## Rarefied Gas Dynamics: Theory and Applications to Vacuum

## Lecture 1: Fundamentals of kinetic theory

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# The presentations can be downloaded from 

 http://fisica.ufpr.br/sharipov/SC
## Outline

- Typical problems.
- Flow regimes.
- Intermolecular potentials.
- Equivalent free path.
- Velocity distribution function
- Boltzmann equation.
- Model equations.
- General form of gas-surface interaction.
- Velocity slip and temperature jump.
- Viscosity.
- Bibliography.


## Poiseuille flow



$$
p_{1}>p_{2}
$$

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## To be calculated:

- $\dot{M}$ mass flow rate?
- density (or pressure) distribution?


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- over the whole range of Kn


## Thermal creep



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## Thermomolecular pressure difference


net flow rate $=0$

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net flow rate $=0$
To be calculated:
$\frac{p_{1}}{p_{2}}=\left(\frac{T_{1}}{T_{2}}\right)^{\gamma}, \quad \gamma=?$

## Couette flow



## Couette flow



To be calculated:

- $P_{x y}$ shear stress
- $u_{x}(y)$ velocity profile

Heat transfer between two plates


## Heat transfer between two plates



To be calculated:

- $q_{x}$ heat flux
- $T(x)$ temperature distribution


## Heat transfer between two cylinders (Pirani sensor)



To be calculated:

- $q_{r}$ heat flux
- $T(r)$ temperature distribution


## Definition

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\begin{equation*}
\mathrm{K} \mathrm{n}=\frac{\text { molecular mean free path }}{\text { characteristic size }}=\frac{\lambda}{a} \tag{2}
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10^{5} \mathrm{~Pa}>\text { pressure }>10^{-9} \mathrm{~Pa}
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## Pressure variation

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\begin{aligned}
& 10^{5} \mathrm{~Pa}>{ }^{\text {pressure }}>10^{-9} \mathrm{~Pa} \\
& 10^{-8} \mathrm{~m}<\text { mean free path }<10^{6} \mathrm{~m}
\end{aligned}
$$

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$10^{-9} \mathrm{~m}<$ size $<1 \mathrm{~m}$

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## Knudsen number variation

$$
10^{15}>\mathrm{Kn}>10^{-8}
$$

## Free molecular regime

$K n \gg 1$

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Every particle moves independently of each other.

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- Test particle Monte Carlo method (afternoon lecture)


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- Test particle Monte Carlo method (afternoon lecture)
- Method of angle elements


## Hydrodynamic regime

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## Continuum mechanics equations are solved

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- The methods are well developed and well known.


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## Continuum mechanics equations are solved

- The methods are well developed and well known.
- There are many commercial codes.


# Transition regime 

$\mathrm{Kn} \sim 1$

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\mathrm{Kn} \sim 1 \tag{6}
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- Direct simulation Monte Carlo method is applied.


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Navier-Stokes eq. is not valid Intermolecular collision cannot be neglected

- Direct simulation Monte Carlo method is applied.
- Kinetic Boltzmann equation is solved


## Hard spheres

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U=\left\{\begin{array}{cc}
\infty & r<d  \tag{7}\\
0 & r>d
\end{array}\right.
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& \mu \approx \frac{5}{16 \sqrt{\pi}} \frac{\sqrt{m k_{\mathrm{B}} T}}{d^{2}} \tag{8}
\end{align*}
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$k_{\mathrm{B}}=1.380649 \times 10^{-23} \mathrm{~J} / \mathrm{K}-$ Boltzmann constant $m$ - mass of molecule
$T$ - temperature of gas

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$$
\begin{equation*}
\lambda=\frac{1}{\sqrt{2} n \pi d^{2}} \quad \text { mean-free-path } \tag{9}
\end{equation*}
$$

$n$ - number density of gas

## Lennard-Jones (LJ) potential

$$
\begin{equation*}
U=4 \epsilon\left[\left(\frac{d}{r}\right)^{12}-\left(\frac{d}{r}\right)^{6}\right] \quad 0 \leq r<\infty \tag{10}
\end{equation*}
$$

Viscosity can be written down as

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\begin{equation*}
\mu=\frac{\sqrt{T}}{d^{2}} \phi\left(\frac{k_{\mathrm{B}} T}{\epsilon}\right) \tag{11}
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Mean-free-path is not well defined.

## Ab initio (AI) potential

Potential energy $U$ of two atoms (or molecules) separated by distance $r$ is calculated applying quantum mechanics (Schrödinger equation).

