Modeling of Gaseous Expansion in Free Jet and Microchannel Flows Using the Modified Moment Method

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Talk outline

- Research goals
- Derivation of hydrodynamic equations from the Boltzmann equation:

  the moment method
- Gaseous expansion in free jet
- Molecular interaction model for gas particle and surface atoms
- Gaseous expansion in micro-channel
- Summary

Research goals

- A fundamental question:

  Can the moment method based on the reduction of information be capable of describing high non-equilibrium gas flows (rarefied and microscsale)?

- Research goals:

  Answering fundamental questions and validation study

  Deriving governing equation and boundary conditions

  -> the basic building block for an **efficient** CFD code

  Providing physical insight and economy of thoughts

- Practical issues**:**

  How to solve the moment equations?

Previous works

- Linear theory: Navier-Stokes

  Suitable for preliminary calculation, very efficient and powerful (modern CFD codes), question of applicability

- Molecular description in phase space: Boltzmann equation, DSMC, MD, etc

  Valid for whole flow regimes, non-trivial issue in computational efficiency

- High order hydrodynamic theories in thermodynamic space:

  Chapman-Enskog method (Burnett, super-Burnett, BGK-Burnnet), Grad's moment method, (rational) extended irreversible thermodynamics, information entropy maximization method…

  Achieving economy of thoughts and description, problem in non-physical solutions and defining the boundary quantities

Strategy

- **Capability**: recover the Navier-Stokes model and extend to the transition regimes [Kn and Kn*M~O(1)]

- **Constraints** on the new model: efficiency, robustness, and mathematical consistency

- Issues:

  Equation types—hyperbolic or parabolic $\Longrightarrow$ no priori restriction

  Boundary conditions—only conserved quantities as independent variables $\Longrightarrow$ no definite information of non-conserved variables on the boundary available

  Balanced treatment of each effects (convective, kinematic, and dissipative) $\Longrightarrow$ dimensionless parameters as a guide

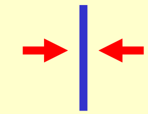
- **Consider a simple problem (benchmark problem)**

  Focus on the big picture

The benchmark problems

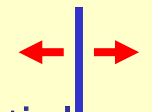
- **Why benchmark problems?**: Simple but preserve the essence of physics; experimental study possible

- 3 cases:

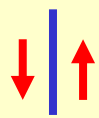


(-) normal velocity gradient—compressive nature—shock wave

(+) normal velocity gradient—expansive nature—free jet



Shear velocity gradient—shear-driven velocity profile—tangential flow near the solid wall

