Physics of polyatomic gases in non-equilibrium based on the second-order Boltzmann-type kinetic theory

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Outline

Part I

2nd-order Boltzmann-type kinetic theory: Boltzmann-based gas dynamics (BGD):

Part II

2nd-order constitutive laws for polyatomic gases

Physics of polyatomic gases in non-equilibrium via

- Topological representation of constitutive laws

- Multi-dimensional flow fields obtained by CFD based on discontinuous Galerkin method
2nd-order Boltzmann-type kinetic theory


PoF 2014, PoF 2016: Balanced closure & validation via MD

PoF 2018: Polyatomic gases (shock-vortex interaction)

Basic information can be found in the Youtube of an Indian GIAN (Global Initiative Academic Networks) Lecture (2017; IIT Kanpur; 15 Lectures)

Rarefied & Microscale Gases and Viscoelastic Fluids: A Unified Framework

https://www.youtube.com/ and search “Rarefied & Microscale Gases”

Other independent NCCR works: Multi-species extension by Ahn & Kim (SNU, Korea, JCP09)

Implicit-FVM implementation by Jiang & Zhao (Zhejiang Univ., China, 2017)

Cf. NCCR: Nonlinear Coupled Constitutive Relation
## Closure-last moment method

\[ \rho u = \iiint m v f(t, r, v) dv_x dv_y dv_z \]

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**Breakdown of moment method:** 1) when the statistical average is meaningless due to too few particles; 2) when thermodynamics is not definable.

**Closure-first approach:** Grad’s 13 moment method (1949) based on polynomial expansion

- Levermore method (1996) based on Gaussian (exponential) expansion

**Closure-last approach:** Eu’s generalized hydrodynamics (1980) based on

- Eu’s closure & equation of transfer
- NCCR (2014) based on balanced closure & equation of transfer
Boltzmann transport equation (BTE)

- A first-order **partial differential** equation with an **integral** collision term

\[
\left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(t, \mathbf{r}, \mathbf{v}) = \frac{1}{Kn} C[f, f_2]
\]

**Movement** Collision (or Interaction)

**Kinematic** Dissipation

C[f, f_2] \sim \int |\mathbf{v} - \mathbf{v}_2| (f^* f_2^* - f_2 f_2) d\mathbf{v}_2

\[= \text{Gain (scattered into)} - \text{Loss (scattered out)} = \left( \frac{\delta f}{\delta t} \right)^+ - \left( \frac{\delta f}{\delta t} \right)^-\]

- **Maxwell’s equation of transfer** for molecular expression \(h^{(n)}\)

\[
\frac{\partial}{\partial t} \left\langle h^{(n)} f \right\rangle + \nabla \cdot \left( \mathbf{u} \left\langle h^{(n)} f \right\rangle + \left( \mathbf{c} h^{(n)} f \right) \right) - \left\langle f \frac{d}{dt} h^{(n)} \right\rangle - \left\langle f \mathbf{c} \cdot \nabla h^{(n)} \right\rangle = \left\langle h^{(n)} C[f, f_2] \right\rangle
\]
Complexity out of simplicity: conservation laws

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

where \( \langle \cdots \rangle = \iiint \cdots dv_x dv_y dv_z \)

Differentiating the statistical definition \( \rho \mathbf{u} = \langle m \mathbf{v} f(t, \mathbf{r}, \mathbf{v}) \rangle \) with time and then combining with BTE (\( t, \mathbf{r}, \mathbf{v} \) are independent and \( \mathbf{v} = \mathbf{u} + \mathbf{c} \))

\[ \frac{\partial}{\partial t} \langle m \mathbf{v} f \rangle = \left\langle m \mathbf{v} \frac{\partial f}{\partial t} \right\rangle = -\left\langle m (\mathbf{v} \cdot \nabla f) \mathbf{v} \right\rangle + \left\langle m \mathbf{v} C[f, f_2] \right\rangle \]

Here \(-\left\langle m (\mathbf{v} \cdot \nabla f) \mathbf{v} \right\rangle = -\nabla \cdot \left\langle m \mathbf{v} \mathbf{v} f \right\rangle = -\nabla \cdot \left\{ \rho \mathbf{u} \mathbf{u} + \left\langle m \mathbf{c} \mathbf{c} f \right\rangle \right\} \)

