Rarefied Gas Dynamics: Theory and Applications to Vacuum

Lecture 3: Gas-surface interaction

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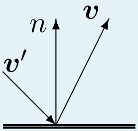
Outline

Diffuse-specular model

Cercignani-Lampis model

Theory based on CL model

General form of boundary condition



$$v_n f(\boldsymbol{v}) = -\int_{v'_n \leq 0} v'_n R(\boldsymbol{v}', \boldsymbol{v}) f(\boldsymbol{v}') \mathrm{d}\boldsymbol{v}' \tag{1}$$

where

$$v_n \geq 0$$

Normalization / impermeability

$$\int_{v_n>0} R(\boldsymbol{v}' \to \boldsymbol{v})\, \mathsf{d}\boldsymbol{v} = 1 \tag{2}$$

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Reciprocity

$$|v_n'| \exp\left(-\frac{mv'^2}{2kT_w}\right) R(\boldsymbol{v}' \to \boldsymbol{v}) \tag{3}$$

$$= |v_n| \exp\left(-\frac{mv^2}{2kT_w}\right) R(-\boldsymbol{v} \to -\boldsymbol{v}') \tag{4}$$

Diffuse-specular scattering

$$R = \alpha_d R_{diff} + (1 - \alpha_d) R_{spec} \tag{5}$$

$$\alpha(\psi) = \frac{J^{incident}(\psi) - J^{reflected}(\psi)}{J^{incident}(\psi) - J^{reflected}_{diff}(\psi)} = \alpha_d \tag{6}$$

for any kind of the property ψ

α_d - unique accommodation coefficient for all properties.

Cerciganani-Lampis model (1971)

$$R_{CL}(\boldsymbol{v}', \boldsymbol{v}) = \frac{v_n}{\pi^2 \alpha_n \, \alpha_t (2 - \alpha_t) v_w^4}$$

$$\times \exp\left\{ -\frac{[\boldsymbol{v}_t - (1 - \alpha_t)\boldsymbol{v}_t']^2}{\alpha_t(2 - \alpha_t)v_w^2} - \frac{v_n^2 + (1 - \alpha_n)v_n'^2}{\alpha_n v_w^2} \right\}$$

$$\times \int_0^{2\pi} \exp\left\{ \frac{2\sqrt{1 - \alpha_n}\, v_n \, v_n' \cos\phi}{\alpha_n v_w^2} \right\} \mathrm{d}\phi \tag{7}$$

$$v_w = \sqrt{\frac{2k_\mathrm{B} T_w}{m}}$$

Cercignani-Lampis model (1971)

$$\psi = mv_t, \quad \alpha(\psi) = \frac{J^{incident}(\psi) - J^{reflected}(\psi)}{J^{incident}(\psi) - J^{reflected}_{diff}(\psi)} = \alpha_t \tag{8}$$

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$0 \leq \alpha_t \leq 2$ tangential momentum accommodation coefficient (TMAC)

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$$\psi = \frac{1}{2} m v_n^2,$$

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$0 \leq \alpha_n \leq 1$ normal energy accommodation coefficient (NEAC)

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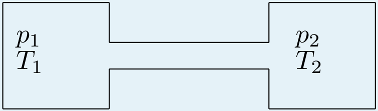
$0 \leq \alpha_n \leq 1$ normal energy accommodation coefficient (NEAC)

$$J^{incident}(\psi) = \int_{v_n<0} |v_n| f(\boldsymbol{v}) \psi(\boldsymbol{v}) \, \mathrm{d}\boldsymbol{v} \tag{10}$$

Eqs.(8) and (9) are NOT dependent on $f(\boldsymbol{v})$ 

Diffuse-specular vs. CL kernel

Scheme of thermo-molecular pressure difference

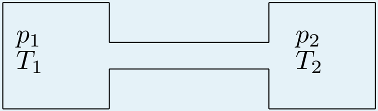


Net flow = 0

$$\frac{p_1}{p_2} = \left(\frac{T_1}{T_2}\right)^{\gamma} \tag{11}$$

Diffuse-specular vs. CL kernel

Scheme of thermo-molecular pressure difference



Net flow $= 0$

$$\frac{p_1}{p_2} = \left(\frac{T_1}{T_2}\right)^{\gamma} \tag{11}$$

Free-molecular regime, diffuse-specular scattering

$$\gamma = \frac{1}{2} \quad \text{for any} \quad \alpha_d \tag{12}$$

Free-molecular regime, experiment

$$0.4 \leq \gamma \leq 0.5 \tag{13}$$

Podgursky, Davis, *J. Phys. Chem.* **65** 1343 (1961) .

Edmonds, Hobson, *J. Vac. Sci. Technol.* **2** 182 (1965).

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Free-molecular regime, CL kernel

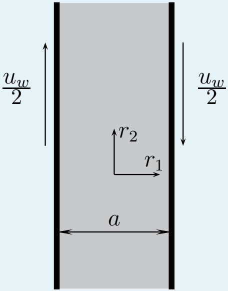
$$0.13 < \gamma < 1 \tag{14}$$

when

$$0.25 \leq \alpha_n \leq 1, \quad \text{and} \quad 0.25 \leq \alpha_t \leq 1.75 \tag{15}$$

Sharipov, *Eur. J. Mech. B/Fluids* **22** (2003)

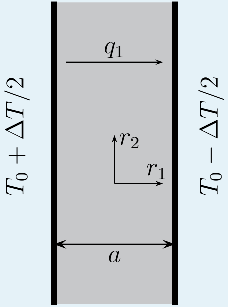
Planar Couette flow, free-molecular regime ($\delta = 0$)



$$P_{12} = -\frac{\alpha_t}{2-\alpha_t}\frac{pu_w}{\sqrt{\pi}v_m}, \quad v_m = \sqrt{\frac{2k_B T}{m}} \tag{16}$$

It depends only on α_t

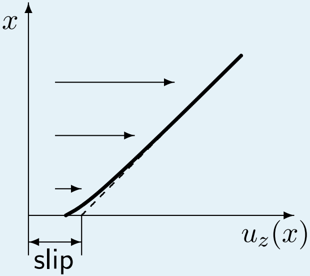
Planar heat transfer, free-molecular regime $\delta = 0$



$$q_1 = -\frac{1}{2}\left[\frac{\alpha_n}{2-\alpha_n} + \frac{\alpha_t(2-\alpha_t)}{2-\alpha_t(2-\alpha_t)}\right]\frac{p\, v_m \Delta T}{\sqrt{\pi} T_0}, \quad \Delta T \ll T_0 \tag{17}$$