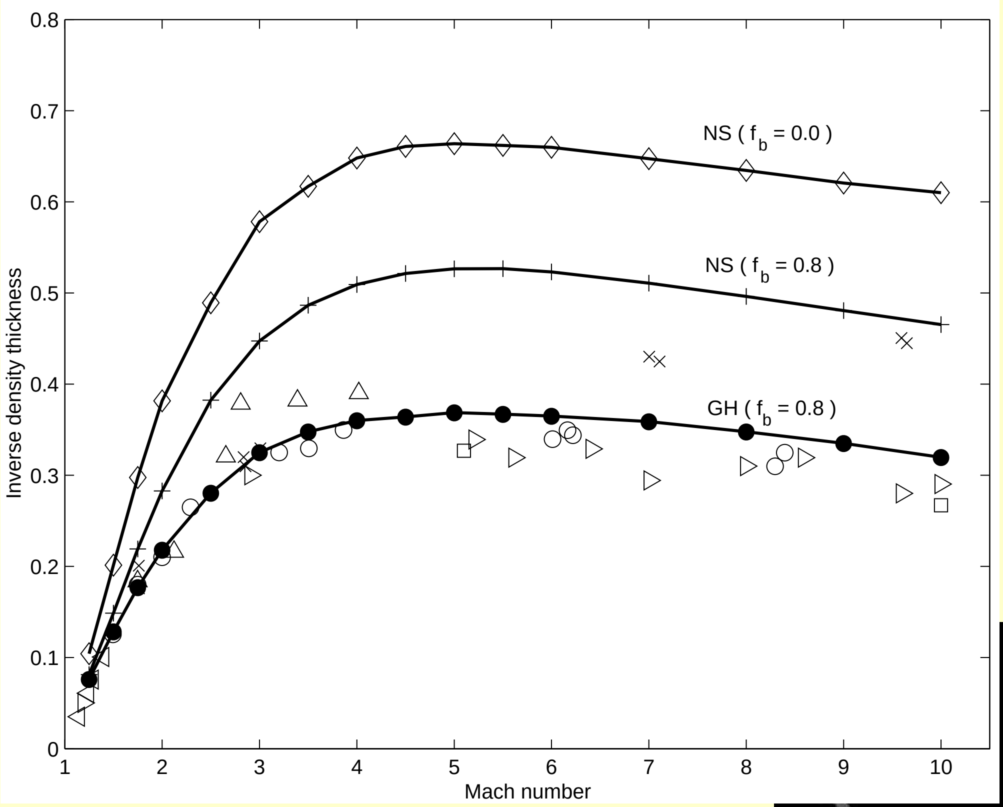


- **Shock wave:**

The most critical problem since the Boltzmann collision integral is directly involved

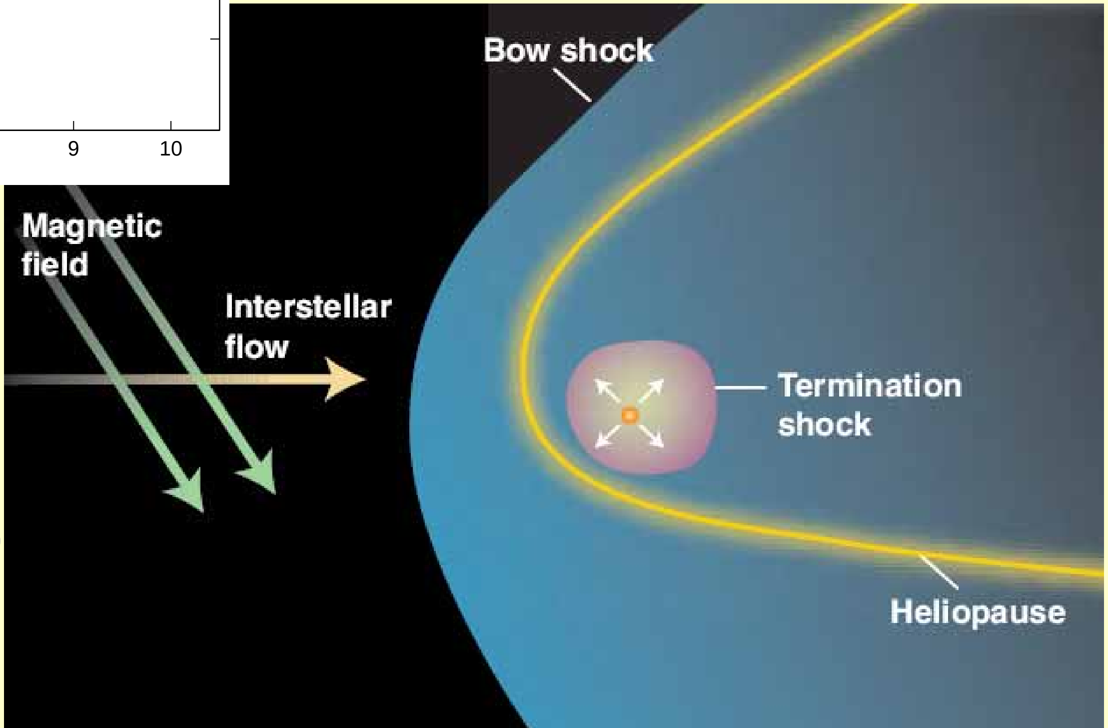
Without the usual complication from the boundary

Shock wave examples



- hypersonic shock wave over a blunt body

- Interaction of the solar wind with interstellar medium (plasma and **neutral hydrogen** gas)



The moment method (Maxwell and Grad)

- **Derivation of the conservation laws and constitutive equations using the concept of statistical average**

