The moment method

\[ \rho = \langle mf(t, r; v) \rangle, \quad \rho u = \langle mvf(t, r; v) \rangle, \quad \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(t, r; \mathbf{v}) = C[f, f_2] \]

Diatonic: \( \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \frac{j}{I} \frac{\partial}{\partial \psi} \right) f(t, r, j, \psi; \mathbf{v}) = R[f, f_2] \)

\[ \rho = \langle mf(t, r; v) \rangle \]

\[ \frac{\partial}{\partial t} \rho = \frac{\partial}{\partial t} \langle mf(t, r; v) \rangle = \left\langle m \frac{\partial f}{\partial t} \right\rangle = \langle mC[f, f_2] \rangle - \langle mv \cdot \nabla f \rangle \]

\[ \frac{\partial \rho}{\partial t} + \langle mv \cdot \nabla f \rangle = \langle mC[f, f_2] \rangle = 0 \]

\[ \frac{\partial \rho}{\partial t} + \langle m \nabla \cdot (\mathbf{f} \mathbf{v}) \rangle - \langle mf \nabla \cdot (\mathbf{v}) \rangle = \frac{\partial \rho}{\partial t} + \langle m \nabla \cdot (\mathbf{f} \mathbf{v}) \rangle = 0 \]

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \langle m \mathbf{v} \rangle = 0 \]

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]
The moment method (I)

\[
\rho \frac{D}{Dt} \left( \frac{\langle h^{(k)} f \rangle}{\rho} \right) + \nabla \cdot \left( c \langle h^{(k)} f \rangle \right) = \left\langle f \left( \frac{D}{Dt} + c \cdot \nabla \right) h^{(k)} \right\rangle + \langle h^{(k)} C[f] \rangle
\]

\[
\rho \frac{D}{Dt} \begin{bmatrix} [I, \rho u, \rho E_t]^T / \rho \\ \Pi / \rho \\ Q / \rho \end{bmatrix} + \nabla \cdot \begin{bmatrix} \Psi^{(I)} \\ \Psi^{(Q)} \end{bmatrix} = \begin{bmatrix} Z^{(I)} + \Lambda^{(I)} \\ Z^{(Q)} + \Lambda^{(Q)} \end{bmatrix}
\]

Main parameter  \( \Pi / p \sim Kn \cdot M \)  (not Kn alone)

Weissenberg No. = \( \tau = \frac{l/a}{T} \sim Kn \cdot M \)

No approximations (no explicit  \( C[f, f_2] \) except for the dissipation term)
The moment method (II)

By differentiating $\Pi \equiv \left\langle m[cc]^2 \right\rangle f(t, r; v)$ with time and combining with the BTE

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

$$\rho \frac{D}{Dt} \left( \frac{\Pi}{\rho} \right) + \nabla \left( m[cc]^2 f \right) = \left\langle f \left( \frac{D}{Dt} + c \cdot \nabla \right) m[cc]^2 \right\rangle + \left\langle m[cc]^2 C[f] \right\rangle$$

Material + high-order flux = $-2 \left[ \Pi \cdot \nabla u \right]^2 - 2 p \left[ \nabla u \right]^2 - \frac{\Pi}{\eta / p} \left\{ fn(p, T, \Pi, Q, \ldots) \right\}$

derivative

Juggling four terms is difficult. By assuming the left-hand term small, we have

$$\frac{\Pi}{\eta / p} \left\{ fn(p, T, \Pi, Q, \ldots) \right\} = -2 \left[ \Pi \cdot \nabla u \right]^2 - 2 p \left[ \nabla u \right]^2$$ : Nonlinear algebraic equations

Constitutive equations for multi-axial (9-dimensional) state of stress and heat flux

Challenging problems in which the NSF theory shows a global failure: Shock structure and force-driven Poiseuille flows
Shock wave structure
The modified moment method: Shock structure

\[
\frac{\Pi}{\eta / p} q(\kappa) = -2[\Pi \cdot \nabla \mathbf{u}]^{(2)} - 2 p[\nabla \mathbf{u}]^{(2)}
\]

There exists a mathematical singularity when

\[
q(\kappa) = 1
\]

A remedy by B. C. Eu (1980) assumes

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

f in an exponential form; cumulant expansion for \( C[f, f_2] \)

and can remove the mathematical singularity.