It depends on both α_t and α_n

Viscous slip coefficient

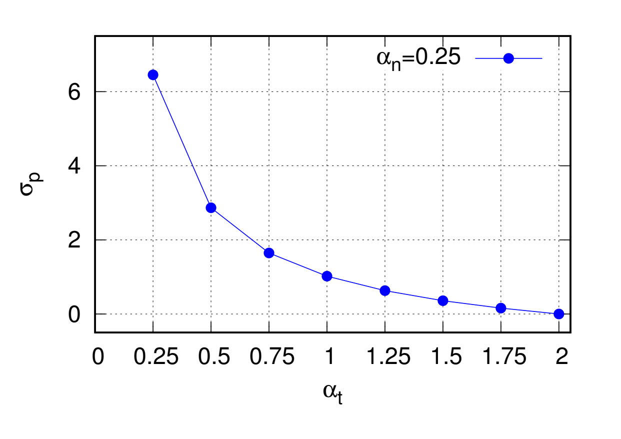


Definition

$$u_z = \sigma_{\mathsf{P}} \ell \frac{\mathsf{d} u_z}{\mathsf{d} x} \quad \text{at} \quad x = 0 \tag{18}$$

σ_{P} - viscous slip coefficient

Viscous slip coefficient σ_P



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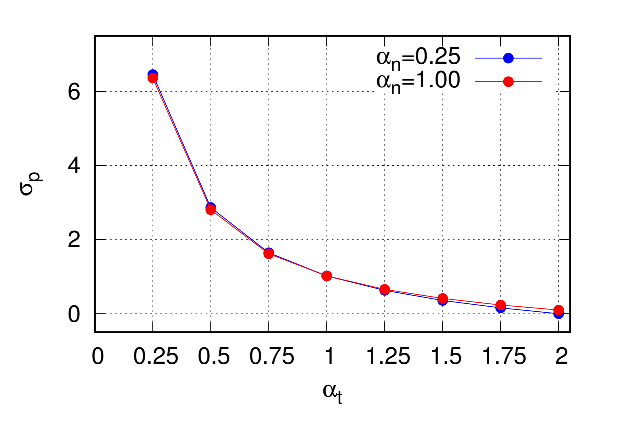
Viscous slip coefficient σ_P



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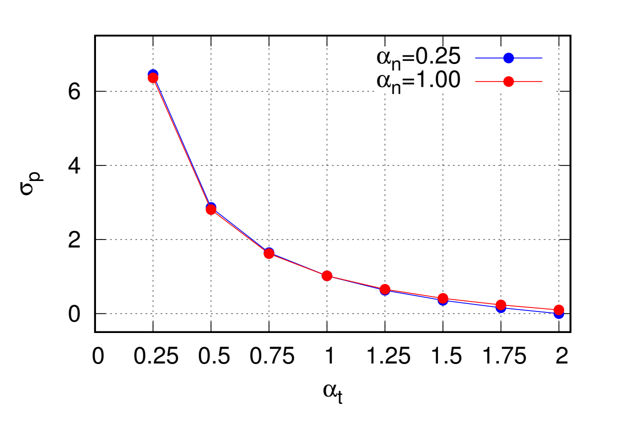
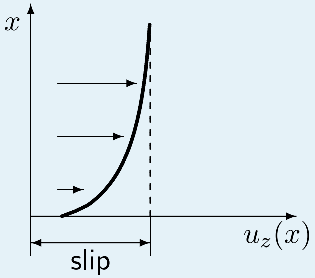
Viscous slip coefficient σ_P



σ_P depends only on α_t

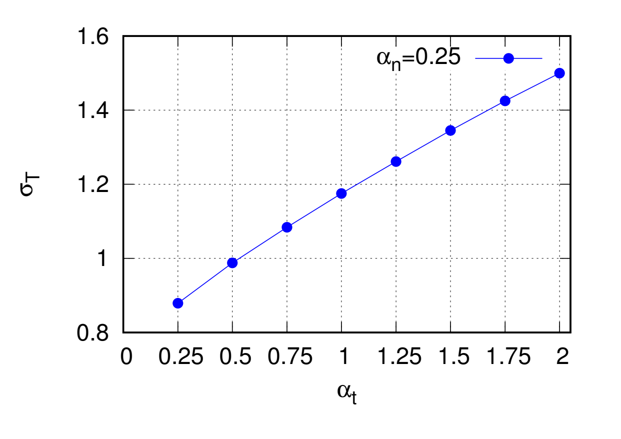
Thermal slip coefficient



Definition

$$u_y = \sigma_{\mathsf{T}} \frac{\mu}{\varrho} \frac{\mathsf{d} \ln T}{\mathsf{d}z} \quad \text{at} \quad x = 0 \tag{19}$$

Thermal slip coefficient σ_T



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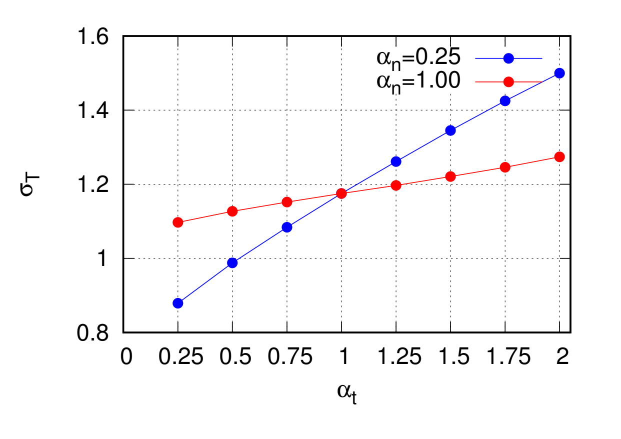

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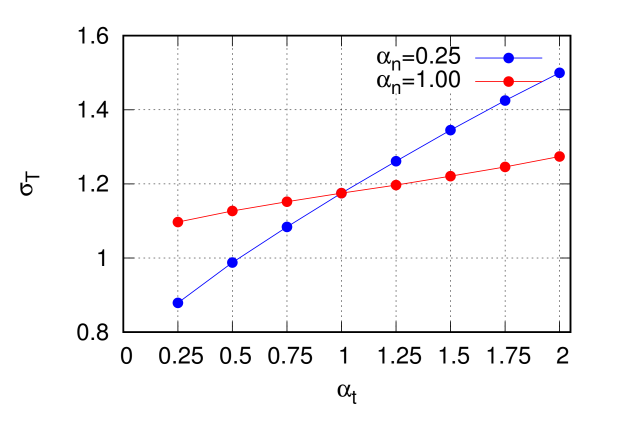
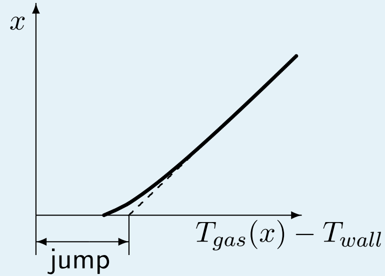


σ_T depends on both α_t and α_n

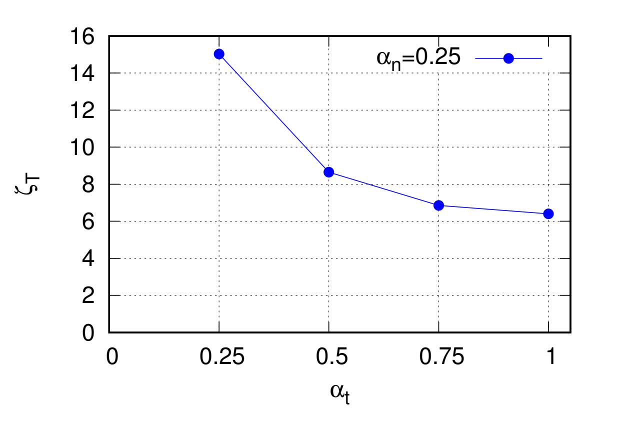
Temperature jump coefficient



Definition

$$T_{gas} - T_{wall} + \zeta_{\mathsf{T}} \ell \frac{\mathsf{d}T}{\mathsf{d}x} \tag{20}$$