By differentiating **stress tensor** $\mathbf{P} = \langle m\mathbf{cc}f(\mathbf{v},\mathbf{r},t)\rangle$ with time and combining with

the Boltzmann equation $\left(\partial_t + \mathbf{v}\cdot\nabla\right)f(\mathbf{v},\mathbf{r},t) = C[f]$,

we obtain $\mathbf{P}_t = -\langle m\mathbf{cc}(\mathbf{v}\cdot\nabla f)\rangle + \mathbf{\Lambda}^{(P)}$ where $\mathbf{\Lambda}^{(P)} \equiv \langle m\mathbf{cc}C[f]\rangle$. $(\mathbf{P} \equiv p\mathbf{I} + \mathbf{\Pi})$

$$\rho\frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right) + \nabla\cdot\boldsymbol{\psi}^{(\Pi)} = -2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} - 2p[\nabla\mathbf{u}]^{(2)} + \mathbf{\Lambda}^{(\Pi)}\left(\equiv\left\langle m[\mathbf{cc}]^{(2)}C[f]\right\rangle\right)$$

substantial derivative of non-conserved variable

+ flux of high order flux = kinematic term + **dissipation term (Boltzmann collision)**

Mathematically, $\mathbf{\Pi}$ = function of conserved variables and their gradients

➡ No approximations; main parameter $\Pi/p \sim \mathrm{Kn}\cdot M$ (not Kn alone)

No explicit C[f(**r**,**v**,t)] except for the dissipation term; not pure hyperbolic

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

Eu's modified moment method

- **Grad's moment method (1949)**

$$\rho \frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right) + \nabla\cdot\boldsymbol{\psi}^{(\Pi)} = -2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} - 2p\left[\nabla\mathbf{u}\right]^{(2)} + \mathbf{\Lambda}^{(\Pi)}\left(\equiv \left\langle m[\mathbf{cc}]^{(2)} C[f]\right\rangle \overset{Grad}{=} -\boxed{\frac{\mathbf{\Pi}}{\eta/p}}\right)$$

Relaxation (BGK) approximation for C[f] and f in a polynomial form

Closure relation: high order moment $\boldsymbol{\psi}^{(\Pi)}$ ~ heat flux

➡ Mathematical singularity for high Kn**M*

Difficulty in defining moments (stress) at the boundary

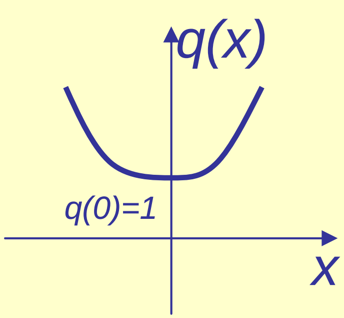
- **Eu's modified moment method (1980, 1992, 1998, 2002)**

$$\rho \frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right) + \nabla\cdot\boldsymbol{\psi}^{(\Pi)} = -2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} - 2p\left[\nabla\mathbf{u}\right]^{(2)} + \mathbf{\Lambda}^{(\Pi)}\left(\equiv \left\langle m[\mathbf{cc}]^{(2)} C[f]\right\rangle \overset{Eu}{=} -\boxed{\frac{\mathbf{\Pi}}{\eta/p} q(\kappa)}\right)$$

f in an exponential form

Cumulant expansion for C[f]