After the decomposition of the stress into pressure and viscous shear stress \( \Pi \)

\[ \mathbf{P} \equiv \left\langle m \mathbf{c} \mathbf{c} f \right\rangle = p \mathbf{I} + \Pi \]

where \( p \equiv \left\langle m \text{Tr}(\mathbf{c} \mathbf{c}) f / 3 \right\rangle \), \( \Pi \equiv \left\langle m [\mathbf{c} \mathbf{c}]^{(2)} f \right\rangle \),

and using the collisional invariance of the momentum, \( \left\langle m \mathbf{v} C[f, f_2] \right\rangle = 0 \),

we have

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

Exact consequence of the original BTE!
Further complexity: constitutive equations

For arbitrary molecular expressions of general moment (viscous shear stress $\Pi$ and heat flux $Q$)

$$
\rho \frac{D}{Dt} \left[ \Pi \left( \equiv \left\langle m [cc]^{(2)} f \right\rangle / \rho \right) \right] + \nabla \cdot \left[ \left\langle mccf \right\rangle - \left\langle mTr(ccc) f \right\rangle I / 3 \right] + \left[ \left\langle mccf \right\rangle : \nabla u \right] + 2 \left[ \Pi \cdot \nabla u \right]^{(2)} + 2p \left[ \nabla u \right]^{(2)} = \left[ \left\langle m[cc]^{(2)} C[f, f_2] \right\rangle \right]
$$

No approximation so far: exact consequence of the original BTE via Maxwell's equation of transfer
Balanced closure: constitutive equations

Conceptual inconsistency of Eu’s closure (1992)

\[
\langle m_{cccf} \rangle - \langle m\text{Tr}(ccc)f \rangle \mathbf{I} / 3 = 0 \implies \text{Vanishing heat flux}
\]

\[
\langle m_{cccf} \rangle = 0 \implies \text{Cannot be zero in general}
\]

New balanced closure with closure-last approach (2014)

2nd-order for kinematic LH = 2nd-order for collision RH

\[
\begin{align*}
\rho \frac{D}{Dt} \left[ \Pi \left( \equiv \left\langle m [cc]^{(2)} f \right\rangle / \rho \right) \right] & + \nabla \cdot \left[ \left\langle m_{cccf} \right\rangle - \left\langle m\text{Tr}(ccc)f \right\rangle \mathbf{I} / 3 \right] + 0 \\
+ \left[ 2 \left[ \Pi \cdot \nabla u \right]^{(2)} \right] & + \left[ 2p \left[ \nabla u \right]^{(2)} \right] = \left[ \left\langle m_{cc} \right\rangle^{(2)} C[f, f_2] \right] \\
\frac{Du}{Dt} \cdot \Pi + Q \cdot \nabla u + \Pi \cdot C_p \nabla T & + \left[ p C_p \nabla T \right] = \left[ \left( mc^2 / 2 - mC_p T \right)C[f, f_2] \right]
\end{align*}
\]
Conservation laws + 2nd-order constitutive relations

**Conservation laws (exact consequence of BTE)**

\[
\rho \frac{D}{Dt} \begin{bmatrix}
\frac{1}{\rho} \\
\mathbf{u} \\
E_t
\end{bmatrix} + \nabla \cdot \begin{bmatrix}
-u \\
pI \\
p\mathbf{u}
\end{bmatrix} + \nabla \cdot \begin{bmatrix}
0 \\
\Pi \\
\Pi \cdot \mathbf{u} + \mathbf{Q}
\end{bmatrix} = 0
\]

In conjunction with the 2nd-order constitutive relations (CR)

\[
\rho \frac{D(\Pi / \rho)}{Dt} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \Pi q_{2nd}(\kappa_1),
\]

**Navier 1st law**

\[
\rho \frac{D(\mathbf{Q} / \rho)}{Dt} + \frac{Du}{Dt} \cdot \Pi + \mathbf{Q} \cdot \nabla \mathbf{u} + \Pi \cdot C_p \nabla T + C_p p \nabla T = -\frac{pC_p}{k_{NS}} \mathbf{Q} q_{2nd}(\kappa_1),
\]

**Fourier 1st law**

Non-hyperbolic

Implicit

\[q_{2nd}(\kappa_1) \equiv \frac{\sinh \kappa_1}{\kappa_1}, \quad \kappa_1 \equiv \frac{T^{1/4}}{p} \left( \frac{\Pi: \Pi}{\mu_{NS}} + \frac{\mathbf{Q} \cdot \mathbf{Q}}{k_{NS}} / T \right)^{1/2}\]
2nd-order theory in elementary flows