Temperature jump coefficient ζ_T



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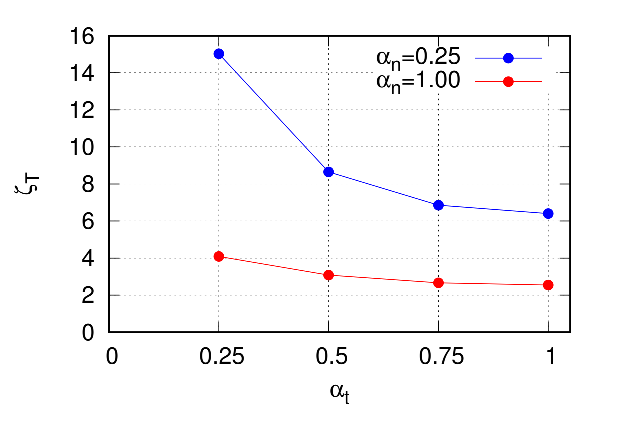

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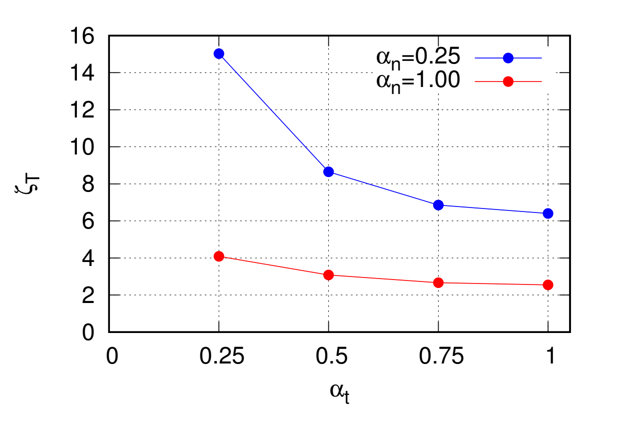
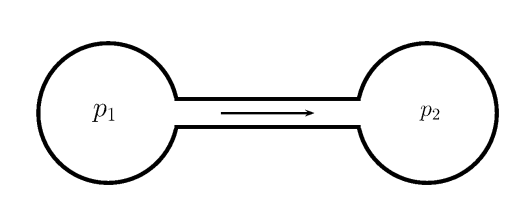
Temperature jump coefficient ζ_T



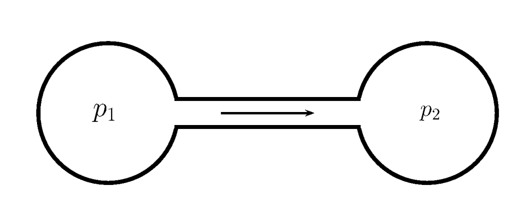
ζ_T depends on both α_t and α_n

Poiseuille flow



$$p_1 > p_2$$

Poiseuille flow

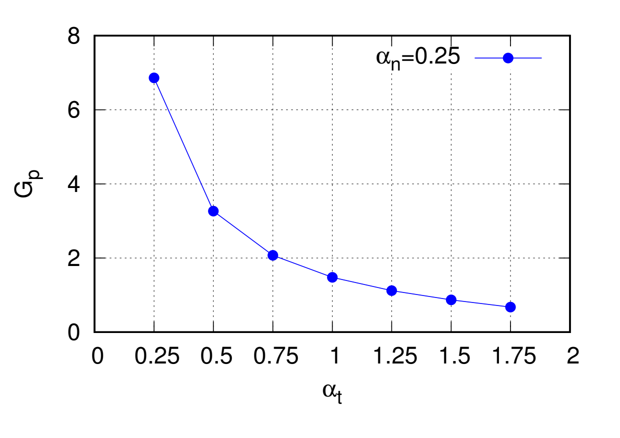


$$p_1 > p_2$$

Definition

$$\dot{M} = \frac{\pi a^3}{v_m} \frac{\mathrm{d}p}{\mathrm{d}x} G_{\mathsf{P}}, \quad G_{\mathsf{P}} = G_{\mathsf{P}}(\delta), \quad \delta = \frac{pa}{\mu v_m} \tag{21}$$

Poiseuille flow through a long circular tube. Free-molecular regime ($\delta = 0.01$)



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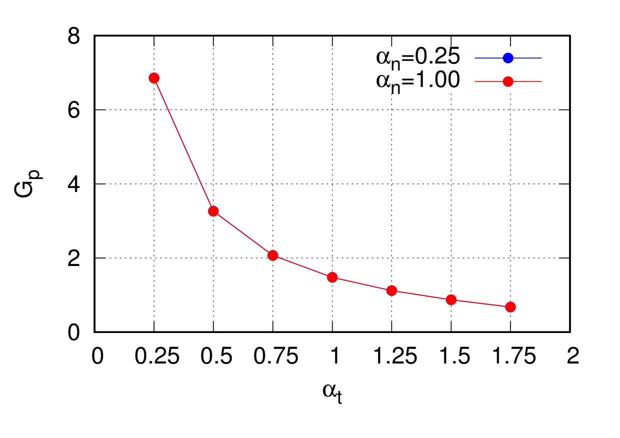

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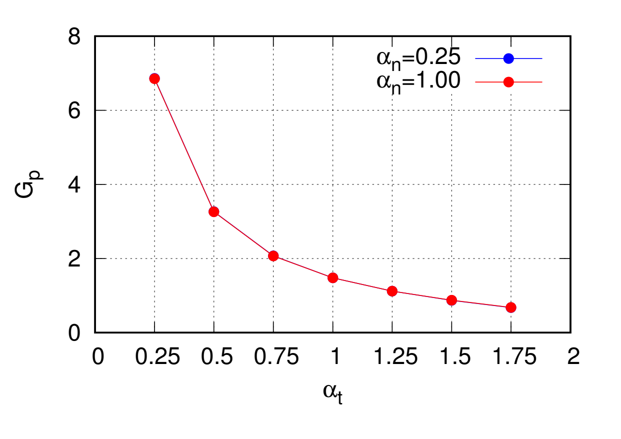
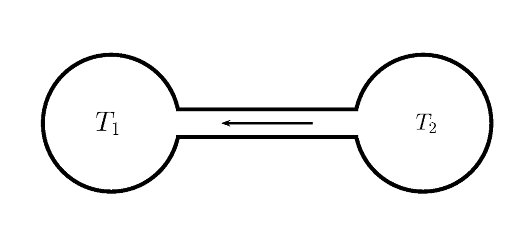


G_p depends only on α_t.