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Numerical values of $U$ are interpolated as

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\begin{equation*}
U(r)=A \mathrm{e}^{-a_{1} r-a_{2} r^{2}}-\sum_{n=3}^{8} \frac{C_{2 n}}{r^{2 n}}\left(1-\mathrm{e}^{-b r} \sum_{k=0}^{2 n} \frac{(b r)^{k}}{k!}\right) \tag{12}
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$a_{1}, a_{2}, b, A, C_{2 n}$ are interpolating coefficients calculated $a b$ initio
Nothing is extracted from experimental data

## Comparison LJ and AI



Al for He: Cencek et al., J. Chem. Phys. 136224303 (2012) Al for Kr: Jäger et al., J. Chem. Phys. 144114304 (2016)

## Definition <br> Mean-free-path is not well defined for arbitrary potential.

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Mean-free-path is not well defined for arbitrary potential.
It is replaced by equivalent-free-path defined in terms of macroscopic quantities: $\mu$ - viscosity, $p$ - pressure

$$
\begin{align*}
& \ell=\frac{\mu v_{m}}{p}  \tag{13}\\
& v_{m}=\sqrt{\frac{2 k_{\mathrm{B}} T}{m}} \text { - most probable molecular speed }
\end{align*}
$$

## Rarefaction parameter

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Free-molecular
$\delta \ll 1$

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Hydrodynamic regime
$\delta \gg 1$
Free-molecular
$\delta \ll 1$

## Transitional regime <br> $\delta \sim 1$

# Definition of velocity distribution function <br> $f(t, \boldsymbol{r}, \boldsymbol{v})$ <br> $t$ - time <br> $\boldsymbol{r}$ - position vector <br> $\boldsymbol{v}$ - molecular velocity 

Definition of velocity distribution function<br>$f(t, \boldsymbol{r}, \boldsymbol{v})$<br>$t$ - time<br>$\boldsymbol{r}$ - position vector<br>$\boldsymbol{v}$ - molecular velocity

$f(t, \boldsymbol{r}, \boldsymbol{v}) \mathrm{d}^{3} \boldsymbol{r} \mathrm{~d}^{3} \boldsymbol{v}$ - number of particles in $\left(\mathrm{d}^{3} \boldsymbol{r} \mathrm{~d}^{3} \boldsymbol{v}\right)$ near $(\boldsymbol{r}, \boldsymbol{v})$ at $t$

## Macroscopic quantities or moments

$$
n(t, \boldsymbol{r})=\int f(t, \boldsymbol{r}, \boldsymbol{v}) \mathrm{d}^{3} \boldsymbol{v}-\text { number density }
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$\boldsymbol{u}(t, \boldsymbol{r})=\frac{1}{n} \int \boldsymbol{v} f(t, \boldsymbol{r}, \boldsymbol{v}) \mathrm{d}^{3} \boldsymbol{v}$ - bulk (hydrodynamic) velocity

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$P_{i j}(t, \boldsymbol{r})=m \int V_{i} V_{j} f(t, \boldsymbol{r}, \boldsymbol{v}) \mathrm{d}^{3} \boldsymbol{v}$ - pressure tensor

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$T(t, \boldsymbol{r})=\frac{m}{3 n k_{\mathrm{B}}} \int V^{2} f(t, \boldsymbol{r}, \boldsymbol{v}) \mathrm{d}^{3} \boldsymbol{v}$ - temperature

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$\boldsymbol{q}(t, \boldsymbol{r})=\frac{m}{2} \int V^{2} \boldsymbol{V} f(t, \boldsymbol{r}, \boldsymbol{v}) \mathrm{d}^{3} \boldsymbol{v}$ - heat flux vector

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$\boldsymbol{q}(t, \boldsymbol{r})=\frac{m}{2} \int V^{2} \boldsymbol{V} f(t, \boldsymbol{r}, \boldsymbol{v}) \mathrm{d}^{3} \boldsymbol{v}$ - heat flux vector
$\boldsymbol{V}=\boldsymbol{v}-\boldsymbol{u}-$ peculiar velocity

## Pressure

$$
\begin{equation*}
p=\frac{1}{3}\left(P_{11}+P_{22}+P_{33}\right) \tag{16}
\end{equation*}
$$

State equation

$$
\begin{equation*}
p=n k_{\mathrm{B}} T \tag{17}
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valid for any state of gas,

