

Solid wall effect on the transport coefficients of gases

FEI Fei, FAN Jing* & JIANG JianZheng

State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

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The diffusion, viscosity and thermal conductivity coefficients of gases between two parallel solid walls have been obtained analytically based on the Green-Kubo relation under a hard-sphere model. They decrease nonlinearly as the Knudsen number defined as the ratio of the mean free path to the wall distance increases. This theoretical prediction was in good agreement by the DSMC results.

transport coefficient, solid wall effect, Green-Kubo relation, Chapman-Enskog theory, DSMC

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Transport phenomenon is an essential feature of fluids [1]. In classical fluid dynamics, the fluxes of mass, momentum, and energy are assumed to be proportional to the gradients of the concentration, velocity and temperature, respectively, i.e.,

$$j = D \frac{dn}{dy}, \quad \tau = \eta \frac{du}{dy}, \quad q = \kappa \frac{dT}{dy}, \quad (1)$$

where n , u and T are the concentration, velocity and temperature, and D , η and κ are the coefficients of diffusion, viscosity and thermal conductivity, respectively, which are phenomenological and usually need to be determined through experimental data.

The Chapman-Enskog (C-E) theory [2] was one of the most important achievements of kinetic studies of gases. It established the relationship between the macroscopic transport coefficients and molecular motion, which has been validated and verified by a number of measured data [1,2]. For hard sphere molecules, according to the C-E theory, the transport coefficients can be written as:

$$\eta = \frac{5}{16} \frac{\sqrt{\pi m k_B T}}{\sigma_T}, \quad \frac{\kappa}{\eta} = \frac{5R}{2(\gamma-1)}, \quad \frac{D}{\eta} = \frac{6}{5\rho}, \quad (2)$$

where m and σ_T are the molecular mass and collision cross section, respectively, k_B is the Boltzmann constant, $R = k_B/m$, and γ is the specific heat ratio.

Another approach to determine transport coefficients originated from Einstein [3]. In the study of the Brownian motion, he demonstrated that the mean square displacement of dust is proportional to the diffusion coefficient of the ambient fluid as time is large enough, that is $\langle \Delta r^2 \rangle = 6Dt$ ($t \rightarrow \infty$). The Einstein relation reveals the relevance between the dissipation and fluctuation of fluids. Later in the 1950s, Kubo et al. [4] developed a linear response theory that extended the Einstein relation. Based on the linear response theory, the transport coefficients have the following expressions that apply to both liquids and gases [4–6]:

$$D = \int_0^\infty \langle v(0)v(t) \rangle dt, \quad (3a)$$

$$\eta = \frac{1}{k_B VT} \int_0^\infty \langle J_{xy}^n(t) J_{xy}^n(0) \rangle dt, \quad (3b)$$

*Corresponding author (email: jfan@imech.ac.cn)

$$\kappa = \frac{1}{k_B VT^2} \int_0^\infty \langle J_y^\kappa(0) J_y^\kappa(t) \rangle dt, \quad (3c)$$

where V and N are the volume and molecular number of a system, respectively, $\langle \rangle$ denotes an ensemble average,

$J_{xy}^n(t) = \sum_{i=1}^N m v_{ix} v_{iy}$ is the microscopic expression of shear

stress flux, and $J_y^\kappa(t) = \sum_{i=1}^N \left[\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right] v_{iy}(t)$ is the microscopic expression of energy flux.

The transport coefficients of gases can be calculated based on the Green-Kubo (G-K) relation (eqs. (3a)–(3c)) using the direct simulation Monte Carlo (DSMC) method [7]. In the DSMC method, gases are represented by a number of model molecules whose trajectories are tracked by a computer. The reliability and accuracy of DSMC were well tested and verified theoretically and experimentally during the past 50 years. An example is shown in Table 1: the transport coefficients of argon gas at the standard conditions obtained by our DSMC calculations are compared to the classical C-E theory (2). The computational domain of DSMC is a square, and the boundary conditions are all periodic. The side length of 10λ is uniformly divided into 50 cells, and the time step $\Delta t = 0.1\tau_c$, where λ and τ_c are the mean free path and mean collision time of argon molecules, respectively. Initially, 50 simulated molecules in an equilibrium state at rest are assigned into each cell following the standard procedures of DSMC. The molecular mass and specific heat ratio of argon are 6.63×10^{-26} kg and $5/3$, respectively [2,7]; for the hard-sphere model, its collision cross section is 4.2×10^{-19} m² [2,7]. Table 1 demonstrates that the DSMC results agree well with the C-E theory, which also verifies our program.

Gas flows in engineering context often involve various interactions between gases and solid walls. They are one of the most important sources of many flow phenomena and patterns. It is easily understood that a solid wall will affect the transport coefficients of gases adjacent to it, because the gas-solid interaction is far different from that between gaseous molecules themselves [8,9]. It is a focus of the present paper to make a quantitative analysis to view such an effect.