Thermal creep

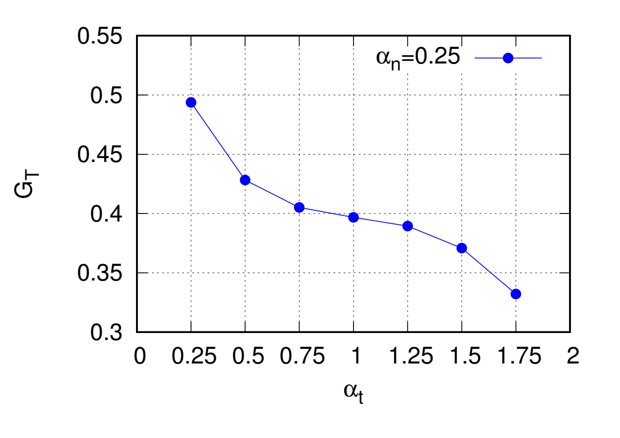


$$T_1 > T_2$$

Definition

$$\dot{M} = \frac{\pi a^3 p}{v_m T} \frac{\mathsf{d}T}{\mathsf{d}x} G_\mathsf{T}, \quad G_\mathsf{T} = G_\mathsf{T}(\delta), \quad \delta = \frac{pa}{\mu v_m} \tag{22}$$

Thermal creep through a long circular tube. Free-molecular regime ($\delta = 0.01$)



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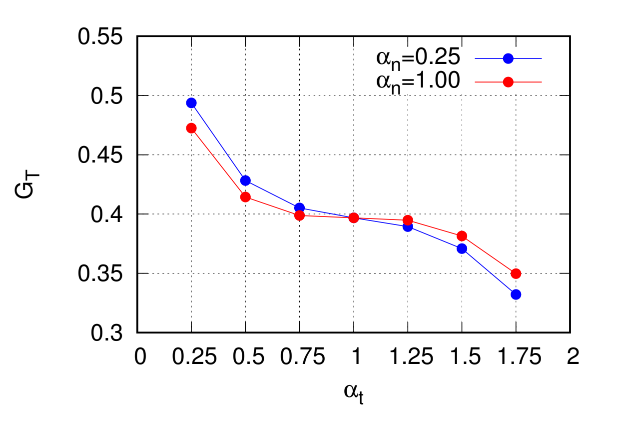

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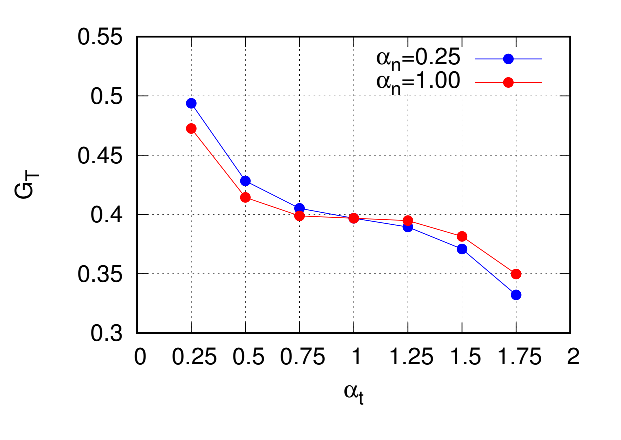
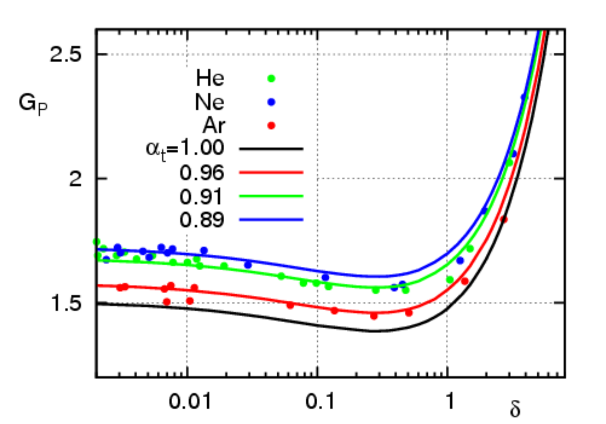


G_T depends on both α_t and α_n

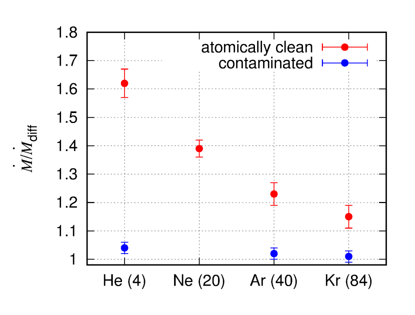
Experiment, Poiseuille flow



Exp.: Porodnov *et al. J. Fluid Mech.* **64**, 417 (1974).
Theory: Sharipov *Eur. J. Mech. B/Fluids* **22**, 145 (2003)

Experiment, free-molecular flow through a tube

Sazhin *et al. J. Vac. Sci. Technol. A* **19**, 2499 (2001).



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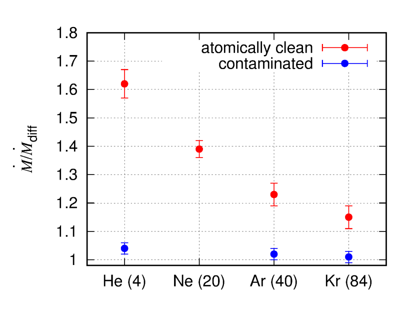
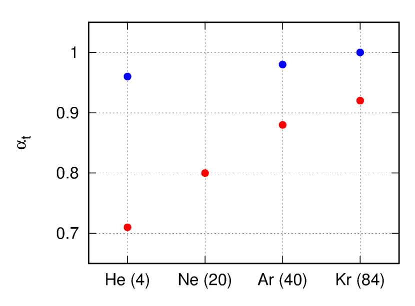
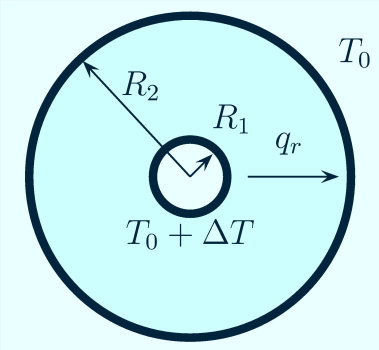




Heat transfer between two cylinders (Pirani sensor)

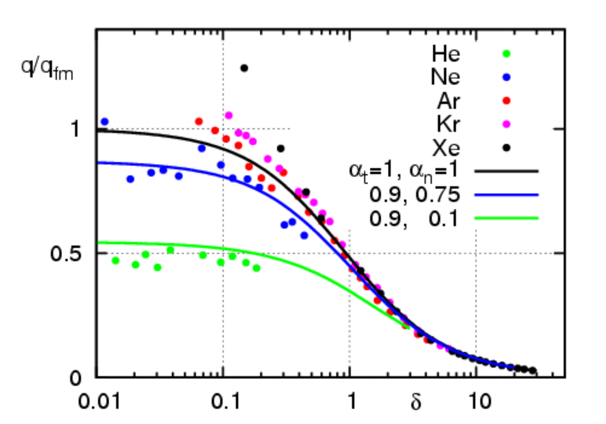


To be calculated:

q_r heat flux

$T(r)$ temperature distribution

Heat transfer between two cylinders



Exp: Semyonov *et al.* *IJHMT* **27**, 1789 (1984).