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$$

valid for any state of gas, even out of equilibrium

## Equilibrium. Global Maxwellian

$$
\begin{align*}
& f^{\mathrm{M}}=n_{0}\left(\frac{m}{2 \pi k_{\mathrm{B}} T_{0}}\right)^{3 / 2} \exp \left(-\frac{m v^{2}}{2 k_{\mathrm{B}} T_{0}}\right)  \tag{18}\\
& n=\int f^{\mathrm{M}} \mathrm{~d}^{3} \boldsymbol{v}=n_{0}=\mathrm{const}  \tag{19}\\
& \boldsymbol{u}=\frac{1}{n} \int \boldsymbol{v} f^{\mathrm{M}} \mathrm{~d}^{3} \boldsymbol{v}=0 \quad \text { no macroscopic motion }  \tag{20}\\
& T=\frac{m}{3 n k} \int V^{2} f^{\mathrm{M}} \mathrm{~d}^{3} \boldsymbol{v}=T_{0}=\text { const } \tag{21}
\end{align*}
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& P_{i j}=m \int V_{i} V_{j} f^{\mathrm{M}} \mathrm{~d}^{3} \boldsymbol{v}=0, \quad i \neq j \quad \text { no shear stress }  \tag{23}\\
& P_{i i}=m \int V_{i} V_{j} f^{\mathrm{M}} \mathrm{~d}^{3} \boldsymbol{v}=p, \quad i=1,2,3  \tag{24}\\
& \boldsymbol{q}=\frac{m}{2} \int V^{2} \boldsymbol{V} f^{\mathrm{M}} \mathrm{~d}^{3} \boldsymbol{v}=0 \quad \text { no heat flux } \tag{25}
\end{align*}
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In equilibrium, Global Maxwellian remains
at ANY gas rarefaction
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In equilibrium, Global Maxwellian remains
at ANY gas rarefaction
even without intermolecular collisions
with gas-surface interaction different from specular.

## New definition of kelvin unity

Old: 1 K is $1 / 273.16$ part of the thermodynamic temperature of the triple point of water.

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Average energy of gaseous particles in equilibrium

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\begin{equation*}
e=\frac{1}{n_{0}} \int \frac{m v^{2}}{2} f^{\mathrm{M}} \mathrm{~d} \boldsymbol{v}=\frac{3}{2} k_{\mathrm{B}} T_{0} \tag{27}
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1 K is a variation of temperature $T$ that results in a change of average energy of gaseous particles by $\frac{3}{2} \times 1.380649 \times 10^{-23} \mathrm{~J}$.

## Boltzmann equation

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& g=\left|\boldsymbol{v}-\boldsymbol{v}_{*}\right| \quad \text { relative speed of collision }  \tag{30}\\
& f=f(\boldsymbol{v}), \quad f_{*}=f\left(\boldsymbol{v}_{*}\right) \quad f^{\prime}=f\left(\boldsymbol{v}^{\prime}\right) \quad f_{*}^{\prime}=f\left(\boldsymbol{v}_{*}^{\prime}\right) \tag{31}
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$\boldsymbol{v}^{\prime}$ and $\boldsymbol{v}_{*}{ }^{\prime}$ - molecular velocities after collision

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\end{align*}
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$\boldsymbol{v}$ and $\boldsymbol{v}_{*}$-molecular velocities before collision
$\boldsymbol{v}^{\prime}$ and $\boldsymbol{v}_{*}{ }^{\prime}$ - molecular velocities after collision
$b, \varepsilon$ - impact parameters

## Scheme of binary collision


azimuthal impact angle $0 \leq \varepsilon \leq 2 \pi$ determines the collision plane

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$$
\begin{equation*}
\boldsymbol{v}, \boldsymbol{v}_{*} \Rightarrow b, \varepsilon, U \Rightarrow \boldsymbol{v}^{\prime}, \boldsymbol{v}_{*}^{\prime}, \tag{32}
\end{equation*}
$$

## Main properties of collision integral $Q$

- It vanishes in equilibrium

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Q\left(f^{M}\right)=0
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- Conservation laws

$$
\begin{equation*}
\int Q \psi(\boldsymbol{v}) \mathrm{d} \boldsymbol{v}=0 \tag{34}
\end{equation*}
$$

where

$$
\begin{equation*}
\psi=m, m \boldsymbol{v}, \frac{m v^{2}}{2} \tag{35}
\end{equation*}
$$