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

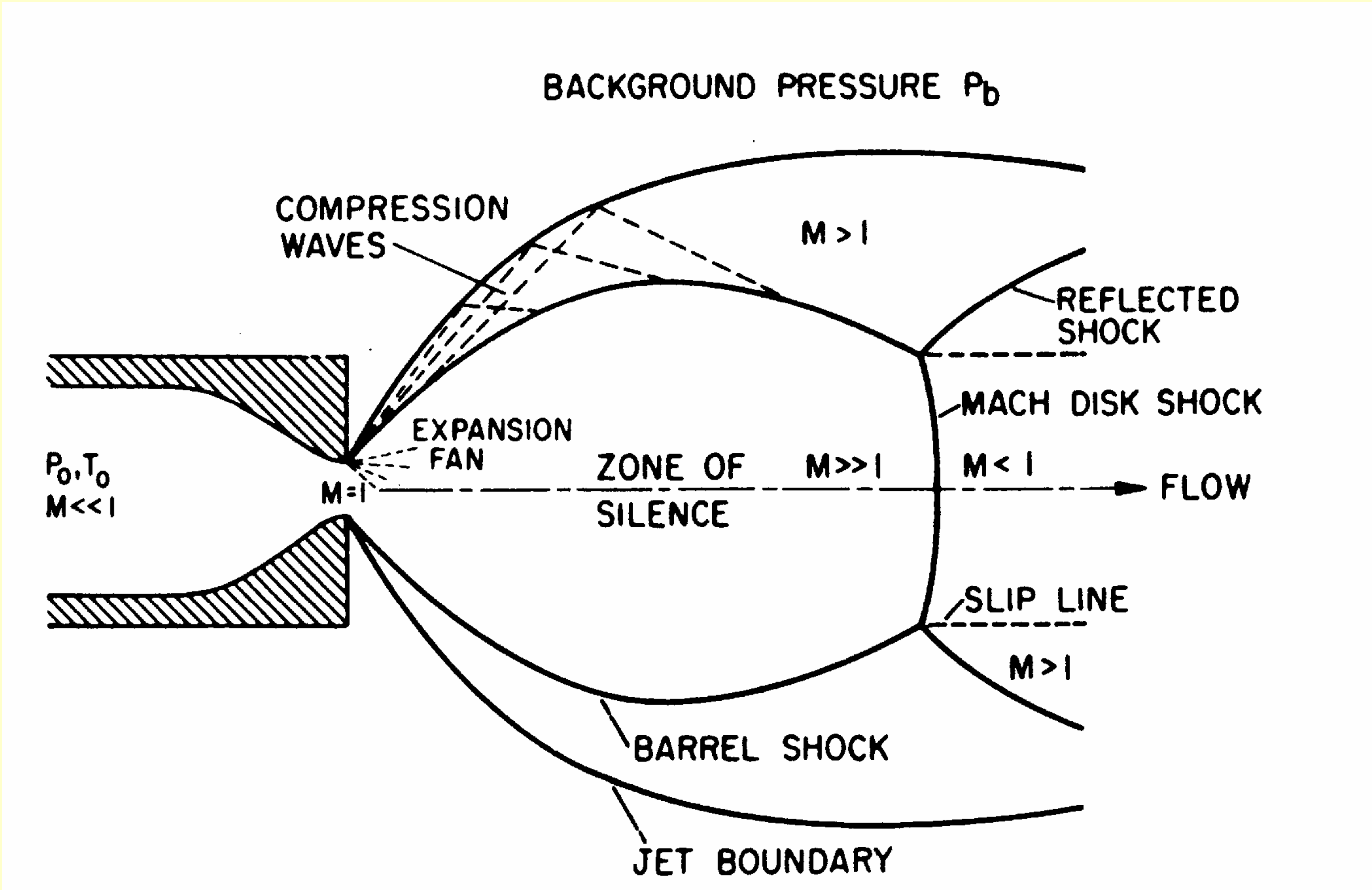


➡ Mathematical singularity is removed

Differential -> algebraic equations -> resolve the boundary problem

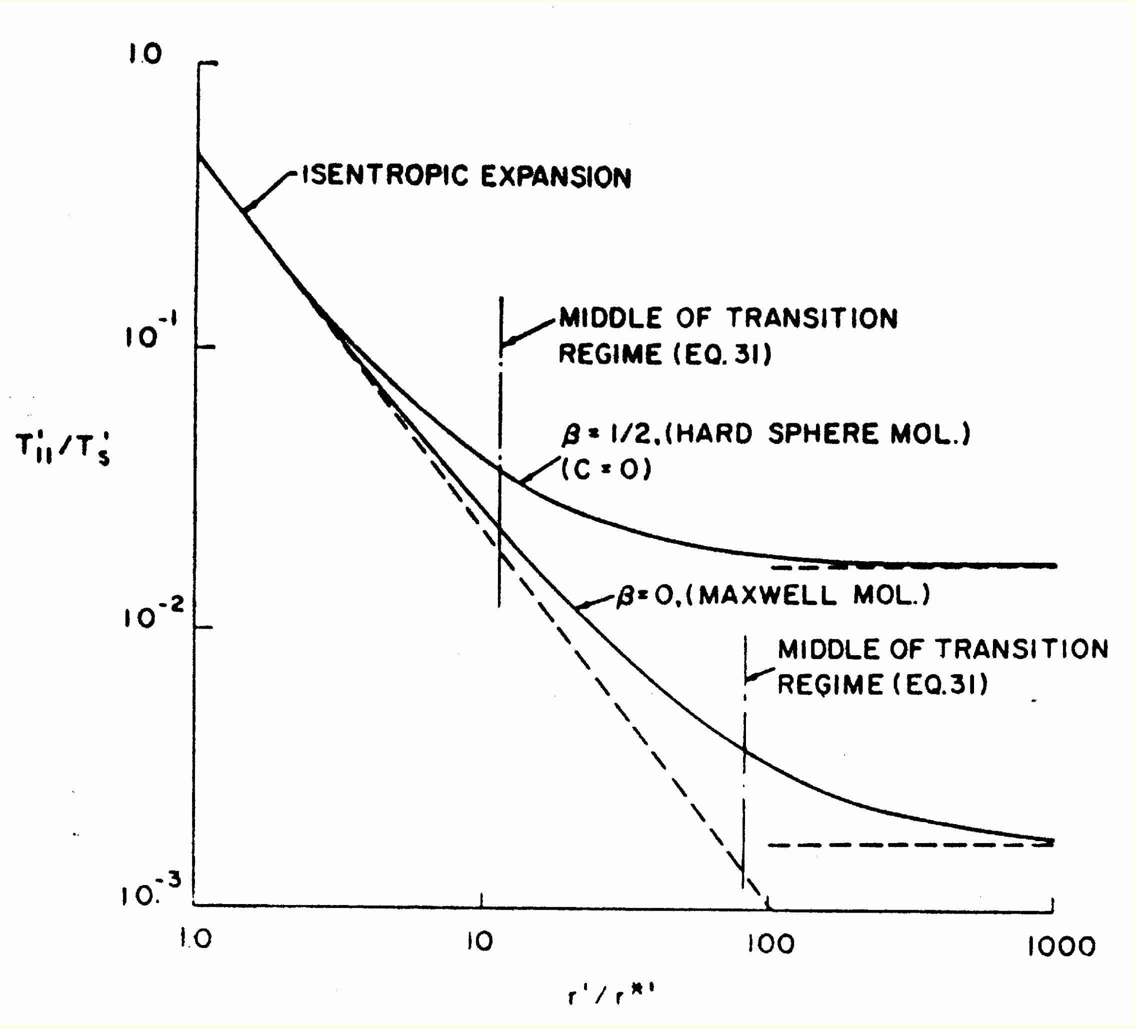
Structure of the free jet

- Practical need of production of high-intensity molecular beam
- Axisymmetric flow configuration: spherically symmetric as an approximation



Pure spherically symmetric source flow

- **Kinetic theory of source flow expansion by Hamel and Willis (1966)**
- **Unusual behavior: freezing of the parallel temperature ($p + \Pi_{rr}$)**



Analysis by the modified moment method (I)

- **Radial dependency only (ρ, u, p, Π_{rr}, Q)**

$$\frac{d}{dr}\begin{bmatrix}\rho u\\ \rho u^2+p\\ \rho\left(h+u^2/2\right)\end{bmatrix}+\frac{2}{r}\rho u\begin{bmatrix}1\\ u\\ h+u^2/2\end{bmatrix}+\begin{bmatrix}0\\ \frac{1}{r^3}\frac{d}{dr}\left(r^3\Pi_{rr}\right)\\ \Pi_{rr}\left(\frac{du}{dr}-\frac{u}{r}\right)+\frac{u}{r^3}\frac{d}{dr}\left(r^3\Pi_{rr}\right)+\frac{1}{r^2}\frac{d}{dr}\left(r^2 Q\right)\end{bmatrix}=0$$

$$\Pi_{rr}q(\kappa)=\Pi_{rr0}\left[1+\frac{\Pi_{rr}}{p}\left(1+\frac{3}{2}\frac{u/r}{du/dr-u/r}\right)\right],$$

dissipation term — kinematic terms — geometrical effect (spherical symmetry)

