RAREFIED GAS DYNAMICS AND ITS APPLICATIONS TO VACUUM TECHNOLOGY

Felix Sharipov

Departamento de Física Universidade Federal do Paraná Curitiba, Brazil http://fisica.ufpr.br/sharipov





 \dot{M} mass flow rate?

 $P_1 > P_2$



 \dot{M} mass flow rate?

Q heat flow rate?

 $P_1 > P_2$



M mass flow rate? *Q* heat flow rate?
density distribution?



$$P_1 > P_2$$

 P_{\sim}

non-isothermal flows, thermal creep



non-isothermal flows, thermal creep

 $T_1 < T_2$



 \dot{M} mass flow rate?

non-isothermal flows, thermal creep

 $T_1 < T_2$



 \dot{M} mass flow rate?

Q heat flow rate?

non-isothermal flows, thermal creep



 \dot{M} mass flow rate?

Q heat flow rate?

density (or pressure) distribution?

non-isothermal flows, thermal creep



 \dot{M} mass flow rate?

Q heat flow rate?

density (or pressure) distribution? over the whole range of Kn

Typical problems Thermomolecular pressure difference



Typical problems Thermomolecular pressure difference



 $\dot{M} = 0$ no mass flow

Typical problems Thermomolecular pressure difference

 P_1, T_1 P_2, T_2

 $\dot{M}=0$ no mass flow

What is the pressure ratio?

Thermomolecular pressure difference



 $\dot{M}=0$ no mass flow

What is the pressure ratio?

$$\frac{P_2}{P_1} = \left(\frac{T_2}{T_1}\right)^{\gamma}$$

Thermomolecular pressure difference



 $\dot{M}=0$ no mass flow

What is the pressure ratio?

$$\frac{P_2}{P_1} = \left(\frac{T_2}{T_1}\right)^{\gamma} \qquad 0 \le \gamma \le 0.5$$

$Kn = \frac{molecular mean free path}{characteristic size}$

$Kn = \frac{molecular mean free path}{characteristic size}$

 $Kn = \frac{molecular mean free path}{characteristic size}$

 $\begin{array}{ll} Kn \gg 1 & Free \ molecular \ regime. \\ Every \ particle \ moves \ independently \ on \ each \ other \end{array}$

Kn≪1 Hydrodynamic regime.Continuum mechanics equations are solved

 $Kn = \frac{molecular mean free path}{characteristic size}$

 $Kn \gg 1$ Free molecular regime. Every particle moves independently on each other

Kn≪1 Hydrodynamic regime.Continuum mechanics equations are solved

Rarefaction parameter

equivalent mean free path

$$\ell = \frac{\mu v_m}{P}$$

Rarefaction parameter equivalent mean free path

$$\ell = \frac{\mu v_m}{P}$$

 μ - viscosity

Rarefaction parameter equivalent mean free path

$$\ell = \frac{\mu v_m}{P}$$

 μ - viscosity

 $v_m = \sqrt{2kT/m}$ most probable molecular vel.

Rarefaction parameter equivalent mean free path

$$\ell = \frac{\mu v_m}{P}$$

 μ - viscosity

 $v_m = \sqrt{2kT/m}$ most probable molecular vel. *P* - pressure

 $f(t, \mathbf{r}, \mathbf{v})$ - velocity distribution function

Boltzmann equation $f(t, \mathbf{r}, \mathbf{v})$ - velocity distribution function $n(t, \mathbf{r}) = \int f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v} - \mathbf{density}$ $\mathbf{u}(t,\mathbf{r}) = \frac{1}{n} \int \mathbf{v} f(t,\mathbf{r},\mathbf{v}) d\mathbf{v}$ - bulk velocity $P(t,\mathbf{r}) = \frac{m}{3} \int V^2 f(t,\mathbf{r},\mathbf{v}) d\mathbf{v}$ - pressure $T(t, \mathbf{r}) = \frac{m}{3nk} \int V^2 f(t, \mathbf{r}, \mathbf{v}) d\mathbf{v}$ - temperature $\mathbf{q}(t,\mathbf{r}) = \frac{m}{2} \int V^2 \mathbf{V} f(t,\mathbf{r},\mathbf{v}) d\mathbf{v}$ - heat flux vector $\mathbf{V} = \mathbf{v} - \mathbf{u}$

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} = Q(ff_*)$$

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} = Q(ff_*)$$

$$Q(ff_*) = \int \left(f'f'_* - ff_* \right) |\mathbf{v} - \mathbf{v}_*| b \mathsf{d} b \, \mathsf{d} \varepsilon \, \mathsf{d} \mathbf{v}_*$$

 \mathbf{v}' and \mathbf{v}_{*}' - pre-collision molecular velocities

 $\mathbf v$ and $\mathbf v_*$ - post-collision molecular velocities

Discrete velocity method:

 $\mathbf{v}_1, \, \mathbf{v}_2, \, \ldots, \mathbf{v}_N,$

Discrete velocity method:

 $\mathbf{v}_1, \, \mathbf{v}_2, \, \ldots, \mathbf{v}_N,$

The BE is split into N differential eqs. coupled via the collisions integral

Till now, a numerical solution of the exact Boltz.Eq. requires great computational efforts