## Main properties

- Irreversibility, H - theorem

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\begin{equation*}
\int Q \ln f \mathrm{~d} \boldsymbol{v} \leq 0 \tag{36}
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- Prandtl number

$$
\begin{equation*}
\operatorname{Pr}=c_{p} \frac{\mu}{\kappa} \simeq \frac{2}{3} \tag{37}
\end{equation*}
$$

$c_{p}$ - specific heat at $p=$ const
$\mu$ and $\kappa$ - viscosity and heat conductivity

## Discrete velocity method:

$$
\boldsymbol{v}_{1}, \boldsymbol{v}_{2}, \ldots, \boldsymbol{v}_{N}
$$

The BE is split into N differential eqs.
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A numerical solution of the exact Boltz.Eq. requires significant computational effort.

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The BE is split into N differential eqs.
coupled via the collisions integral (next lecture)

A numerical solution of the exact Boltz.Eq. requires significant computational effort.

Model equation is a simplified Boltzmann equation

## Bhatnagar, Gross, Krook (BGK) model

$$
\begin{equation*}
Q=\nu\left(f_{l o c}^{\mathrm{M}}-f\right) \tag{39}
\end{equation*}
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$$

$\nu$ - frequency of intermolecular collisions
$f_{l o c}^{\mathrm{M}}$ local Maxwellian

$$
\begin{equation*}
f_{l o c}^{\mathrm{M}}=n\left(\frac{m}{2 \pi k_{\mathrm{B}} T}\right)^{3 / 2} \exp \left[-\frac{m(\boldsymbol{v}-\boldsymbol{u})^{2}}{2 k_{\mathrm{B}} T}\right] \tag{40}
\end{equation*}
$$

$n(t, \boldsymbol{r}), \boldsymbol{u}(t, \boldsymbol{r})$ and $T(t, \boldsymbol{r})$ are unknown
and calculated via $f$

## Main properties

$$
Q=\nu\left(f^{M}-f\right)
$$

## Main properties

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- $Q\left(f^{\mathrm{M}}\right)=0:$ Yes!
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- H - theorem: Yes!
- Prandtl number:=1 NOT 2/3

Mass or heat transfer is described.

## S model

$$
\begin{equation*}
Q=\frac{p}{\mu}\left\{f^{\mathrm{M}}\left[1+\frac{2 m(\boldsymbol{q} \cdot \boldsymbol{V})}{15 n(k T)^{2}}\left(\frac{m V^{2}}{2 k T}-\frac{5}{2}\right)\right]-f\right\} \tag{42}
\end{equation*}
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- H - theorem: Not proved
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Mass and heat transfer are described.

## Ellipsoidal model

$$
\begin{align*}
& Q=\frac{2 p}{3 \mu}\left\{n \sqrt{\frac{\operatorname{det} A}{\pi^{3}}} \exp \left[-\sum_{i, j=1}^{3} A_{i j}\left(v_{i}-u_{i}\right)\left(v_{j}-u_{j}\right)\right]-f\right\}  \tag{43}\\
& A=B^{-1}, \quad B_{i j}=(k T / m)\left(3 \delta_{i j}-P_{i j} / p\right) \tag{44}
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Mass and heat transfer are described.

## Accommodation coefficient

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\begin{equation*}
\alpha(\psi)=\frac{J^{-}(\psi)-J^{+}(\psi)}{J^{-}(\psi)-J_{d i f f}^{+}(\psi)} \tag{45}
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if $\psi=m \boldsymbol{v}$, then $\alpha$ is momentum accommodation coefficient if $\psi=\frac{1}{2} m v^{2}$, then $\alpha$ is energy accommodation coefficient

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ACs depend on the incident distribution function via $J^{-}$.


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 $A C$ is dependent on gas flow.

## Accommodation coefficient

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& J^{+}(\psi)=\int_{v_{n}>0}\left|v_{n}\right| f(\boldsymbol{v}) \psi(\boldsymbol{v}) \mathrm{d} \boldsymbol{v}  \tag{49}\\
& J^{-}(\psi)=\int_{v_{n}<0}\left|v_{n}\right| f(\boldsymbol{v}) \psi(\boldsymbol{v}) \mathrm{d} \boldsymbol{v} \tag{50}
\end{align*}
$$

specular reflection $\Rightarrow J^{+}=J^{-} \Rightarrow \alpha=0$

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\end{align*}
$$

specular reflection $\Rightarrow J^{+}=J^{-} \Rightarrow \alpha=0$
complete accommodation $\Rightarrow J^{+}=J_{\text {diff }}^{+} \Rightarrow \alpha=1$

