Velocity and Temperature Boundary-Layer Modeling Using Averaged Molecule cluster Transport Equations

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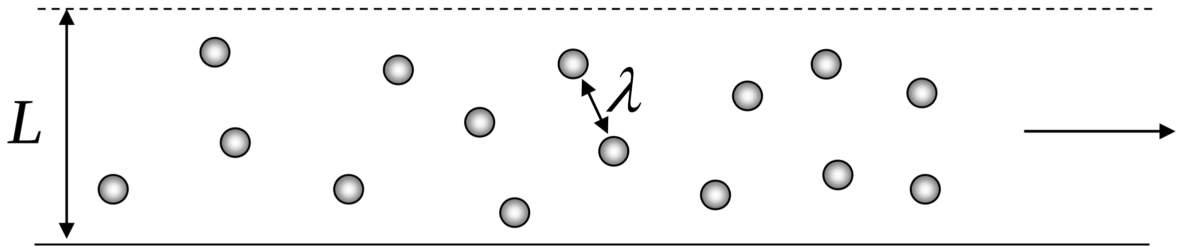
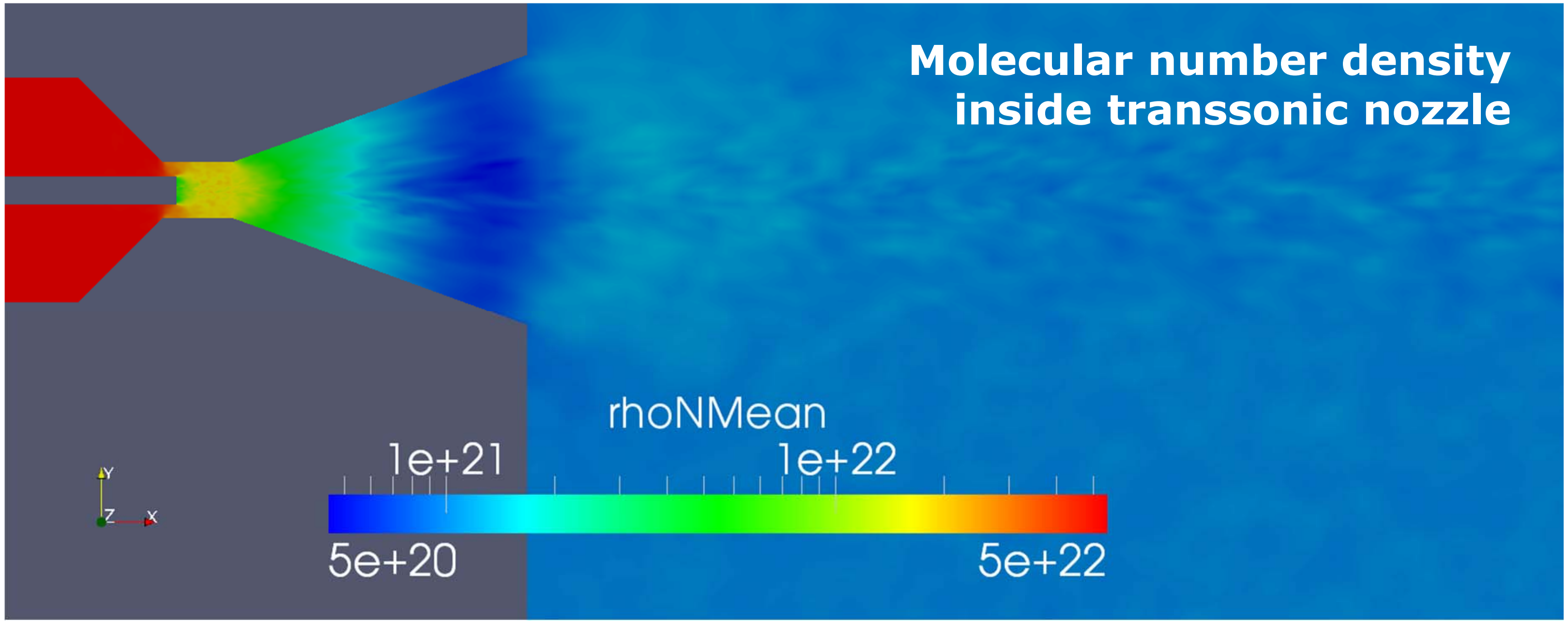
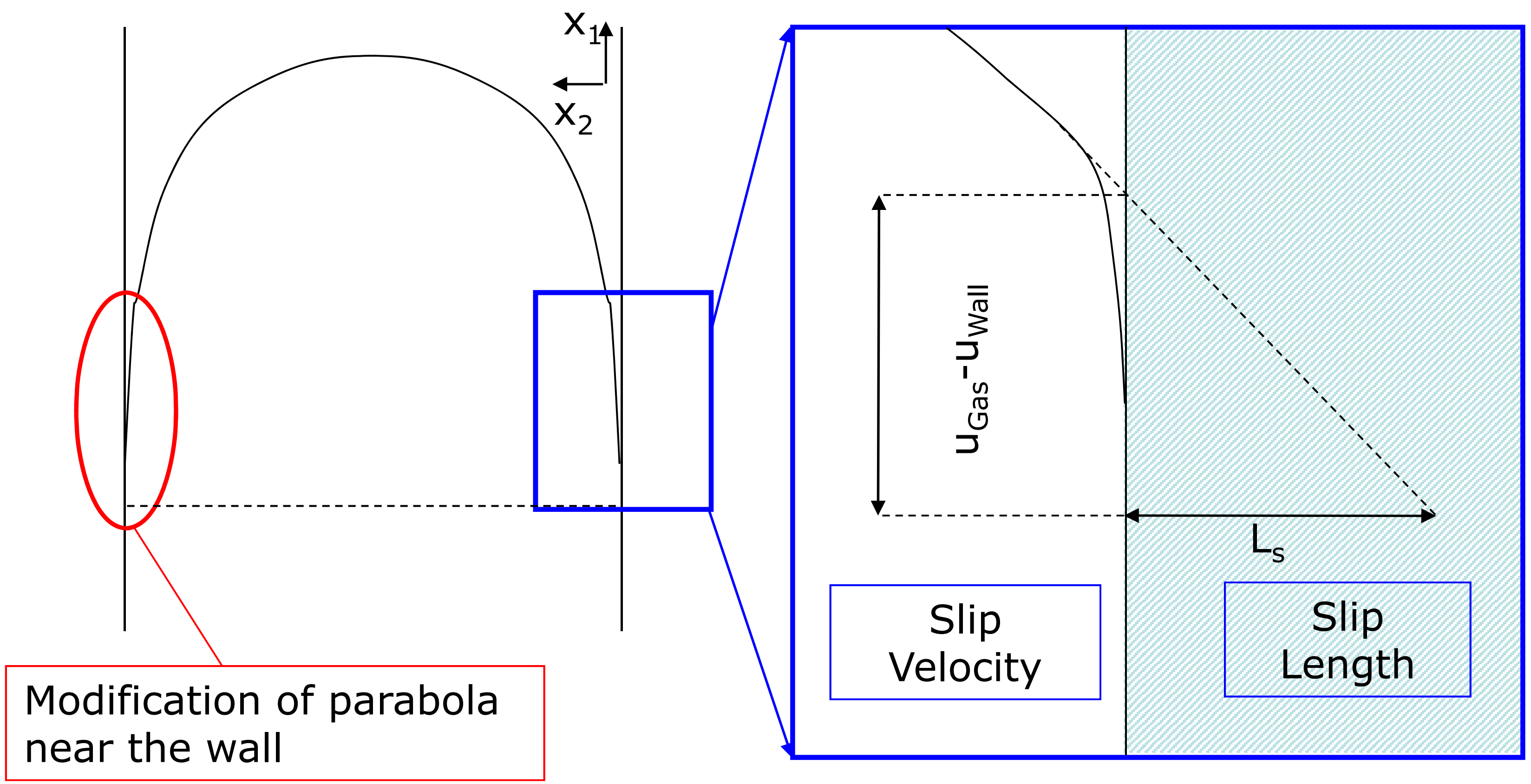
Micro- und macroscopic approach