Before a further analysis, we firstly perform a preliminary calculation to look at how much solid walls affect the transport coefficients of their neighboring gases. The calculation is similar to Table 1, and the main difference is the upper and lower sides that are replaced by solid walls. In

Table 1 Comparison of diffusion, viscosity and thermal conductivity coefficients of argon gas in the standard conditions obtained by the DSMC calculations based on the G-K relation (3) and the C-E theory (2)

Coefficients	DSMC + G-K relation	C-E theory
D (cm ² /s)	1.43×10^{-1}	1.43×10^{-1}
μ (Ns/m ²)	2.15×10^{-5}	2.12×10^{-5}
κ (J/msK)	1.69×10^{-2}	1.65×10^{-2}

kinetic studies [1–7], a solid wall is often assumed to be fully diffusely reflecting, as does it in this paper. The wall temperatures are 273 K, which is the same as the argon gas. As an example, the procedure to calculate the viscosity coefficient is described as follows:

(1) At the i th time step t_i , $t_i = i\Delta t$ ($i = 1, 2, \dots, N_0$), the microscopic shear stress $J_{xy}^n(t_i) = \sum_{i=1}^N m v_{ix} v_{iy}$ is obtained through a statistical mean of the known velocity components of each simulated molecule;

(2) For certain time interval Δt^* , the autocorrelation function of viscosity at time t_i is obtained by an ensemble averaging, i.e.,

$$\langle J_{xy}^n(t_i) J_{xy}^n(0) \rangle = \frac{1}{N_t + 1} \sum_{k=0}^{N_t} J_{xy}^n(t_i + k\Delta t^*) J_{xy}^n(k\Delta t^*),$$

where $N_t = (N_0 \Delta t - t_i) / \Delta t^*$, and $\Delta t^* = 100\Delta t$ in the present calculations.

(3) Substitute $\langle J_{xy}^n(t_i) J_{xy}^n(0) \rangle$ into the G-K relation (3b), and numerically integrate to obtain the viscosity coefficient.

As shown in Table 2, the transport coefficients of argon gas decrease significantly as the distance between the upper and lower plates L decreases. Compared to the viscosity coefficient without the effect of solid walls 2.15×10^{-5} Ns/m² given in Table 1, μ^* (the superscript * denotes the effect of solid walls) decreases about 2%, 19% and 69% when $L = 100\lambda$, 10λ and λ , respectively.

1 Transport coefficients of gases between two parallel solid walls

The velocity autocorrelation function of gaseous molecules in a system,

$$C^D(t) \equiv \langle v_x(0) v_x(t) \rangle = \frac{1}{N} \sum_{i=1}^N v_{xi}(0) v_{xi}(t), \quad (4)$$

with the initial value

$$C^D(0) = \langle v_x^2 \rangle = k_B T / m = 0.5 c_m^2, \quad (5)$$

where $c_m = \sqrt{2k_B T / m}$ is the most probable speed of thermal motion.

During a time interval Δt , the velocity autocorrelation

Table 2 Transport coefficients of argon in the standard condition between two solid plates at three different distances obtained by the DSMC calculations based on the G-K relation (eqs. (3a)–(3c))

Coefficients	100λ	10λ	λ
D^* (cm ² /s)	1.41×10^{-1}	1.31×10^{-1}	7.65×10^{-2}
μ^* (Ns/m ²)	2.10×10^{-5}	1.74×10^{-5}	6.70×10^{-6}
κ^* (J/msk)	1.60×10^{-2}	1.17×10^{-2}	3.25×10^{-3}

function near a solid wall changes owing to two different mechanisms. One is collisions between the gaseous molecules themselves, and the other is the interaction between the gaseous molecules and walls. Therefore, we have

$$\Delta C^D(t_0) = C^D(t_0 + \Delta t) - C^D(t_0) = \Delta C_{\text{bulk}}^D(t_0) + \Delta C_{\text{wall}}^D(t_0). \quad (6)$$

For the first mechanism, the velocity autocorrelation function decays exponentially due to the collisions between the gaseous molecules themselves [6],

$$\begin{aligned} \Delta C_{\text{bulk}}^D(t_0) &= [C^D(t_0 + \Delta t) - C^D(t_0)]_{\text{bulk}} \\ &= C^D(t_0)e^{-g\Delta t} - C^D(t_0) = -C^D(t_0)g\Delta t, \end{aligned} \quad (7)$$

where $g = C^D(0) / D$.