## General form

solid


$$
\begin{equation*}
v_{n} f(\boldsymbol{v})=-\int_{v_{n}^{\prime}<0} v_{n}^{\prime} R\left(\boldsymbol{v}^{\prime} \rightarrow \boldsymbol{v}\right) f\left(\boldsymbol{v}^{\prime}\right) \mathrm{d} \boldsymbol{v}^{\prime} \quad \text { for } \quad v_{n}>0 \tag{51}
\end{equation*}
$$

$R\left(\boldsymbol{v}^{\prime} \rightarrow \boldsymbol{v}\right)$ - scattering kernel

## Normalization / impermeability

$$
\begin{equation*}
\int_{v_{n}>0} R\left(\boldsymbol{v}^{\prime} \rightarrow \boldsymbol{v}\right) \mathrm{d} \boldsymbol{v}=1 \tag{52}
\end{equation*}
$$

## Normalization / impermeability

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\int_{v_{n}>0} R\left(\boldsymbol{v}^{\prime} \rightarrow \boldsymbol{v}\right) \mathrm{d} \boldsymbol{v}=1 \tag{52}
\end{equation*}
$$

## Reciprocity

$$
\begin{align*}
& \left|v_{n}^{\prime}\right| \exp \left(-\frac{m v^{\prime 2}}{2 k T_{w}}\right) R\left(\boldsymbol{v}^{\prime} \rightarrow \boldsymbol{v}\right)  \tag{53}\\
& \quad=\left|v_{n}\right| \exp \left(-\frac{m v^{2}}{2 k T_{w}}\right) R\left(-\boldsymbol{v} \rightarrow-\boldsymbol{v}^{\prime}\right)
\end{align*}
$$

Details in Lecture 3

## Velocity slip and temperature jump boundary conditions

Moderate rarefaction $(\delta>10)$ can be considered by
the Navier-Stokes equations subject to
the velocity slip and temperature jump boundary conditions

## Viscous slip coefficient



## Definition

$$
\begin{equation*}
u_{z}=\sigma_{\mathrm{P}} \ell \frac{\mathrm{~d} u_{z}}{\mathrm{~d} x} \quad \text { at } \quad x=0 \tag{55}
\end{equation*}
$$

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

## Application to Couette flow



No slip condition

$$
\begin{equation*}
P_{x y}=\mu \frac{u_{w}}{a} \tag{56}
\end{equation*}
$$

## Application to Couette flow



No slip condition

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Slip condition

$$
\begin{equation*}
P_{x y}=\mu \frac{u_{w}}{a}\left(1+2 \sigma_{\mathrm{P}} \frac{\ell}{a}\right)^{-1} \tag{57}
\end{equation*}
$$

## Thermal slip coefficient



## Definition

$$
\begin{equation*}
u_{y}=\sigma_{\mathrm{T}} \frac{\mu}{\varrho} \frac{\mathrm{~d} \ln T}{\mathrm{~d} z} \quad \text { at } \quad x=0 \tag{58}
\end{equation*}
$$

## Temperature jump coefficient



## Definition

$$
\begin{equation*}
T_{g a s}-T_{w a l l}=\zeta_{T} \ell \frac{\mathrm{~d} T}{\mathrm{~d} x} \tag{59}
\end{equation*}
$$

## Application to heat transfer



No jump condition

$$
\begin{equation*}
q_{x}=\kappa \frac{\Delta T}{a} \tag{60}
\end{equation*}
$$

## Application to heat transfer



No jump condition

$$
\begin{equation*}
q_{x}=\kappa \frac{\Delta T}{a} \tag{60}
\end{equation*}
$$

Jump condition

$$
\begin{equation*}
q_{x}=\kappa \frac{\Delta T}{a}\left(1+2 \zeta_{\mathrm{T}} \frac{\ell}{a}\right)^{-1} \tag{61}
\end{equation*}
$$

## Diffuse scattering

$\sigma_{\mathrm{P}}$ calculated from kinetic equation with gas-surface boundary condition

## Diffuse scattering

$\sigma_{\mathrm{P}}$ calculated from kinetic equation with gas-surface boundary condition
$\sigma_{\mathrm{P}}=1.016 \quad$ solution of BGK model
$\sigma_{\mathrm{P}}=1.018$
solution of $S$ model
$\sigma_{\mathrm{P}}=0.985$
solution of Boltzmann Eq for HS
$\sigma_{\mathrm{P}}=1.00$
solution of Boltzmann Eq for LJ, He at T=300 K