Characteristic layer thickness





Poiseuille flow of high Knudsen numbers



Molecule number density and statistical filters

Molecule number N

Control volume V_0

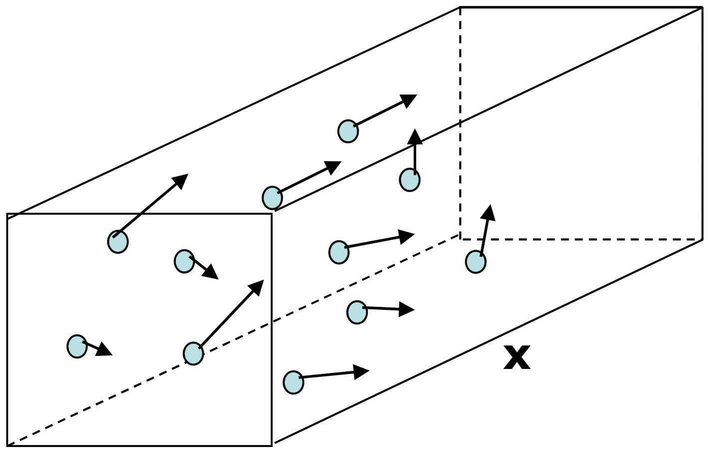
Number density $n = \lim_{V_0 \to 0} \frac{N}{V_0}$

Molecule velocity ξ_i

Mean velocity $\overline{n\xi_i} = \int_{\delta\Psi} \xi_i f_B(t,\vec{x},\vec{\xi})d\psi$

Number-density weighted $u_i = \tilde{\xi}_i = \frac{1}{\overline{n}}\overline{n\xi_i}$

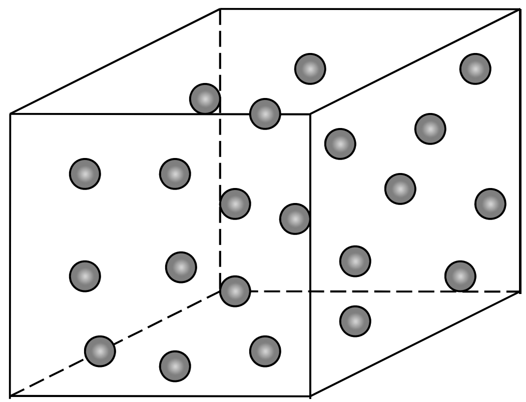
Velocity deviation $\xi_i'' = \xi_i - \tilde{\xi}_i$



Continuity of molecular diffusion

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j}\left(n\xi_j\right) = 0 \quad \Rightarrow \quad \frac{\partial \bar{n}}{\partial t} + \frac{\partial}{\partial x_j}\left(\overline{n\xi_j}\right) = 0$$

$$\Rightarrow \quad \frac{\partial \bar{n}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{n}\bar{\xi}_j\right) = -\frac{\partial}{\partial x_j}\underbrace{\left(\overline{n'\xi_j}\right)}_{-D\frac{\partial \bar{n}}{\partial x_j}}$$



Velocity correlation

$$\overline{n'\xi_j} = -D\frac{\partial \bar{n}}{\partial x_j}$$

$$\overline{n'\xi_i\xi_j} = -D\left(\frac{\partial}{\partial x_j}\overline{n\xi_i} + \frac{\partial}{\partial x_i}\overline{n\xi_j}\right)$$

Analogy of macroscopic values

$$\rho = m\bar{n} \qquad T = \frac{m}{\kappa k_B}\square\xi_k''\xi_k''$$

$$u_i = \tilde{\xi}_i \qquad \mu = m\bar{n}D \quad [\mathrm{Sc}=1]$$

$$p = m\frac{\bar{n}}{\kappa}\square\xi_k''\xi_k'' \qquad = \frac{2}{3}\frac{m}{E\left(d_m^2\right)}\sqrt{\frac{\square\xi_k''\xi_k''}{\kappa\pi^3}}$$

Number-density weighted averaging

Molecule velocity ξ

$$\tilde{\xi}_j = \frac{E(n\xi_j)}{E(n)} = \frac{\overline{n\xi}}{\overline{n}} \qquad \frac{\partial n}{\partial t} + \frac{\partial}{\partial x_j}(n\xi_j) = 0 \quad \Rightarrow \quad \frac{\partial \overline{n}}{\partial t} + \frac{\partial}{\partial x_j}(\overline{n}\tilde{\xi}_j) = 0$$