- Critical role of $q_{2nd}(\kappa_1)$ term in compression case
- Negligible role of $q_{2nd}(\kappa_1)$ term in expansion & velocity shear
  (simple shear thinning – decreasing viscosity)
A model for 1-D compression & expansion

\[ \rho \frac{D(\Pi / \rho)}{Dt} + 2[\Pi \cdot \nabla u]^{(2)} + 2p[\nabla u]^{(2)} = -\frac{p}{\mu_{NS}} \Pi \left( \frac{\sinh \kappa_1}{\kappa_1} \right), \quad \kappa_1 \equiv \frac{T^{1/4}}{p} \left( \frac{\Pi : \Pi / \mu_{NS}}{k_{NS}} + \frac{Q \cdot \hat{Q}}{T} \right)^{1/2} \]

No heat flux

\[ \rho \frac{D(\Pi / \rho)}{Dt} (\mu_{NS}) + [\Pi \cdot (-2\mu_{NS}) \nabla u]^{(2)} + p(-2\mu_{NS})[\nabla u]^{(2)} = p\Pi \left( \frac{\sinh \kappa_1}{\kappa_1} \right), \quad \kappa_1 \equiv \frac{T^{1/4}}{p} \left( \frac{\Pi : \Pi / \mu_{NS}}{k_{NS}} \right)^{1/2} \]

One-dimension

\[ \Pi_{NS} \equiv -2\mu_{NS} [\nabla u]^{(2)} \]

\[ \hat{t} \equiv \frac{t}{\mu_{NS} / p}, \quad \hat{\Pi} \equiv \frac{\Pi}{p}, \quad \Pi_{NS} \equiv -\frac{4}{3} \mu_{NS} \frac{\partial u}{\partial x} \]

\[ \frac{D\hat{\Pi}}{Dt} - \hat{\Pi}_{NS}\hat{\Pi}_{NS} - \hat{\Pi}_{NS} = -\hat{\Pi} q(|\hat{\Pi}|), \quad \text{where} \quad q(|\hat{\Pi}|) \equiv \sinh |\hat{\Pi}| / |\hat{\Pi}| \]

\[ t_{\text{stress}} (10^{-8} \text{ sec}) \ll t_{\text{flow}} \]

Or steady-state

\[ \hat{\Pi}_{NS} + \hat{\Pi}_{NS} = \hat{\Pi} q(|\hat{\Pi}|) \]

2nd-order 1st-order 1st-order x 2nd-order

Kinematic motion Collision
2nd-order constitutive laws in compression/expansion

1-D compression and expansion

\[ \Pi / p \]

Viscous stress / pressure

\[ \frac{\Pi}{p} \]

Grad non-classical model (1952)

\[
q = 1 \text{ by assuming Maxwellian molecule}
\]

\[
\dot{\Pi}_{NS} + \dot{\Pi}_{NS} = \dot{\Pi} \cdot 1
\]

Singularity

Navier classical model (1822)

\[
q = \frac{\sinh(\Pi/p)}{\Pi/p}
\]

Myong non-classical model (1999, 2014)

\[
\dot{\Pi}_{NS} + \dot{\Pi}_{NS} = \dot{\Pi}q(\Pi)
\]

\[ q(x) \]

\[ q(0) = 1 \]

\[ x \]

Velocity gradient / pressure

\[ \Pi_{NS} / p \]

Expansion

Compression

Normal (linear viscosity)

0 + \( \dot{\Pi}_{NS} = \dot{\Pi} \cdot 1 \)
1-D shock result: inverse shock thickness

New 2nd-order & 2nd-order: **Best**

Navier 1st-order & 1st-order: **Reference**

Grad 2nd-order & 1st-order: **Singularity**

\[ 0 + \hat{\Pi}_{NS} = \hat{\Pi}_q(\hat{\Pi}) \]

Quasi-linear 1st-order & 2nd-order: **Worse** than Navier

**Importance of balanced closure**

Shock density thickness of argon gas

Shock temperature-density distance

2\textsuperscript{nd}-order constitutive laws in velocity shear

\[
\rho \frac{D(\Pi / \rho)}{Dt} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \Pi q_{2nd}(\kappa_1),
\]

\[
\rho \frac{D(\mathbf{Q} / \rho)}{Dt} + \frac{Du}{Dt} \cdot \Pi + \mathbf{Q} \cdot \nabla \mathbf{u} + \Pi \cdot C_p \nabla T + C_p p \nabla T = -\frac{pC_p}{k_{NS}} \mathbf{Q} q_{2nd}(\kappa_1)
\]