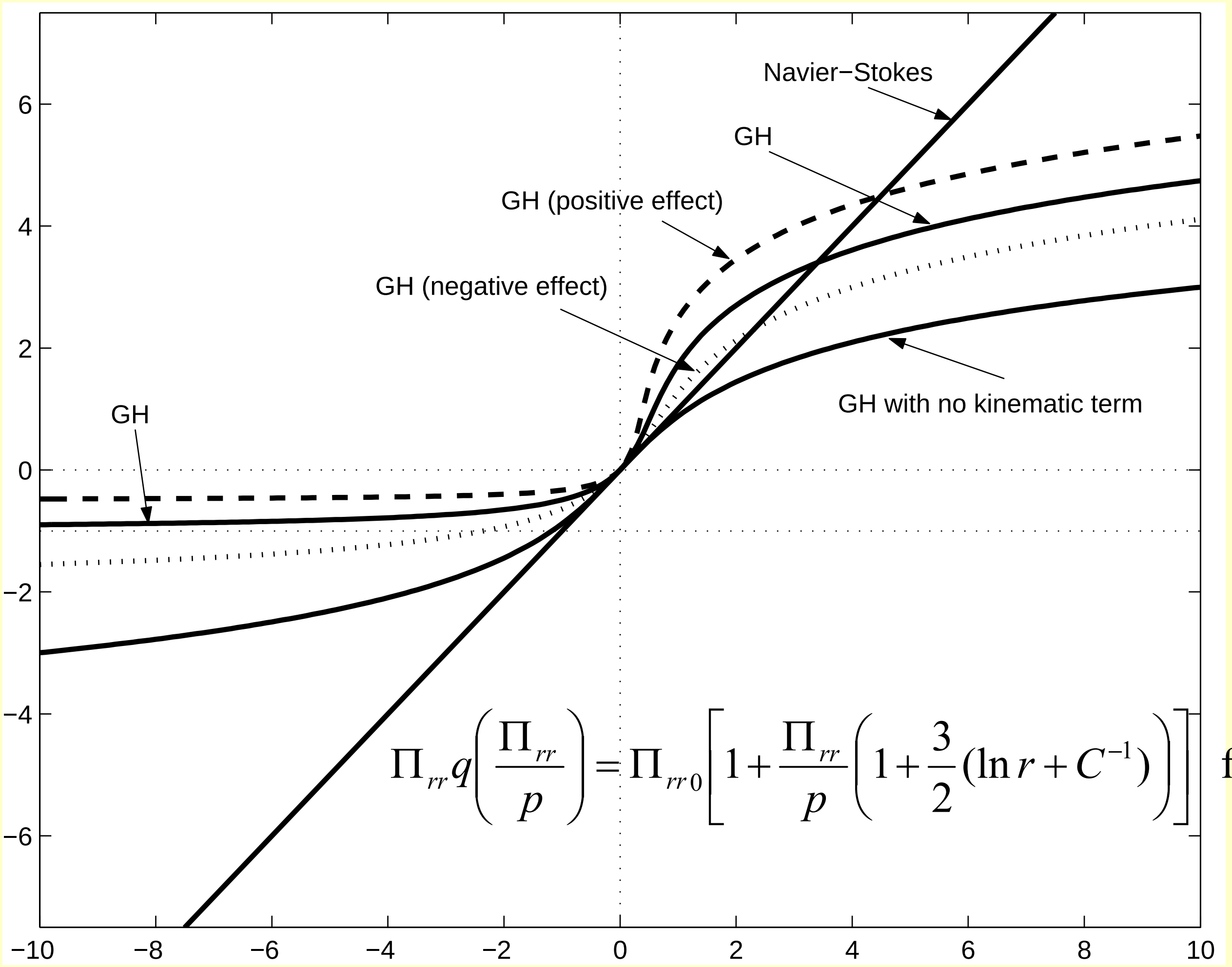
$$Qq(\kappa)=Q_0\left[1+\frac{\Pi_{rr}}{p}\right]\quad \text{where}\quad \kappa=\frac{\left(mk_BT\right)^{1/4}}{p\sqrt{2}d}\left[\frac{3/2\Pi^2{}_{rr}}{2\eta}+\frac{Q^2}{\lambda}\right]^{1/2}$$

$$\Pi_{rr0}=-\frac{4\eta}{3}r\frac{d}{dr}\left(\frac{u}{r}\right),\quad Q_0=-\lambda\frac{d}{dr}\left(\ln T\right)$$

Analysis by the modified moment method (II)

- $p+\Pi_{rr}$ decreases in expanding flow as the radius increases -> a possible explanation of freezing of the parallel temperature $p+\Pi_{rr}$