Momentum transport equation

$$\frac{\partial}{\partial t}(n\xi_i) + \frac{\partial}{\partial x_j}(n\xi_i\xi_j) = 0 \quad \Rightarrow \quad \frac{\partial}{\partial t}(\overline{n}\tilde{\xi}_i) + \frac{\partial}{\partial x_j}(\overline{n}\tilde{\xi}_i\tilde{\xi}_j) = -\frac{\partial}{\partial x_j}\left(\frac{\overline{n}}{\kappa}\widetilde{\xi_i''\xi_j''}\right)$$

$$+\frac{\partial}{\partial x_j}\left[D\overline{n}\left(\frac{\partial\tilde{\xi}_i}{\partial x_j} + \frac{\partial\tilde{\xi}_j}{\partial x_i} - \frac{2}{\kappa}\frac{\partial\tilde{\xi}_k}{\partial x_k}\delta_{ij}\right)\right]$$

$$-\frac{\partial}{\partial x_j}\left[\frac{D^2}{\overline{n}}\left(\frac{\partial\overline{n}}{\partial x_i}\frac{\partial\overline{n}}{\partial x_j} - \frac{1}{\kappa}\frac{\partial\overline{n}}{\partial x_k}\frac{\partial\overline{n}}{\partial x_k}\delta_{ij}\right)\right]$$

(red)	Unsteady
(green)	Convection
(blue)	Source
(yellow)	Diffusion
(orange)	Conversion

Turbulence analogy

$$\zeta = \frac{1}{2}\overline{\xi_k''\xi_k''} \qquad \overline{\xi_i''\xi_j''} = \frac{2}{\kappa}\zeta\delta_{ij} + \underbrace{\frac{D^2}{\bar{n}^2}\left[\frac{\partial\bar{n}}{\partial x_i}\frac{\partial\bar{n}}{\partial x_j} - \frac{1}{\kappa}\frac{\partial\bar{n}}{\partial x_k}\frac{\partial\bar{n}}{\partial x_k}\delta_{ij}\right] - D\left[\frac{\partial\tilde{\xi}_j}{\partial x_i} + \frac{\partial\tilde{\xi}_i}{\partial x_j} - \frac{2}{\kappa}\frac{\partial\tilde{\xi}_k}{\partial x_k}\delta_{ij}\right]}_{\Phi_{ij}}$$

Energy transport equation

$$\frac{\partial}{\partial t}(n\zeta) + \frac{\partial}{\partial x_j}(n\zeta\xi_j) = 0 \Rightarrow \frac{\partial}{\partial t}(\bar{n}\zeta) + \underbrace{\frac{\partial}{\partial x_j}(\bar{n}\zeta\tilde{\xi}_j)}_{\text{convection}} = \underbrace{\frac{\partial}{\partial x_j}\left(D\bar{n}\frac{\kappa+2}{\kappa}\frac{\partial\zeta}{\partial x_j}\right)}_{\text{diffusion}} \underbrace{-\bar{n}\frac{2}{\kappa}\zeta\frac{\partial\tilde{\xi}_k}{\partial x_k}}_{\text{compression}} \underbrace{-\bar{n}\Phi_{ij}\frac{\partial\tilde{\xi}_i}{\partial x_j}}_{\text{dissipation}}$$

$$\underbrace{-\frac{\partial}{\partial x_j}\left[\left(D\bar{n}\frac{\kappa+2}{\kappa}\frac{\partial\tilde{\xi}_i}{\partial x_i} - \frac{1}{\kappa}\frac{D^2}{\bar{n}}\frac{\partial\bar{n}}{\partial x_i}\frac{\partial\bar{n}}{\partial x_i}\right)\frac{D}{\bar{n}}\frac{\partial\bar{n}}{\partial x_j}\right]}_{\text{conversion}}$$

Terms of kinetic dissipation and other energetic production

Depending on velocity and number density gradients

Energy Diffusion without density gradients works with **Pr=<u>κ/(κ +2) = 1/γ < 1</u>** .