Theory: Sharipov & Bertoldo, *J. Vac. Sci. Technol. A* **24** 2087 (2006)

Heat transfer between two planar plates. Free-molecular regime, Eq(17)

Gas	Surface	$\tilde{q}$	α_t	α_n
He	SS[a]	0.168 ± 0.010[c]	0.49	0.01
	Al[d]	0.173 ± 0.010	0.51	0.01
	Pl[e]	0.230 ± 0.011	0.68	0.01
	SS-pl[f]	0.132 ± 0.009	0.40	0.01
	Al-pl[g]	0.132 ± 0.009	0.40	0.01
	Pl-pl[h]	0.198 ± 0.010	0.58	0.01
Ar	SS	0.510 ± 0.021	0.95	0.92
	Al	0.521 ± 0.021	1.0	0.93
	Pl	0.521 ± 0.021	1.0	0.93
	SS-pl	0.462 ± 0.019	0.9	0.84
	Al-pl	0.471 ± 0.019	0.9	0.85
	Pl-pl	0.500 ± 0.020	0.95	0.90

[a]Machined stainless steel.
[d]Machined aluminum.
[e]Machined platinum.
[f]Machined stainless steel treated by plasma.
[g]Machined aluminum treated by plasma.
[h]Machined platinum treated by plasma.

Exp.: Trott *et al.*, *Rev. Sci. Instrum* **82** 035120 (2011).

Theory: Sharipov and Moldover, *J. Vac. Sci. Technol. A* **34** (2016).

Experiment values of temperature jump coeff. ζ_T

Gas	Surface	References	ζ_T	α_t	α_n
He	ETP-Cu[a]	[1]	6.67 ± 0.32	0.7	0.037
	ETP-Cu	[2]	6.805 ± 0.022	0.7	0.027
	OFHC-Cu[e]	[3]	7.1 ± 0.2	0.7	0.007
	SS[f]	[4]	7.1 ± 1.3	0.7	0.007
Ar	Al[g]	[5]	2.30 ± 0.25	0.9	0.85
	ETP-Cu	[6]	2.55 ± 0.16	0.9	0.76
	ETP-Cu	[7]	2.62 ± 0.07	0.9	0.74

[a]Electrolytic-tough-pitch copper.
[e]Oxygen-free-high-conductivity copper.
[f]Stainless steel.
[g]Aluminum alloy.

[1] Gavioso et al., *Metrologia* **52**, S274 (2015).
[2] Pitre et al., *Metrologia* **52**, S263 (2015).
[3] Gavioso et al., *Int. J. Thermophys.* **32**, 1339 (2011).
[4] Gavioso et al. *Metrologia* **47**, 387 (2010).
[5] Ewing et al. *Metrologia* **22**, 93 (1986).
[6] Pitre et al. *Int. J. Thermophys.* **32**, 1825 (2011).
[7] de Podesta et al. *Metrologia* **50**, 354 (2013).

Theory: Sharipov and Moldover, *J. Vac. Sci. Technol. A* **34**, 061604 (2016).

CL kernel was used to redefine kelvin (K)

In the past, kelvin was defined *via* the triple point of water.

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Since 2019, the Boltzmann constant is fixed

$$k_{\mathsf{B}} = 1.380649 \times 10^{-23} \mathsf{J/K} \tag{23}$$

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kelvin is now defined *via* the Boltzmann constant

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$$k_{\mathsf{B}} = 1.380649 \times 10^{-23} \mathsf{J/K} \tag{23}$$

kelvin is now defined *via* the Boltzmann constant

Sound speed in dilute gas

k_{B} is extracted from

$$c = \sqrt{\gamma \frac{k_{\mathsf{B}} T}{m}}, \quad \gamma = \frac{c_p}{c_v} = \frac{5}{3} \quad \text{for noble gas} \tag{24}$$

Acoustic resonator

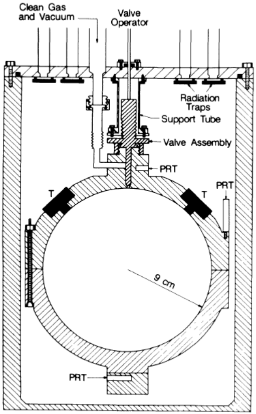

FIG. 1. Cross section of resonator and pressure vessel. The transducer assemblies are indicated by T, and the locations of the capsule thermometers are indicated by PRT. The pressure vessel is immersed in a stirred liquid bath (not shown) which is maintained at T_t.

Moldover *et al. Phys. Rev. Letters* **60**, 249 (1988).

Boundary condition for temperature

$$T_g = T_s + \zeta_{\mathsf{T}} \ell \frac{\mathrm{d}T}{\mathrm{d}x_n} \tag{25}$$

$\ell = \mu v_m / p$ is the equivalent free path of molecules
$\ell \sim 0.1$ μm at $p = 1$ atm.

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$$\zeta_{\mathsf{T}} = \zeta_{\mathsf{T}}(\alpha_t, \alpha_n) \tag{26}$$

ζ_{T} was calculated for helium and the resonator surface applying the CL kernel. (Sharipov & Moldover, *J. Vac. Sci. Technol. A* **34** (2016)).

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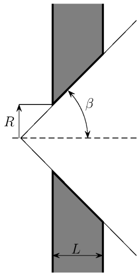
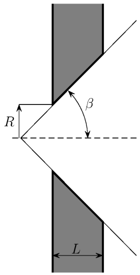
ζ_{T} was calculated for helium and the resonator surface applying the CL kernel. (Sharipov & Moldover, *J. Vac. Sci. Technol. A* **34** (2016)).
As a result, the experimental accuracy of k_{B} was significantly improved.
Then, its value was fixed as $k_{\mathsf{B}} = 1.380649^{-23}$ J/K.

Free-molecular flow though a conical orifice



(a)

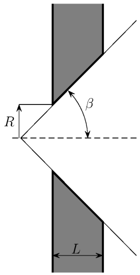
Free-molecular flow though a conical orifice



(a)

Conductance is well known for diffuse gas-surface interaction.

Free-molecular flow though a conical orifice



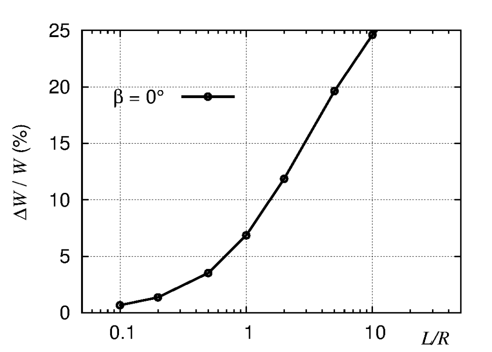
(a)

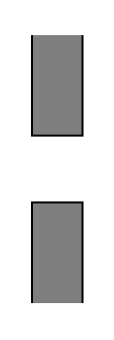
Conductance is well known for diffuse gas-surface interaction.