Till now, a numerical solution of the exact Boltz.Eq. requires great computational efforts

BGK model

$$Q(ff_*) = \nu \left(f^M - f \right)$$

Till now, a numerical solution of the exact Boltz.Eq. requires great computational efforts

BGK model

$$Q(ff_*) = \nu \left(f^M - f \right)$$

S model

$$Q(ff_*) = \nu \left\{ f^M \left[1 + \frac{2m(\mathbf{q} \cdot \mathbf{V})}{15n(kT)^2} \left(\frac{mV^2}{2kT} - \frac{5}{2} \right) \right] - f \right\}$$

Till now, a numerical solution of the exact Boltz.Eq. requires great computational efforts

BGK model

$$Q(ff_*) = \nu \left(f^M - f \right)$$

S model

$$Q(ff_*) = \nu \left\{ f^M \left[1 + \frac{2m(\mathbf{q} \cdot \mathbf{V})}{15n(kT)^2} \left(\frac{mV^2}{2kT} - \frac{5}{2} \right) \right] - f \right\}$$

$$f^{M} = n \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left[-\frac{m(\mathbf{v}-\mathbf{u})^{2}}{2kT}\right]$$

 $\nu = P/\mu$ - frequency of intermolecular collisions

Viscous slip coefficient



Viscous slip coefficient



The most used formula

$$u_y = \frac{2 - \alpha}{\alpha} \lambda \frac{du_y}{du_x}$$

- α -accommodation coefficient
- λ mean free path
Viscous slip coefficient All disagreements with experiments are eliminated by fitting α :

 $0.1 \le \alpha \le 2,$

while in reality

 $0.9 \le \alpha \le 1,$





$$u_y = \sigma_{\mathsf{P}} \ell \frac{\mathsf{d} u_y}{\mathsf{d} x} \quad \text{at} \quad x = 0$$

 $\sigma_{\rm P}$ - viscous slip coefficient

ℓ equivalent mean free path

Diffuse scattering

 $\sigma_{\rm P} = \sqrt{\pi}/2 = 0.886$ estimation by Maxwell

Diffuse scattering $\sigma_{\rm P} = \sqrt{\pi}/2 = 0.886$ $\sigma_{\rm P} = 1.016$ $\sigma_{\rm P} = 1.018$ $\sigma_{\rm P} = 0.985$

estimation by Maxwell solution of BGK model solution of S model solution of Boltzmann Eq.

Non-diffuse scattering

Estimation by Maxwell

$$\sigma_{\mathsf{P}} = 0.886 \frac{2-\alpha}{\alpha}$$

Non-diffuse scattering

Estimation by Maxwell

$$\sigma_{\mathsf{P}} = 0.886 \frac{2-\alpha}{\alpha}$$

S model with CL bound.cond., (Sharipov-2003)

$$\sigma_{\mathsf{P}} = 1.018 \frac{2 - \alpha_t}{\alpha_t} - 0.264 \frac{1 - \alpha_t}{\alpha_t}$$

 $\sigma_{\rm P}$ is sensitive to the gas-surface interaction

Gas-surface interaction law

Experiment by Porodnov et al. (1974) technical (contaminated) surface

gas	He	Ne	Ar	Kr	Xe	H_2	N_2	CO_2
$lpha_t$	0.88	0.85	0.92	1.0	1.0	0.95	0.91	0.99

Gas-surface interaction law

Experiment by Porodnov et al. (1974) technical (contaminated) surface

gas	He	Ne	Ar	Kr	Xe	H_2	N_2	CO_2
$lpha_t$	0.88	0.85	0.92	1.0	1.0	0.95	0.91	0.99

For a technical surface α_t is very close to unity for the most of gases

Thermal slip coefficient

$$u_y = \sigma_{\mathsf{T}} \frac{\mu}{\varrho} \frac{\mathsf{d} \ln T}{\mathsf{d} y} \quad \text{at} \quad x = 0$$

Diffuse scattering $\sigma_{T} = 0.75$ estimation by Maxwell $\sigma_{T} = 1.175$ solution of S model $\sigma_{T} = 1.01$ solution of Boltzmann Eq.

Temperature jump coefficient

$$T_g = T_w + \zeta_{\mathsf{T}} \ell \frac{\mathsf{d}T}{\mathsf{d}x}$$

Diffuse scattering $\zeta_T = 1.662$ estimation by Maxwell $\zeta_T = 1.954$ solution of S model

$$\dot{M} = \frac{\pi a^2 P}{v_m} \left(-G_P \frac{a}{P} \frac{\mathrm{d}P}{\mathrm{d}x} + G_T \frac{a}{T} \frac{\mathrm{d}T}{\mathrm{d}x} \right)$$

 $G_P = G_P(\delta)$ $G_T = G_T(\delta)$

$$\delta = \frac{a}{\ell}$$

Free molecular regime $\delta = 0$

$$G_P = \frac{8}{3\sqrt{\pi}}, \qquad G_T = \frac{1}{2}G_P$$

Hydrodynamic regime $\delta \to \infty$

$$G_P = \frac{\delta}{4} + \sigma_{\rm P}, \qquad G_T = \frac{\sigma_{\rm T}}{\delta}$$