Π_{rr}/p



$$\Pi_{rr}\,q\left(\frac{\Pi_{rr}}{p}\right)=\Pi_{rr0}\left[1+\frac{\Pi_{rr}}{p}\left(1+\frac{3}{2}\left(\ln r+C^{-1}\right)\right)\right]\quad \text{for } u=r\left(1+C\ln r\right)$$

Π_{rr0}/p

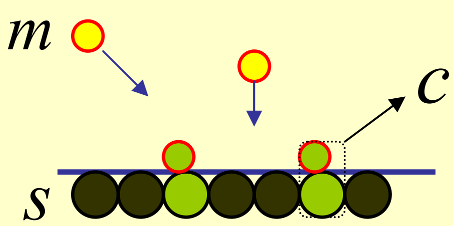
Boundary condition based on Langmuir adsorption isotherm

N : number of sites (s) per unit area of the surface interacting with gas molecules (m)

$N\alpha$: number of sites which are covered

$N(1-\alpha)$: number of sites which are not covered

Let us assume that m and s form the complex c. Then the equilibrium constant K becomes



$$K = \frac{C_c}{C_m C_s} = \frac{N\alpha}{[p/k_B T_w]N(1-\alpha)},$$

that is,

$$\boxed{\alpha = \frac{\beta p}{1+\beta p}} \quad \text{where} \quad \beta = \frac{K}{k_B T_w}.$$

$m + s \Rightarrow c$

Slip Boundary Conditions

- **Langmuir slip condition (Dirichlet type)**

$$u = \alpha u_w + (1-\alpha)u_r, \quad T = \alpha T_w + (1-\alpha)T_r \quad \text{where } \alpha = \frac{p/4\omega Kn}{1+p/4\omega Kn}$$

$$\omega = \omega_0(\nu)\left(\frac{T_w}{T_r}\right)^{1+2/(\nu-1)} \exp\left(-\frac{D_e}{k_B T_w}\right) = \underline{fn(\nu, T_w, D_e)}$$

D_e : Heat of adsorption [$O(10^{-1} \sim 10)$ kcal/mol]

- **Maxwell slip condition (Neumann type)**

$$u = u_w + \varsigma \Pi_w = u_w + \sigma_v \ell \left(\frac{\partial u}{\partial n}\right)_w, \quad T = T_w + \sigma_T \frac{1}{\Pr}\frac{2\gamma}{\gamma+1}\ell\left(\frac{\partial T}{\partial n}\right)_w$$

Cf. We can prove $\omega \sim \sigma_v \left(\equiv (2-\theta)/\theta\right)$ in the case of microchannel flow.

As a result, **a physical meaning can be assigned to** $\sigma_{v,T}$.

$$\sigma_{v,T} \sim \omega = \omega_0(\nu)\left(\frac{T_w}{T_r}\right)^{1+2/(\nu-1)} \exp\left(-\frac{D_e}{k_B T_w}\right)$$

Analysis and validation study

- Pressure-driven compressible flow in microchannel with finite length

$$\frac{\partial(pu)}{\partial x} + \frac{\partial(pv)}{\partial y} = 0$$

$$\frac{dp}{dx} = \frac{\partial^2 u}{\partial y^2}$$

with $\boxed{\text{slip b.c.}}$ ⇨ $p(x), u(x,y), v(x,y)$

Ex. $$\frac{u(y)}{u_{ave}} = \frac{1/4 - y^2 + Kn}{1/6 + Kn}$$

For high Kn*M flow ⇨ $$\frac{dp}{dx} = -\frac{\partial \Pi_{xy}}{\partial y}$$ with $$\boxed{\Pi_{xy}\, q\left(CN_\delta \left|\Pi_{xy}\right| / p\right) = -\frac{\partial u}{\partial y}}$$

Ex. $$\frac{u(y)}{u_{ave}} = \frac{1 - \cosh(\Phi/2) - \alpha[1 - \cosh(\Phi y)]}{1 - \cosh(\Phi/2) - \alpha[1 - q(\Phi/2)]}$$