## Diffuse scattering

$\sigma_{\mathrm{P}}$ calculated from kinetic equation with gas-surface boundary condition
$\sigma_{\mathrm{P}}=1.016 \quad$ solution of BGK model
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$\sigma_{\mathrm{P}}=1.00 \quad$ solution of Boltzmann Eq for LJ, He at T=300 K
$\sigma_{\mathrm{P}} \approx 1.00$ weakly sensitive to intermolecular collisions

## Diffuse scattering

$\sigma_{\mathrm{T}}$ calculated from kinetic equation with gas-surface boundary condition

$$
\begin{array}{ll}
\sigma_{\mathrm{T}}=1.175 & \text { solution of S model } \\
\sigma_{\mathrm{T}}=1.02 & \text { solution of Boltzmann Eq. for } \mathrm{HS} \\
\sigma_{\mathrm{T}}=1.08 & \text { solution of Boltzmann Eq. for LJ, He at } \mathrm{T}=300 \mathrm{~K}
\end{array}
$$

## Diffuse scattering

$\sigma_{\mathrm{T}}$ calculated from kinetic equation with gas-surface boundary condition

$$
\begin{array}{ll}
\sigma_{\mathrm{T}}=1.175 & \text { solution of S model } \\
\sigma_{\mathrm{T}}=1.02 & \text { solution of Boltzmann Eq. for } \mathrm{HS} \\
\sigma_{\mathrm{T}}=1.08 & \text { solution of Boltzmann Eq. for } \mathrm{LJ}, \mathrm{He} \text { at } \mathrm{T}=300 \mathrm{~K} \\
\sigma_{\mathrm{T}} \approx 1.00 \text { sensitive to intermolecular collisions }
\end{array}
$$

## Diffuse scattering

$\zeta_{T}$ calculated from kinetic equation with gas-surface boundary condition
$\zeta_{T}=1.954 \quad$ solution of $S$ model
$\zeta_{\mathrm{T}}=1.89$
solution of Boltz. eq. for HS
$\zeta_{\mathrm{T}}=1.91$
solution of Boltz. eq. for LJ, He at 293 K

## Diffuse scattering

$\zeta_{T}$ calculated from kinetic equation with gas-surface boundary condition
$\zeta_{T}=1.954 \quad$ solution of $S$ model
$\zeta_{\mathrm{T}}=1.89 \quad$ solution of Boltz. eq. for HS
$\zeta_{T}=1.91 \quad$ solution of Boltz. eq. for LJ, He at 293 K
$\zeta_{\mathrm{T}} \approx 1.9$ weakly sensitive to intermolecular collisions

## Viscosity ab initio

## needed to calculate equivalent free path

$$
\begin{equation*}
\ell=\frac{\mu v_{m}}{p} \tag{62}
\end{equation*}
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needed to calculate equivalent free path

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Viscosity is calculated from the linearized Boltzmann equation with $a b$ initio potential over a wide range of temperature with a high accuracy.

## Viscosity of He at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

Experiment: Berg \& Burton, Mol.Phys. 111 (2013)

$$
\begin{equation*}
\mu=(19.8253 \pm 0.0059) \times 10^{-6} \text { Pa s, } \quad u_{r}=3 . \times 10^{-4} \tag{63}
\end{equation*}
$$

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\end{equation*}
$$

Theory: Cencek et al. J. Chem. Phys. 136 (2012)

$$
\begin{equation*}
\mu=(19.82533 \pm 0.00019) \times 10^{-6} \text { Pa s, } \quad u_{r}=9.6 \times 10^{-6} \tag{64}
\end{equation*}
$$

Relative difference $=1.5 \times 10^{-6}$

## Viscosity of Ne at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

Experiment: Berg \& Burton, Mol.Phys. 111 (2013)

$$
\begin{equation*}
\mu=(31.6880 \pm 0.0096) \times 10^{-6} \text { Pa s, } \quad u_{r}=3 . \times 10^{-4} \tag{66}
\end{equation*}
$$

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\end{equation*}
$$

Theory: Bich et al. Mol. Phys. 106 (2008).