Transitional regime G_P



Cercignani et al. (1966)

Transitional regime G_P



Cercignani et al. (1966) Sharipov, 1996

Transitional regime G_P



Cercignani et al. (1966) Sharipov, 1996 Loyalka & Hamoodi (1991)

Transitional regime G_P



Transitional regime G_T





Transitional regime G_T



Loyalka (1994) Sharipov, 1996

Transitional regime G_T



Loyalka (1994) Sharipov, 1999 Loyalka & Hickey, 1991

Transitional regime G_T



Loyalka (1994) Sharipov, 1999 Loyalka & Hickey, 1991

BGK does not, while S provides reliable results for non-isothermal flows

Numerical data on G_P and G_T can be found in

Sharipov & Seleznev, Data on Internal Rarefied gas Flows *J. Phys. Chem. Ref. Data* **27**, 657-706 (1998)

Numerical calculations of \dot{M} can be carried out on-line

http://fisica.ufpr.br/sharipov

Direct Simulation Monte Carlo M particles are considered simultaneously

 $M \sim 10^7 - 10^8$

Direct Simulation Monte Carlo M particles are considered simultaneously

 $M \sim 10^7 - 10^8$

- Free motion of particles
- Interaction with solid surface, Elimination and Generation of particles
- Simulation of collisions
- Calculation of macroscopic quantities

Orifice flow





$$W = \frac{\dot{M}}{\dot{M}_0}, \qquad \dot{M}_0 = \frac{\sqrt{\pi a^2}}{v_m} P_0$$











Orifice flow at $P_1 > 0$



Orifice flow at $P_1 > 0$ Flowfield at $P_0/P_1 = 100$ and $\delta = 1000$



Orifice flow at $P_1 > 0$ Flowfield at $P_0/P_1 = 10$ and $\delta = 1000$



Felix Sharipov – p. 37

Holweck pump



Holweck pump



Holweck pump. First stage Four problems are solved

- Poiseuille flow in x direction $G_x^{(P)}(\delta)$
- Poiseuille flow in z direction $G_z^{(P)}(\delta)$
- Couette flow in x direction $G_x^{(C)}(\delta)$
- Couette flow in z direction $G_z^{(C)}(\delta)$



It takes long CPU time
Holweck pump. Second stage S - pumping speed

$$G_{\eta} = \frac{S}{v_m \ell^2}$$

$$\ell \frac{dP}{d\eta} = \sin \alpha \frac{\frac{U}{v_m} P \cos \alpha [G_z^{(C)} - \frac{\ell_z}{\ell} G_x^{(C)}] - G_\eta P_h}{G_z^{(P)} \sin^2 \alpha + \frac{\ell_z}{\ell} G_x^{(P)} \cos^2 \alpha}$$

It takes short CPU time

Holweck pump. Second stage

It allows us easily to change many parameters such as:

- groove inclination
- fore vacuum and high vacuum pressures
- angular velocity of rotating cylinder,
- species of gas
- temperature of the gas

Holweck pump. Results Limit compression pressure ratio



Holweck pump. Results Dimensional pumping speed



 Velocity slip coefficients of single gas for different gas-surafce interaction laws

- Velocity slip coefficients of single gas for different gas-surafce interaction laws
- Velocity slip coefficients for gaseous mixtures

- Velocity slip coefficients of single gas for different gas-surafce interaction laws
- Velocity slip coefficients for gaseous mixtures
- Temperature jump coefficient of single gas for different gas-surafce interaction laws

- Velocity slip coefficients of single gas for different gas-surafce interaction laws
- Velocity slip coefficients for gaseous mixtures
- Temperature jump coefficient of single gas for different gas-surafce interaction laws
- Temperature jump coefficient for gaseous mixtures

over the whole range of the gas rarefaction

 Single gas flows through long tubes and channels

- Single gas flows through long tubes and channels
- Mixture gas flows through long tubes and channels

- Single gas flows through long tubes and channels
- Mixture gas flows through long tubes and channels
- Gas flow through orifices and slits

- Single gas flows through long tubes and channels
- Mixture gas flows through long tubes and channels
- Gas flow through orifices and slits
- Couette flow of a single gas

- Single gas flows through long tubes and channels
- Mixture gas flows through long tubes and channels
- Gas flow through orifices and slits
- Couette flow of a single gas
- Couette flow of mixtures

- Single gas flows through long tubes and channels
- Mixture gas flows through long tubes and channels
- Gas flow through orifices and slits
- Couette flow of a single gas
- Couette flow of mixtures
- Modelling of vacuum pumps

Numerical programs

Some calculations of flow rate through tubes, channels and orifices can be carried out in dimensional quantities on line

http://fisica.ufpr.br/sharipov/

Numerical programs

Some calculations of flow rate through tubes, channels and orifices can be carried out in dimensional quantities on line

http://fisica.ufpr.br/sharipov/

Thank you for your attention