Conductance for CL model: Sharipov & Barreto, *Vacuum* **121**, 22-25 (2015).

Deviation of W at $\alpha_t = 0.8$ from that at $\alpha_t = 1$

$$\Delta W = W|_{\alpha_t=0.8} - W|_{\alpha_t=1}$$





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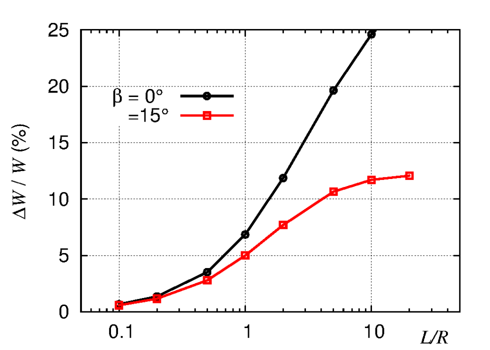

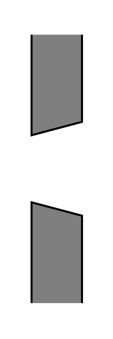

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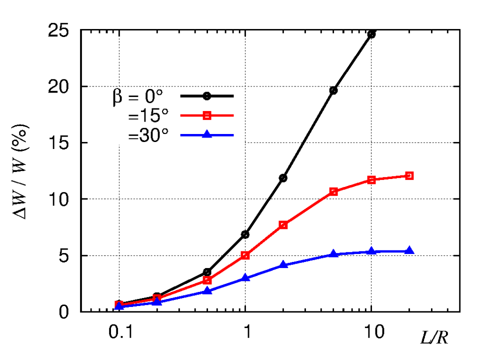

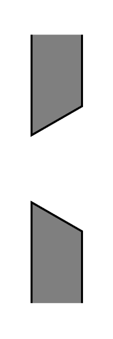

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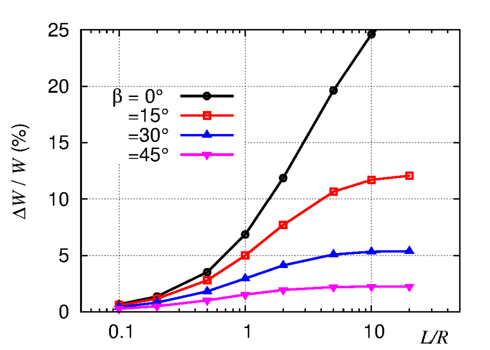

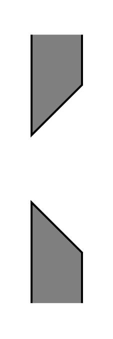

Deviation of W at $\alpha_n = 0.1$ from that at $\alpha_n = 1$

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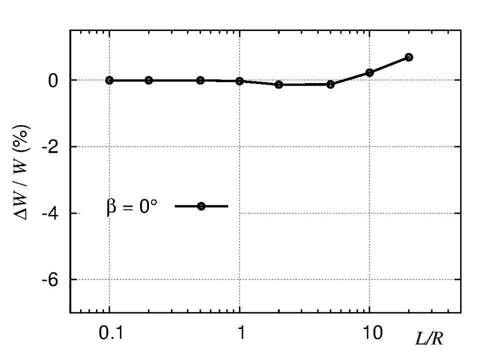

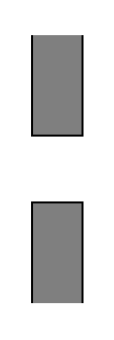

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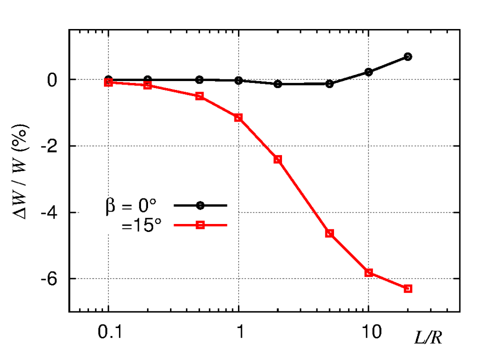

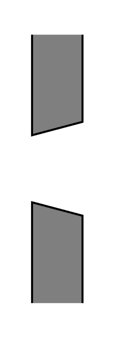

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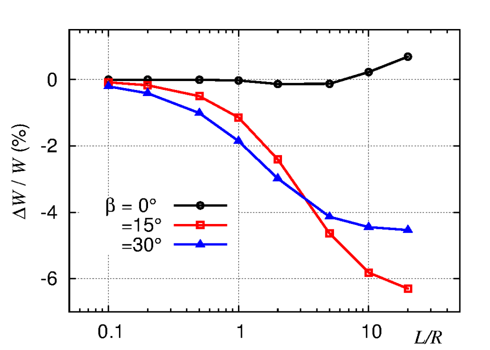

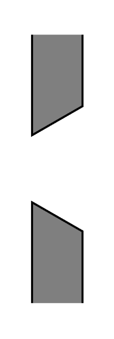

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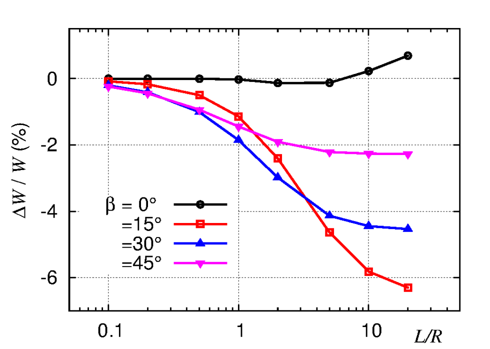
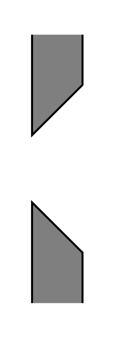
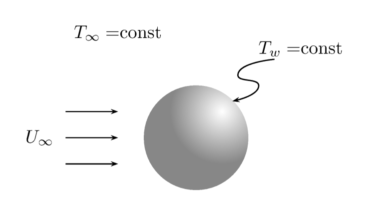




Drag force on a sphere



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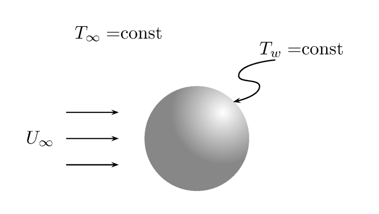
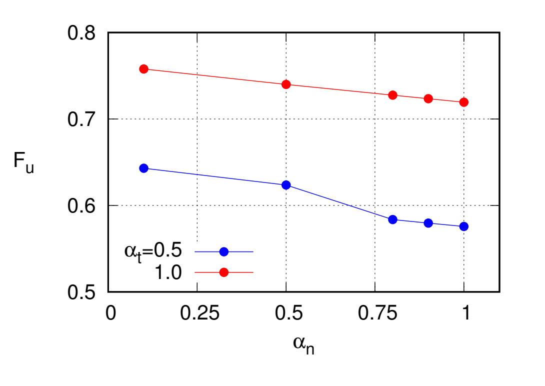


$$F = 4\pi R^2 p_\infty \frac{U_\infty}{v_0} F_u \tag{27}$$

$$\delta = \frac{R}{\ell_0}, \quad U_\infty \ll v_0 \tag{28}$$

$F_u = F_u(\delta, \alpha_t, \alpha_n)$ calculated via the Boltzmann equation (29)