This may indicate that the dissipation term \( q(\kappa) \) plays a critical role in the shock structure problem.

Cf. \( q(\kappa) = 1 + \frac{1}{6} \kappa^2 + O(\kappa^4) \)
Constitutive relations for shock structure

Stress

New implicit model
\[ \hat{\Pi}_{xx}q(\hat{\Pi}_{xx}) = \hat{\Pi}_{xx0} + \hat{\Pi}_{xx} \hat{\Pi}_{xx0} \]

Dissipation = Therm. Force + Kinematics

Nonlinearity

Asymmetry

Cf. Navier-Stokes' model
\[ \hat{\Pi}_{xx} = \hat{\Pi}_{xx0} = -2\eta [\nabla u]^2 \]

Cf. Karlin's explicit model (1997) based on the resummation technique
\[ \hat{\Pi}_{xx} = \frac{-3 + 2\hat{\Pi}_{xx0} + 3\sqrt{1 - 4\hat{\Pi}_{xx0}/3 + 4\hat{\Pi}^2}}{4\hat{\Pi}_{xx0}} \]
An example of shock structure solution: Monatomic and diatomic gases

Myong (JCP 2004) by a model constitutive equation
Constitutive relations in one-dimensional shear flow (I)

\[ 0 = -2[\Pi \cdot \nabla u]^{(2)} - 2p[\nabla u]^{(2)} - \frac{\Pi}{\eta/p} q(\kappa) \]

In dimensionless form

\[ 0 = \left[ \hat{\Pi} \cdot \nabla \hat{u} \right]^{(2)} + \hat{\Pi}_0 - \hat{\Pi}q(\hat{\kappa}) \quad \text{where} \quad \hat{\kappa}^2 = \hat{\Pi} : \hat{\Pi} + \hat{Q} \cdot \hat{Q} \]

Cf. \( 0 = \hat{\Pi}_0 - \hat{\Pi}q(\hat{\Pi}) \Rightarrow \hat{\Pi} = \sinh^{-1} \hat{\Pi}_0 : \text{Eyring - Ree empirical formula in rheology} \)

When only shear velocity \( dv/dx \) exists,

\[ \hat{\Pi}_{xx}q(\hat{\kappa}) = -\frac{2}{3} \hat{\Pi}_{xy} \hat{\Pi}_{xy0} \]

\[ \hat{\Pi}_{xy}q(\hat{\kappa}) = (1 + \hat{\Pi}_{xx}) \hat{\Pi}_{xy0} \quad \text{where} \quad \hat{\kappa}^2 = 3\hat{\Pi}_{xx} (\hat{\Pi}_{xx} - 1) \]

I) Symmetric, but \textbf{nonlinear and coupled} (\( \hat{\Pi}_{xx} \) induced by \( \hat{\Pi}_{xy0} \))

II) Yielding \textbf{a stress constraint} \( \hat{\Pi}_{xy}^2 = -1.5(1 + \hat{\Pi}_{xx})\hat{\Pi}_{xx} \)
Constitutive relations in one-dimensional shear flow (II)

Shear-thinning (viscoelastic) behavior!
(Cross fluid in rheology)
Force-driven Poiseuille 1-d gas flow: An analytical solution (I)

- Identified as one of three surprising hydrodynamic results discovered by DSMC (A.L. Garcia, 1997)
- Global failure of the NSF theory in predicting non-uniform pressure profile and the central minimum in the temperature profile -> Hydrodynamic theories in trouble
- Further studied numerically by K. Xu (2003; Super-Burnett) and Torrilhon & Struchtrup (2008; Regularized 13-moment equations)
By applying pure 1-d assumption, a closure relation, and \( q(k)=1 \)