1-D velocity shear \hspace{1cm} \text{No heat flux}

\[
\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla = 0
\]

\[
\frac{1}{\mu_{NS}}\begin{bmatrix}
2\Pi_{xy} \Pi_{xy/NS} / 3 \\
-\Pi_{yy} \Pi_{xy/NS}
\end{bmatrix}
- \frac{1}{\mu_{NS}} \begin{bmatrix}
0 \\
p \Pi_{xy/NS}
\end{bmatrix}
= -\frac{p}{\mu_{NS}} \begin{bmatrix}
\Pi_{yy} \\
\Pi_{xy}
\end{bmatrix} q_{2nd}(\kappa_1)
\]

\[
\hat{\Pi}^2_{xy} = -\frac{3}{2} \left(1 + \hat{\Pi}_{yy} \right) \hat{\Pi}_{yy}
\]

Kinematic stress constraint due to 2\textsuperscript{nd}-order coupling!

No such thing in 1\textsuperscript{st}-order Navier law!

MD: Molecular Dynamics(2014)

MD
DSMC
NCCR
NSF

Rod Climbing Effect

Newtonian
Visco-elastic

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Talk 13/27
R. S. Myong, Gyeongsang National University, South Korea
Multi-dimensional CFD based on DG

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Convergence property

Super-parallel performance (via the rate of cost reduction) (C&F, 2017)
Two-dimensional shock structure around cylinder

Computed Mach contours over cylinder (Mach 5.48, Kn=0.2)

NCCR: Nonlinear Coupled Constitutive Relation

Monatomic, diatomic, and (linear) polyatomic gases

- Once the Stokes assumption is abandoned, an additional constitutive law of the excess normal stress $\Delta$ related to the bulk viscosity will appear:
  \[ \Delta = \mu_b (\Delta \cdot \mathbf{u}). \]
- The inner structure of strong shock waves (Emanuel and Argrow 1994)
- Dilatational waves in transition in hypersonic boundary layers (Zhu et al. 2016)
Monatomic, diatomic, and (linear) polyatomic gases

- Once the Stokes assumption is abandoned, an additional constitutive law of the excess normal stress $\Delta$ related to the bulk viscosity will appear

$$\Delta = \mu_b (\Delta \cdot \mathbf{u}).$$

- The inner structure of strong shock waves (Emanuel and Argrow 1994)
- Dilatational waves in transition in hypersonic boundary layers (Zhu et al. 2016)
Boltzmann-Curtiss equation for polyatomic gases

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

\[\rho \mathbf{u} \equiv \langle m \mathbf{v} f (\mathbf{v}, \mathbf{r}, j, \psi, t) \rangle\]

- \( I \) = moment of inertia
- \( j \) = angular momentum
- \( \psi \) = azimuthal angle

\[\rho \equiv \langle mf (\mathbf{v}, \mathbf{r}, j, \psi, t) \rangle\]

\[\rho E \equiv \left\langle \left( \frac{1}{2} mc^2 + H_{rot} \right) f (\mathbf{v}, \mathbf{r}, j, \psi, t) \right\rangle\]

\[\langle \ldots \rangle \equiv \int \int \int ... d\nu_x d\nu_y d\nu_z j dj d\psi d\Omega\]

\[\rho \frac{d}{dt} \begin{bmatrix} 1/ \rho \\ \mathbf{u} \\ E_t \end{bmatrix} + \nabla \cdot \begin{bmatrix} -\mathbf{u} \\ p \mathbf{I} \\ pu \end{bmatrix} + \nabla \cdot \begin{bmatrix} 0 \\ \Pi + \Delta \mathbf{I} \\ (\Pi + \Delta \mathbf{I}) \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.
\]