Drag force on a sphere at $\delta = 1$
Kalempa & Sharipov, *J. Fluid Mech.* **900** (2020)



F_u increases by increasing α_t

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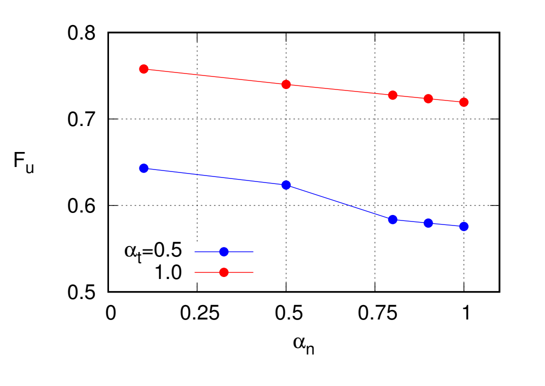
Kalempa & Sharipov, *J. Fluid Mech.* **900** (2020)



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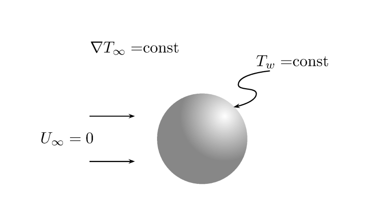
F_u decreases by increasing α_n

Thermophoresis on a sphere at $\delta = 1$



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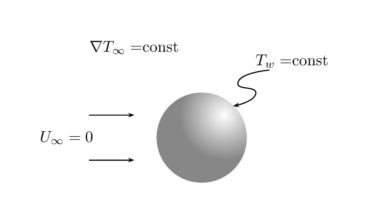
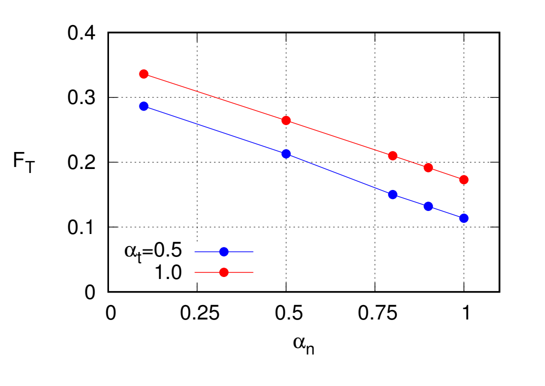


$$F = 4\pi R^2 p_\infty \ell_0 \left(\nabla \ln T\right) F_T \tag{30}$$

$$\delta = \frac{R}{\ell_0}, \quad \ell_0 = \frac{p_\infty}{\mu v_0} \quad v_0 = \sqrt{\frac{2k_\mathrm{B} T_\infty}{m}} \tag{31}$$

$$F_T = F_T(\delta, \alpha_t, \alpha_n) \quad \text{calculated via the Boltzmann equation} \tag{32}$$

Thermophoresis on a sphere at $\delta = 1$
Kalempa & Sharipov, *J. Fluid Mech.* **900** (2020)



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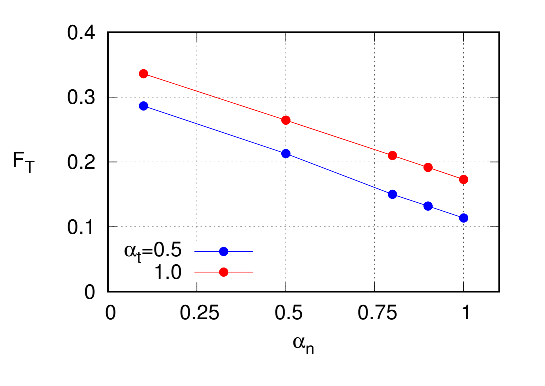
Kalempa & Sharipov, *J. Fluid Mech.* **900** (2020)

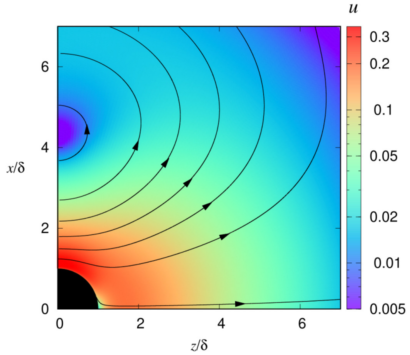


F_T increases by increasing α_t

F_T decreases by increasing α_n

Thermophoresis. Speed u and streamlines at $\delta = 10$ and $\alpha_t = 0.5$. Kalempa & Sharipov, *J. Fluid Mech.* **900** (2020)

. $\alpha_n = 0.1$ $\alpha_n = 1$



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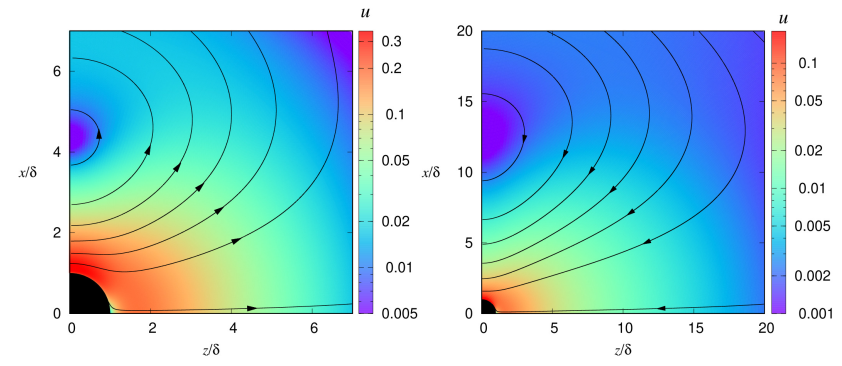
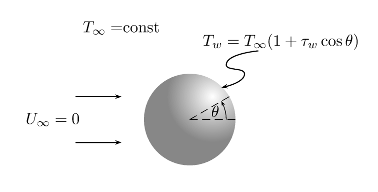


Flow-field changes qualitatively by increasing α_n.