\[
\begin{align*}
\rho \frac{D}{Dt} & \begin{bmatrix} 1, \rho u, \rho E_1 \end{bmatrix}^{\Gamma} / \rho \\
& \begin{bmatrix} \Pi / \rho \\
Q / \rho \\
\end{bmatrix} \\
+ \nabla \cdot \begin{bmatrix} u, p I + \Pi, (p I + \Pi) \cdot u + Q \end{bmatrix}^T \\
& = \begin{bmatrix} \rho a \\
Z^{(\Pi)} + \Lambda^{(\Pi)} \\
Z^{(Q)} + \Lambda^{(Q)} \\
\end{bmatrix}
\end{align*}
\]

\[
\begin{align*}
\frac{d}{dy} & \begin{bmatrix} p I + \Pi \\
(p I + \Pi) \cdot u + Q \\
0 \\
0 \\
\end{bmatrix} \\
& = \begin{bmatrix} \rho a \\
0 \\
Z^{(\Pi)} - \frac{\Pi}{\eta / p} \\
Z^{(Q)} - \frac{Q}{k / C_p p} \\
\end{bmatrix}
\end{align*}
\]
The analytical solutions are

\[
\frac{p(y)}{p_{y=0}} = 1 + \tan^2\left(\sqrt{\frac{2}{3}}\varepsilon_h \frac{y}{h}\right), \quad \frac{\Pi_{xy}(y)}{p_{y=0}} = \sqrt{\frac{3}{2}} \tan\left(\sqrt{\frac{2}{3}}\varepsilon_h \frac{y}{h}\right)
\]

\[
\frac{T(y)}{T_{y=0}} = \sec^c\left(\sqrt{\frac{2}{3}}\varepsilon_h \frac{y}{h}\right) \left\{ 1 - \left[ 1 - \frac{T_w}{T_{y=0}} \sec^c\left(\sqrt{\frac{2}{3}}\varepsilon_h \frac{0.5}{h}\right) \right] \frac{F\left(\sqrt{\frac{2}{3}}\varepsilon_h \frac{y}{h}\right)}{F\left(\sqrt{\frac{2}{3}}\varepsilon_h \frac{0.5}{h}\right)} \right\}
\]

where \( c = \frac{3(\gamma - 1)}{2\gamma} \), \( F(y) \equiv \frac{\sin^2(y)}{\cos^{4-c}(y)} + \frac{2}{2-c} \left( 1 - \frac{1}{\cos^{2-c}(y)} \right) \)

and \( \varepsilon_h \equiv \frac{ah}{RT_w} \) (Rayleigh no. in case of gravitational force).
Force-driven Poiseuille 1-d gas flow: An analytical solution (IV)

\[ \varepsilon_h = 0.8 \]

\[ T_w = 0.9 T_{y=0} \]
Summary

• Constitutive equations: Multi-axial, viscoelastic flow in stress/pressure domain (rheology)
• Subtle interplay of terms in the constitutive equations
  1) Nonlinearity (dissipation) and asymmetry (kinematics) in 1-d compression and expansion flow
  2) Stress coupling and constraint (kinematics) in 1-d shear flow; minor role of the dissipative term
• Solved the force-driven Poiseuille flow by a hydrodynamic model

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A missing component in the moment method

Molecular (Probabilistic) \[ \beta = \frac{1}{k_B T} \]

Phase Space
\[ f(t, \mathbf{r}; \mathbf{v}) \]

Boltzmann
\[ \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(t, \mathbf{r}; \mathbf{v}) = C[f, f_2] \]

\[ \rho = \langle m f(t, \mathbf{r}; \mathbf{v}) \rangle \]
\[ \rho \mathbf{u} = \langle m \mathbf{v} f(t, \mathbf{r}; \mathbf{v}) \rangle \]
\[ \langle \cdots \rangle = \iiint \cdots dv_x dv_y dv_z \]

Continuum (Hydrodynamic)
\[ \left( \rho, \mathbf{u}, T, \Pi, Q, \cdots \right)(t, \mathbf{r}) \]

Thermodynamic Space

Navier-Stokes-Fourier

Not far from LTE

Conservation Laws

Moment Equation

\[ \frac{\rho}{D t} + \nabla \cdot (p \mathbf{I} + \Pi) = 0 \]