- \( \Pi \) : normal stress tensor = \(-2 \mu_{NS} [\nabla \mathbf{u}]^{(2)}\)
- \( \Delta \) : excess normal stress = \(-\mu_b \nabla \cdot \mathbf{u}\)
- \( Q \) : heat flux vector = \(-k \nabla T\)

\[\Delta = \left\langle m \text{Tr} (\mathbf{c} \mathbf{c}) f / 3 - m \text{Tr} (\mathbf{c} \mathbf{c}) f^{(0)} / 3 \right\rangle, \quad p = \left\langle m \text{Tr} (\mathbf{c} \mathbf{c}) f^{(0)} / 3 \right\rangle\]
2\textsuperscript{nd}-order constitutive relations for polyatomic gases

\[ \Pi = \langle h^{(1)} f \rangle \quad h^{(1)} = m [cc]^{(2)} \]
\[ \Delta = \langle h^{(2)} f \rangle \quad h^{(2)} = mc^2 / 3 - p / n \]
\[ Q = \langle h^{(3)} f \rangle \quad h^{(3)} = \left[ mc^2 / 3 + H_{rot} - m\hat{h} \right] c \]

2\textsuperscript{nd}-order

\[ [\hat{\Pi} \cdot \nabla \hat{u}]^{(2)} + (f_b \hat{\Delta} + 1) \hat{\Pi}_{NF} = \hat{\Pi} q_{2nd} (c\hat{R}) \]
\[ \frac{3}{2} f_b \left( \hat{\Pi} + f_b \hat{\Delta} I \right) : \nabla \hat{u} + \hat{\Delta}_{NF} = \hat{\Delta} q_{2nd} (c\hat{R}) \]
\[ \hat{\Pi} \cdot \hat{Q}_{NS} + (f_b \hat{\Delta} + 1) \hat{Q}_{NF} = \hat{Q} q_{2nd} (c\hat{R}) \]

1\textsuperscript{st}-order

Linearization

\[ \hat{\Pi}_{NS} = -2\mu [\nabla u]^{(2)} \]
\[ \hat{\Delta}_{NS} = -\mu_b \nabla \cdot u \]
\[ \hat{Q}_{NS} = -k \nabla T \]

Topological representation of constitutive relations is possible!
Topology of 2nd-order CR (compression/expansion)

1st-order

2nd-order

Viscous shear stress

Argon $\mu_{\text{bulk}}=0$

$N_2$ $\mu_{\text{bulk}}=\mu_{\text{shear}}$

$CO_2$ $\mu_{\text{bulk}}=2,000\mu_{\text{shear}}$
Topography of 2nd-order CR (compression/expansion)

First-order

Argon $\mu_{\text{bulk}} = 0$

$N_2$ $\mu_{\text{bulk}} = \mu_{\text{shear}}$

$CO_2$ $\mu_{\text{bulk}} = 2,000 \mu_{\text{shear}}$

Second-order

Heat flux

$\dot{Q}$
Trajectory of shock structure in topology of CR

Mach number = 5.0

$f_b=0.0$

$f_b=0.8$
Inverse density thickness of shock wave (nitrogen)

Symbols-

- experiment

- NSF (fb=0)
- NF (fb=0.8)
- NCCR (fb=0.8)

Bulk viscosity effect
2nd-order effect
Multi-dimensional case: shock-vortex interaction

\[
\text{Enstrophy}(t) = \int_{\partial A} \left( \Omega_z^2(x, y, t) \right) dx dy,
\]

\[
\text{Vorticity} \; \Omega_z = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}
\]
Multi-dimensional case: shock-vortex interaction

Shock Mach = 2.0  
Vortex Mach = 0.8  
Knudsen = 0.001

Argon  
$f_b = 0$  
$\gamma = 1.667$

Nitrogen  
$f_b = 0.75$  
$\gamma = 1.4$

Methane  
$f_b = 1.33$  
$\gamma = 1.289$
Multi-dimensional case: shock-vortex interaction

Macro SVI

Micro SVI

(a) Argon gas, $f_b = 0.0$
(b) Nitrogen gas, $f_b = 0.8$
(c) Methane gas, $f_b = 1.33$

Effects of diatomic and polyatomic gases on macro SVI with $M_s = 2.0, M_v = 0.8, r_i = 1000\lambda$ (top) and micro SVI with $M_s = 2.0, M_v = 0.8, r_i = 10\lambda$ (bottom): sound pressure at $t = 1000\text{ ns}$.
Dusty gas flows in Lunar landing

Dust-gas Interaction

Plume-Surface Simulation in Rarefied Condition

Erosion Modeling

Dust-gas Interaction

NCCR

DSMC

nd [m⁻³]

2.00E+23
6.32E+22
2.00E+22
6.32E+21
2.00E+21
6.32E+20
2.00E+20

Δ [m]