$$
\begin{equation*}
\mu=(31.728 \pm 0.032) \times 10^{-6} \mathrm{~Pa} \mathrm{~s}, \quad u_{r}=1 . \times 10^{-3} \tag{67}
\end{equation*}
$$

Relative difference $=1.3 \times 10^{-3}$

## Viscosity of Ar at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

Experiment: Berg \& Burton, Mol.Phys. 111 (2013)

$$
\begin{equation*}
\mu=(22.5539 \pm 0.0067) \times 10^{-6} \text { Pa s, } \quad u_{r}=3 . \times 10^{-4} \tag{68}
\end{equation*}
$$

## Viscosity of Ar at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

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\begin{equation*}
\mu=(22.5539 \pm 0.0067) \times 10^{-6} \text { Pa s, } \quad u_{r}=3 . \times 10^{-4} \tag{68}
\end{equation*}
$$

Theory: Vogel et al. Mol. Phys. 108 (2010)

$$
\begin{equation*}
\mu=22.552 \times 10^{-6} \mathrm{~Pa} \mathrm{~s}, \tag{69}
\end{equation*}
$$

Relative difference $=8.4 \times 10^{-5}$

## Viscosity of Kr at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

Experiment: Berg \& Burton, Mol.Phys. 111 (2013)

$$
\begin{equation*}
\mu=(25.2812 \pm 0.0076) \times 10^{-6} \text { Pa s, } \quad u_{r}=3 . \times 10^{-4} \tag{70}
\end{equation*}
$$

## Viscosity of Kr at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

Experiment: Berg \& Burton, Mol.Phys. 111 (2013)

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\mu=(25.2812 \pm 0.0076) \times 10^{-6} \text { Pa s, } \quad u_{r}=3 . \times 10^{-4} \tag{70}
\end{equation*}
$$

Theory: Jäger J. Chem.Phys. 144 (2016)

$$
\begin{equation*}
\mu=(25.279 \pm 0.020) \times 10^{-6} \text { Pa s, } \quad u_{r}=7.9 \times 10^{-4} \tag{71}
\end{equation*}
$$

Relative difference $=8.7 \times 10^{-5}$

## Viscosity of Xe at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

Experiment: Berg \& Burton, Mol.Phys. 111 (2013)

$$
\begin{equation*}
\mu=(23.0162 \pm 0.0040) \times 10^{-6} \mathrm{~Pa} \mathrm{~s}, \quad u_{r}=1.7 \times 10^{-4} \tag{72}
\end{equation*}
$$

## Viscosity of Xe at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

Experiment: Berg \& Burton, Mol.Phys. 111 (2013)

$$
\begin{equation*}
\mu=(23.0162 \pm 0.0040) \times 10^{-6} \mathrm{~Pa} \mathrm{~s}, \quad u_{r}=1.7 \times 10^{-4} \tag{72}
\end{equation*}
$$

Sharipov \& Benites, Physical Chemistry Chemical Physics 23 (2021)

$$
\begin{equation*}
\mu=(23.028 \pm 0.069) \times 10^{-6} \text { Pa s, } \quad u_{r}=3 \times 10^{-3} \tag{73}
\end{equation*}
$$

Relative difference $=5.3 \times 10^{-4}$

## Viscosity of Xe at $25^{\circ} \mathrm{C}$ : theory vs. Experiment

Experiment: Berg \& Burton, Mol.Phys. 111 (2013)

$$
\begin{equation*}
\mu=(23.0162 \pm 0.0040) \times 10^{-6} \mathrm{~Pa} \mathrm{~s}, \quad u_{r}=1.7 \times 10^{-4} \tag{72}
\end{equation*}
$$

Sharipov \& Benites, Physical Chemistry Chemical Physics 23 (2021)

$$
\begin{equation*}
\mu=(23.028 \pm 0.069) \times 10^{-6} \text { Pa s, } \quad u_{r}=3 \times 10^{-3} \tag{73}
\end{equation*}
$$

Relative difference $=5.3 \times 10^{-4}$

## Viscosity ab initio

are most complete and most reliable data.