Thermodynamic consistence of transport equations

$$de = Tds + pdv$$ Constitutive equation

$$\dot{\zeta} = \dot{e} \quad \Rightarrow \quad \bar{n}T\dot{s} = \bar{n}\dot{\zeta} - \bar{n}\underbrace{p}_{\frac{2}{\kappa}\zeta}\dot{v}$$ Variation energy / intrinsic energy

Entropy increase

$$\Rightarrow \quad \bar{n}T\dot{s} = \underbrace{-\bar{n}\Phi_{ij}\frac{\partial \tilde{\xi}_i}{\partial x_j}}_{\text{dissipation}} + \underbrace{\frac{\partial}{\partial x_j}\left(\frac{1}{\kappa}\frac{D^3}{\bar{n}^2}\frac{\partial \bar{n}}{\partial x_i}\frac{\partial \bar{n}}{\partial x_i}\frac{\partial \bar{n}}{\partial x_j} - D^2\gamma\frac{\partial \tilde{\xi}_i}{\partial x_i}\frac{\partial \bar{n}}{\partial x_j}\right)}_{\text{conversion}} + \underbrace{\frac{\partial}{\partial x_j}\left(D\bar{n}\gamma\frac{\partial \zeta}{\partial x_j}\right)}_{\text{diffusion}}$$

Compression $\rightarrow$ Energy increase Expansion $\rightarrow$ Entropy increase

$$\frac{\partial}{\partial t}(\rho e) + \underbrace{\frac{\partial}{\partial x_j}(\rho e u_j)}_{\text{convection}} = \rho T\dot{s} \underbrace{- \rho e(\gamma - 1)\frac{\partial u_k}{\partial x_k}}_{\text{compression}}$$

Only for γ>1

Boundary conditions

Well-known
wall shear stress

$$\boxed{\tau_w = \frac{\mu}{L_w} = \frac{\rho}{L_w} \cdot \sqrt{2\zeta}\,\frac{\lambda}{3}}$$

$$\tau_w^* = \frac{\tau_w L_w}{\mu_0} = \frac{\rho}{\mu_0}\sqrt{2\zeta}\,\frac{\lambda}{3} = \frac{1}{3}\underbrace{\frac{\rho L_w^2 p_0}{\mu_0^2}}_{\rho^*}\underbrace{\frac{\sqrt{2\zeta}\,\mu_0}{L_w p_0}}_{c^*}\underbrace{\frac{\lambda}{L_w}}_{Kn_w} = \boxed{\frac{Kn_w}{3}\rho^* c^*}$$

Modeled influence of large mean-free-paths on wall shear stress

$$\tau_w = \frac{\mu}{L_w} \quad \Rightarrow \quad \boxed{\tilde{\tau}_w = \frac{\mu}{L_w + \sqrt[3]{L_w \cdot \lambda \cdot \lambda}} = \frac{\mu}{L_w}\left(\frac{1}{1+\left(\lambda / L_w\right)^{2/3}}\right)}$$

$$\tilde{\tau}_w^* = \frac{\tilde{\tau}_w L_w}{\mu_0} = \frac{\mu}{\mu_0}\left(\frac{1}{1+\left(\lambda / L_w\right)^{2/3}}\right) = \boxed{\frac{\tau_w^*}{1+Kn_w^{2/3}}}$$

Computational resuts

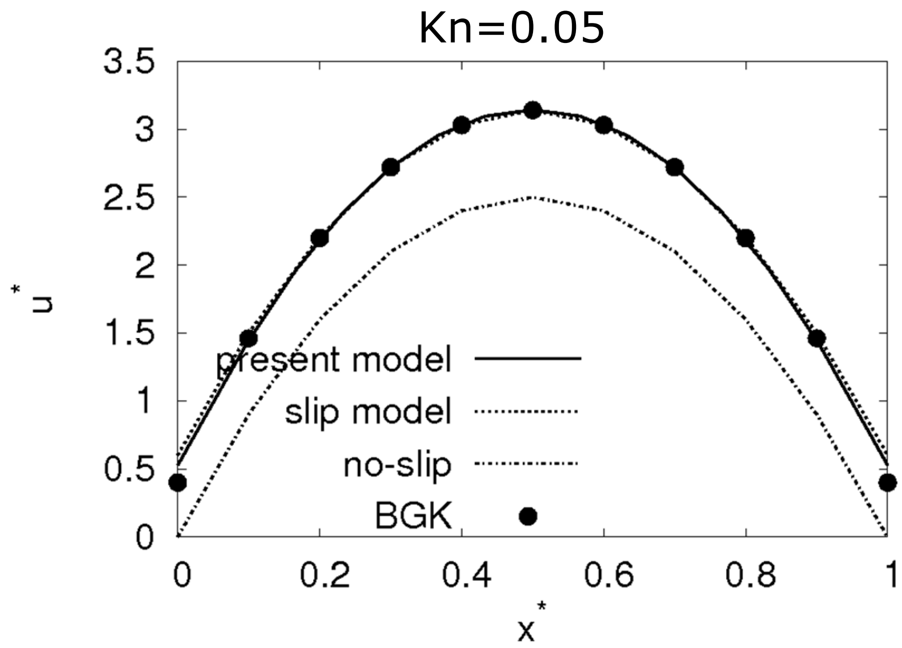
Pressure gradient condition:

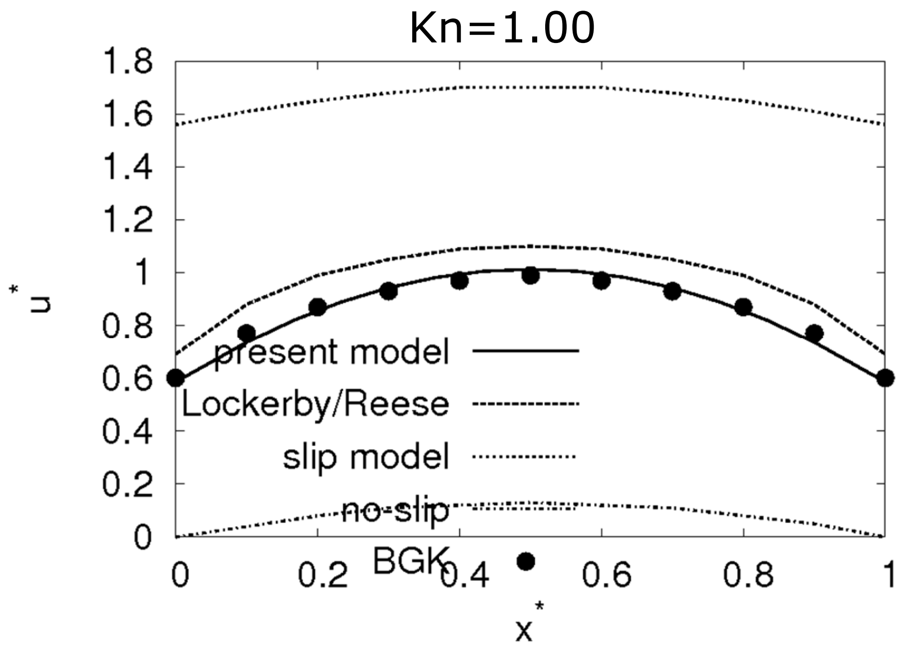
$$\frac{dp^*}{dx^*} = -Kn_0$$

Non-dimensional values:

$$u_i^* = \frac{u_i \mu_0}{H p_0} \qquad p^* = \frac{p}{p_0}$$

$$Kn_0 = \frac{\lambda}{L_0} \qquad x^* = \frac{x}{L_0}$$





Conclusions

Continuity, momentum and ernergy are calculated by transport equations of *number density n* and the *first and second statistical moments of the molecular velocity*. **(→ statistical modelling)**

$$\overline{n\xi_i} = \int_{\delta\Psi} \xi_i f_B(t,\vec{x},\vec{\xi})d\psi \qquad u \equiv \tilde{\xi}_j = \frac{E\left(n\xi_j\right)}{E\left(n\right)} = \frac{\overline{n\xi}}{\overline{n}} \qquad e \equiv \zeta = \frac{1}{2}\overline{\xi_k''\xi_k''}$$

Analogy of macroscopic values

Algebraic model describes scalar diffusion coefficient

(→ diffusion modelling)

$$\mu = \frac{2}{3}\frac{m}{E\left(d_m^2\right)}\sqrt{\frac{\xi_k''\xi_k''}{\kappa\pi^3}}$$

For high Knudsen numbers : Diffusion is described by formulation of dilute gases

(→ slip modelling)

$$\tau^* = \frac{\mu}{L}\frac{1}{1+Kn_w^{2/3}}$$

Many thanks for
your attention!