where $$\Phi = -C\varepsilon \frac{d(\ln p)}{dx}$$

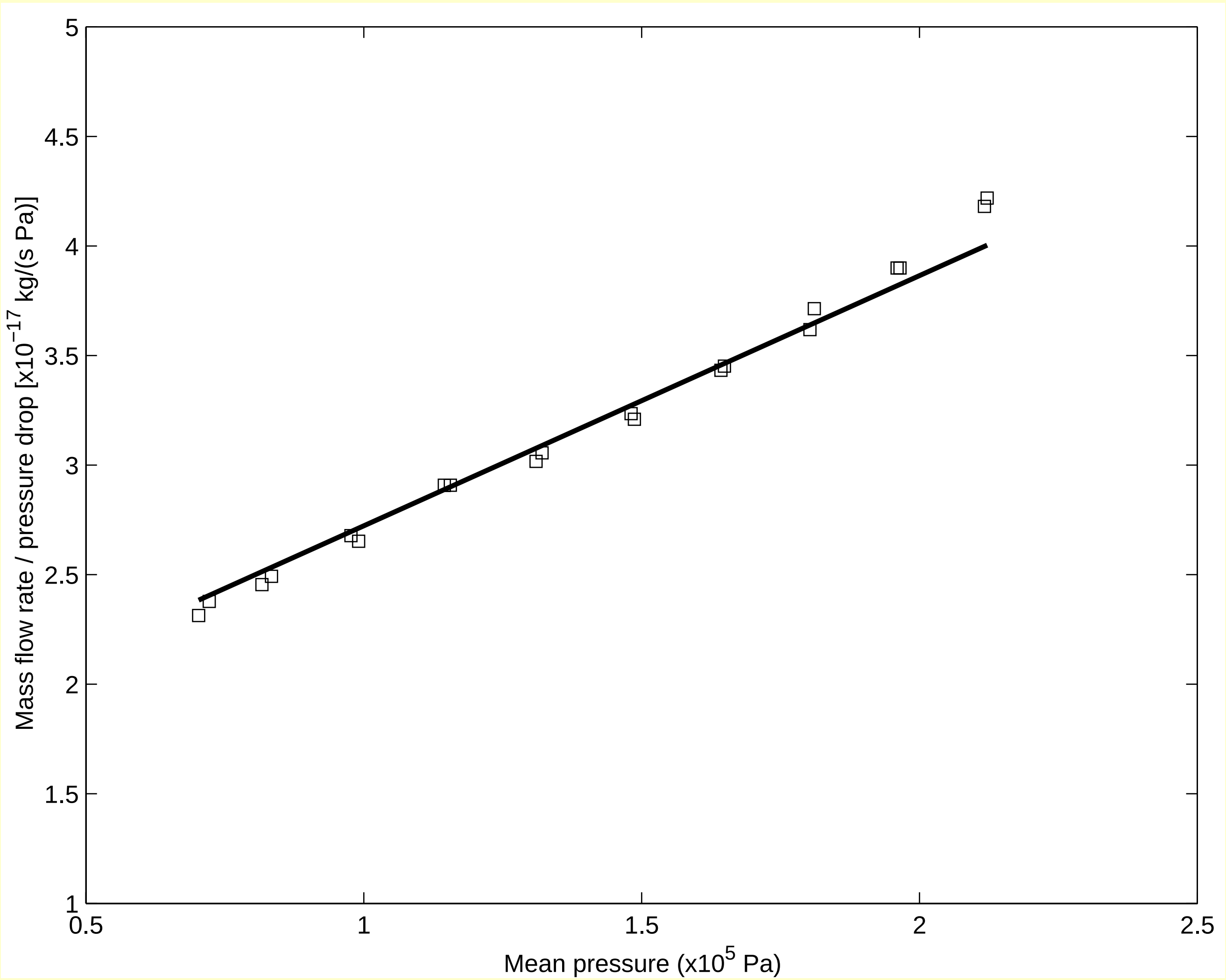
Numerical solutions for o. d. e. of pressure distribution

Ex. Arkilic's experiment in micro-channel

(silicon, $H = 1.33\mu m, W = 52.3\mu m, L = 7.5mm$)

Helium gas (exit $\mathbf{Kn} = 2.5$)

Mass flow rate of helium gas exhausting to an exit pressure of 6.5 kPa (Kn=2.5) (Arkilic's 1997 data)



Summary

- The modified moment method is applied to the study of benchmark problems; pressure-driven free jet and microchannel flows.

- The kinetic term associated with the ratio of radial stress components in the spherical geometry seems to be responsible for the freezing of the parallel temperature.

- The full results of the spherically symmetric source flow remains to be seen.