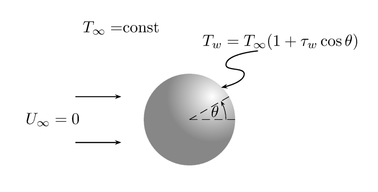
Radiometric force

Radiometer

Radiometric force on a sphere



Radiometric force on a sphere



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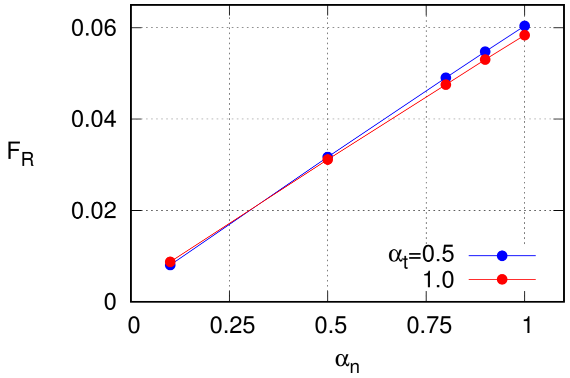
$$\delta = \frac{R}{\ell_0}, \quad \ell_0 = \frac{p_\infty}{\mu v_0} \quad v_0 = \sqrt{\frac{2k_\mathrm{B} T_\infty}{m}} \tag{34}$$

$F_R = F_R(\delta, \alpha_t, \alpha_n)$ calculated via the Boltzmann equation (35)

Radiometric force of sphere at $\delta = 1$
Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)



F_R weakly depends on α_t

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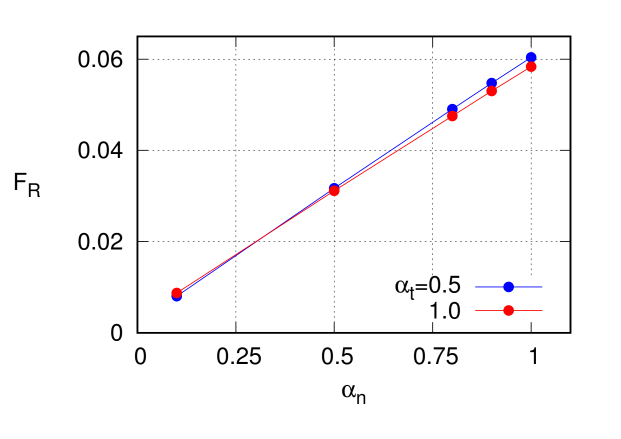
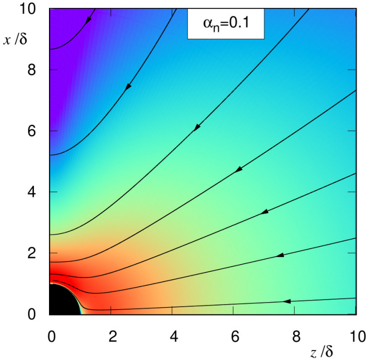
Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)



F_R weakly depends on α_t

F_R increases by increasing α_n

Radiometric force. Speed and streamlines at $\alpha_t = 1$ and $\delta = 0.1$. Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)



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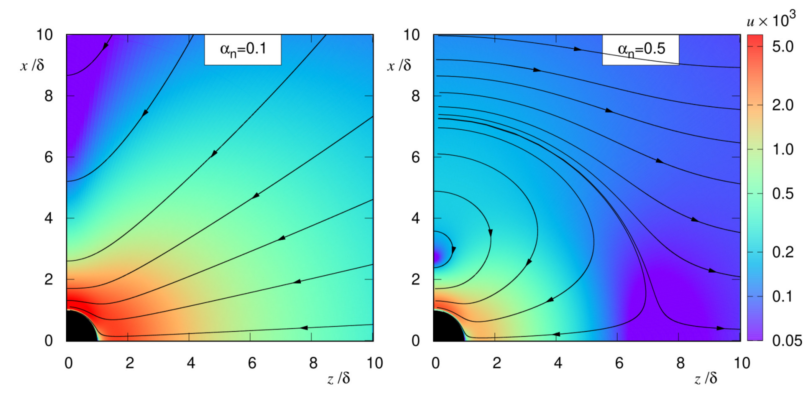
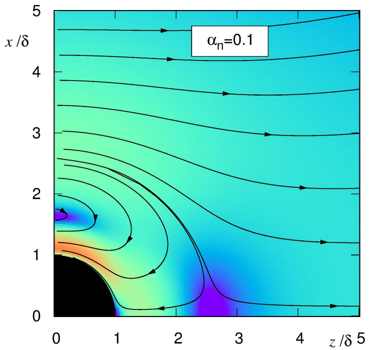


Flow-field changes qualitatively by increasing α_n from 0.1 to 0.5.

Radiometric force. Speed and streamlines at $\alpha_t = 1$ and $\delta = 1$. Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)



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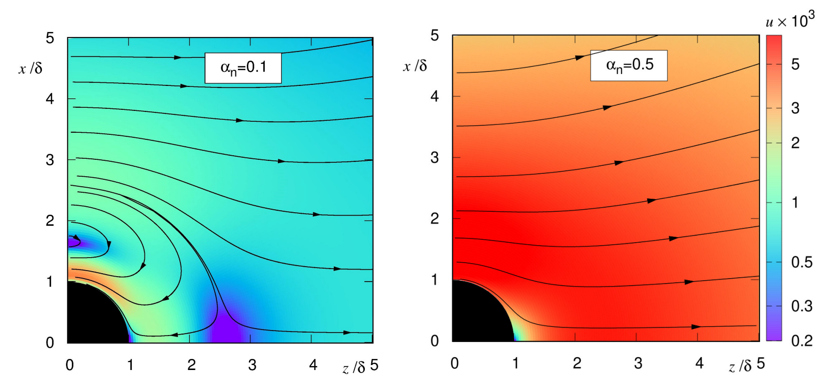
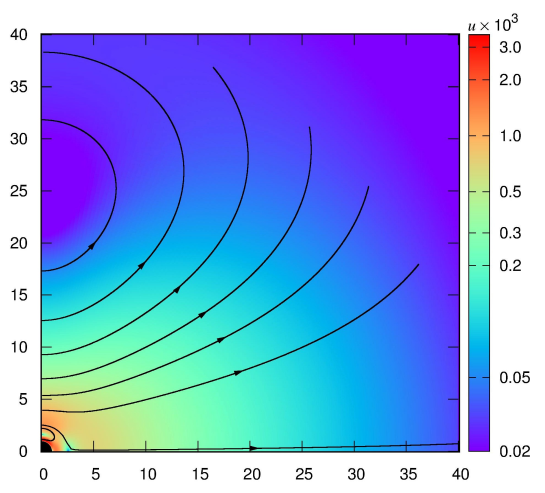


Flow-field changes qualitatively by increasing α_n from 0.1 to 0.5.

Radiometric force. Speed and streamlines at $\alpha_t = 1$, $\alpha_n = 0.1$ and $\delta = 1$. Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)



There are two vortices

Radiometric force. Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)

In the free-molecular regime ($\delta = 0$)

diffuse scattering ($\alpha_t = 1$ and $\alpha_n = 1$):

Radiometric force. Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)

In the free-molecular regime ($\delta = 0$)

diffuse scattering ($\alpha_t = 1$ and $\alpha_n = 1$): the gas is at rest

Radiometric force. Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)

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Radiometric force. Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)

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The same behaviour was detected by Kosuge, Aoki *et al.* in their work:

Phys. Fluids **23** 030603 (2011)

Radiometric force. Kalempa & Sharipov, *Phys. Fluids* **33**, 073602 (2021)

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The same behaviour was detected by Kosuge, Aoki *et al.* in their work:

Phys. Fluids **23** 030603 (2011)

Their conclusion: "For the CL model, ... a steady flow is induced by the nonuniform temperature distribution of the plates even in the free-molecular limit. This is in contrast to the fact that such a flow vanishes in the free-molecular limit for the Maxwell-type model"

THE END
of Lecture 3, Part 1

Thank you for your attention

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