## Equivalent free path for mixtures

$$
\begin{equation*}
\ell=\frac{\mu v_{m}}{p}, \quad v_{m}=\sqrt{\frac{2 k_{\mathrm{B}} T}{\bar{m}}}, \quad \bar{m}=\sum_{i} x_{i} m_{i} \tag{74}
\end{equation*}
$$

$\bar{m}$ is mean molecular mass
$\mu$ is viscosity of mixture calculated from system of Boltzmann equations
$\mu$ is a function of temperature $T$ and chemical composition $x_{i}$

## Viscosity of mixture Ne-Ar at $T=273 \mathrm{~K}, \mathrm{HS}$ vs AI

HS: Tipton et al. Eur. J. Mech. B-Fluids 28, 335 (2009).
AI: Sharipov \& Benites Fluid Phase Equilibria 498, 23-32 (2019).


$$
\begin{equation*}
\frac{\left|\mu^{(H S)}-\mu^{(A I)}\right|}{\mu^{(A I)}} \times 100 \%=2.1 \% \tag{75}
\end{equation*}
$$

## Viscosity of mixture He-Kr at $T=273 \mathrm{~K}, \mathrm{HS}$ vs AI

HS: Tipton et al. Eur. J. Mech. B-Fluids 28, 335 (2009).
AI: Sharipov \& Benites Phys. Fluids. 32, 077104 (2020)


$$
\begin{equation*}
\frac{\left|\mu^{(H S)}-\mu^{(A I)}\right|}{\mu^{(A I)}} \times 100 \%=7.8 \% \tag{76}
\end{equation*}
$$

## Viscosity of He-Ne mixture vs. temperature.

 Ab initio. Quantum approach.

Sharipov \& Benites J. Chem. Phys. 147, 224302 (2017).

## Viscosity of He-Ne mixture vs. temperature.

Ab initio. Quantum approach.


Sharipov \& Benites J. Chem. Phys. 147, 224302 (2017).

## Viscosity of He -Ne mixture vs. temperature.

Ab initio. Quantum approach.


Sharipov \& Benites J. Chem. Phys. 147, 224302 (2017).
No general expression of $\mu=F\left(\mu_{1}, \mu_{2}, \ldots\right)$

## Viscous as function of temperature

$$
\begin{equation*}
\mu=\mu_{r e f}\left(\frac{T}{T_{r e f}}\right)^{\omega}, \quad \omega=\mathrm{const} \tag{77}
\end{equation*}
$$

## Viscous as function of temperature

$$
\begin{equation*}
\mu=\mu_{\text {ref }}\left(\frac{T}{T_{r e f}}\right)^{\omega}, \quad \omega=\mathrm{const} \tag{77}
\end{equation*}
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However, $\omega$ is not constant


## Viscous as function of temperature

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\begin{equation*}
\mu=\mu_{\text {ref }}\left(\frac{T}{T_{r e f}}\right)^{\omega}, \quad \omega=\mathrm{const} \tag{77}
\end{equation*}
$$

However, $\omega$ is not constant


Interpolation (??) is used for $T \approx T_{r e f}$.

## Book

## Felix Sharipov

## Rarefied Gas Dynamics

Fundamentals for Research and Practice


## Handbook

Edited by
Karl Jousten

## Handbook of <br> Vacuum Technology

Second Edition


## Ab initio potentials

- He: Przybytek, et al. Phys. Rev. Lett. 104, 183003 (2010).
- Ne: Hellmann, et al. Mol. Phys. 105, 3013-3023 (2007).
- Ar: Jäger, et al. Mol. Phys. 107, 2181-2188 (2009).
- Kr: Jäger, et al. J. Chem. Phys. 144114304 (2016).
- Xe: Hellmann, et al. J. Chem. Phys. 147034304 (2017)
- He-Ne, He-Ar, Ne-Ar: Cacheiro, et al. Mol. Phys. 102, 101-110
(2004)
- He-Kr: Jäger et al. J. Chem. Phys. 146, 214302 (2017)


## Data on viscosity of mixtures based on ab initio potential

He-Ar: Sharipov \& Benites J. Chem. Phys. 143 (2015)
He-Ne: Sharipov \& Benites J. Chem. Phys. 147 (2017)
He-Ar, Ne-Ar: Sharipov \& Benites, Fluid Phase Equilibria 498 (2019). He-Kr: Jäger \& Bich J. Chem. Phys. 146 (2017)

Ternary and quaternary mixtures of $\mathrm{He}, \mathrm{Ne}, \mathrm{Ar}, \mathrm{Kr}$ : Sharipov \& Benites, Phys. Fluids. 32 (2020).

Isotopic mixtures of Ne, Ar, Kr, and Xe: Sharipov \& Benites, Physical Chemistry Chemical Physics 23, 16664 (2021)

# THE END of Lecture 1 

## Thank you

# for your attention 

http://fisica.ufpr.br/sharipov