For the second mechanism, during the interval Δt , all the gaseous molecules in the system can be divided into two parts: one collide with the walls, while the other do not. Consequently,

$$\begin{aligned} C^D(t_0) &= \frac{1}{N} \sum_{i=1}^N v_{xi}(0)v_{xi}(t_0) \\ &= \frac{1}{N} \left(\sum_{i=1}^{N_{\text{wall}}} v_{xi}(0)v_{xi}(t_0) + \sum_{i=N_{\text{wall}}+1}^N v_{xi}(0)v_{xi}(t_0) \right), \end{aligned} \quad (8a)$$

$$\begin{aligned} C^D(t_0 + \Delta t) &= \frac{1}{N} \sum_{i=1}^N v_{xi}(0)v_{xi}(t_0 + \Delta t) \\ &= \frac{1}{N} \left(\sum_{i=1}^{N_{\text{wall}}} v_{xi}(0)v_{xi}(t_0 + \Delta t) \right. \\ &\quad \left. + \sum_{i=N_{\text{wall}}+1}^N v_{xi}(0)v_{xi}(t_0 + \Delta t) \right), \end{aligned} \quad (8b)$$

where N_{wall} is the number of molecules striking the solid walls during the time interval, which can be expressed as follows [1,2,7]:

$$N_{\text{wall}} = 2 \times \frac{1}{4} nc\Delta t = \frac{1}{2} \times \frac{N}{L} \times \frac{2c_m}{\sqrt{\pi}} \Delta t = N \times \frac{c_m \Delta t}{\sqrt{\pi} L}. \quad (9)$$

When we are concerned only the effect of the solid walls, the velocity autocorrelation function of the part of the molecules without colliding with the walls will remain unchanged. Thus,

$$\begin{aligned} \Delta C_{\text{wall}}^D(t_0) &= [C^D(t_0 + \Delta t) - C^D(t_0)]_{\text{wall}} \\ &= \frac{1}{N} \sum_{i=1}^{N_{\text{wall}}} v_{xi}(0)v_{xi}(t_0 + \Delta t) - \frac{1}{N} \sum_{i=1}^{N_{\text{wall}}} v_{xi}(0)v_{xi}(t_0). \end{aligned} \quad (10)$$

According to the diffuse reflection model, the velocities of a molecule before and after hitting a wall are irrelevant, i.e.,

$$\sum_{i=1}^{N_{\text{wall}}} v_{xi}(0)v_{xi}(t_0 + \Delta t) = 0. \quad (11)$$

Substitution of eq. (11) into eq. (10) yields

$$\begin{aligned} \Delta C_{\text{wall}}^D(t_0) &= -\frac{1}{N} \sum_{i=1}^{N_{\text{wall}}} v_{xi}(0)v_{xi}(t_0) \\ &= -\frac{N_{\text{wall}}}{N} \times \frac{1}{N_{\text{wall}}} \sum_{i=1}^{N_{\text{wall}}} v_{xi}(0)v_{xi}(t_0). \end{aligned} \quad (12)$$

At time t_0 , the part of molecules that will collide with the solid walls in the succeeding time interval equals $C^D(t_0)$.

Substituting eq. (9) into eq. (12), we have

$$\Delta C_{\text{wall}}^D(t_0) = -\frac{c_m}{\sqrt{\pi} L} C^D(t_0) \Delta t. \quad (13)$$

Substituting eqs. (13) and (7) into eq. (6), after solving the differential equation, we have

$$C^D(t) = C^D(0) \exp[-(1 + \phi_D)gt], \quad (14)$$

with

$$\phi_D = \frac{c_m}{\sqrt{\pi} L g} = \frac{c_m}{\sqrt{\pi} L} \times \frac{mD}{k_B T} = \frac{3}{4} Kn, \quad (15)$$

where $Kn = \lambda / L$, and $\lambda = 1 / (\sqrt{2} n \sigma_T)$.

Substitution of eq. (14) into eq. (3a) gives rise to the diffusion coefficient between the two parallel solid walls,

$$D^* = \int_0^\infty C^D(t) dt = \frac{C^D(0)}{(1 + \phi_D)g} = \frac{D}{1 + \phi_D}, \quad (16)$$

or

$$\frac{D^*}{D} = \frac{1}{1 + 3Kn/4}. \quad (17)$$

Similarly, the viscosity and thermal conductivity coefficients are obtained, with the details given in Appendix.

$$\frac{\eta^*}{\eta} = \frac{1}{1 + 5\alpha_\eta Kn/4}, \quad (18)$$

$$\frac{\kappa^*}{\kappa} = \frac{1}{1 + 39\alpha_\kappa Kn/16}. \quad (19)$$

As derived in Appendix, the parameters α_η and α_κ satisfy the following equations, respectively:

$$\frac{4}{5\alpha_\eta} + \exp\left[-\left(\frac{4}{5} + Kn\alpha_\eta\right)\right] = 1 - Kn, \quad (20)$$

$$\frac{8}{15\alpha_\kappa} + \exp\left[-\left(\frac{8}{15} + \frac{13}{10}Kn\alpha_\kappa\right)\right] = 1 - \frac{13}{10}Kn. \quad (21)$$

As shown in Figure 1, based upon the exact numerical solutions of eqs. (20) and (21), the relations of α_η and α_κ to

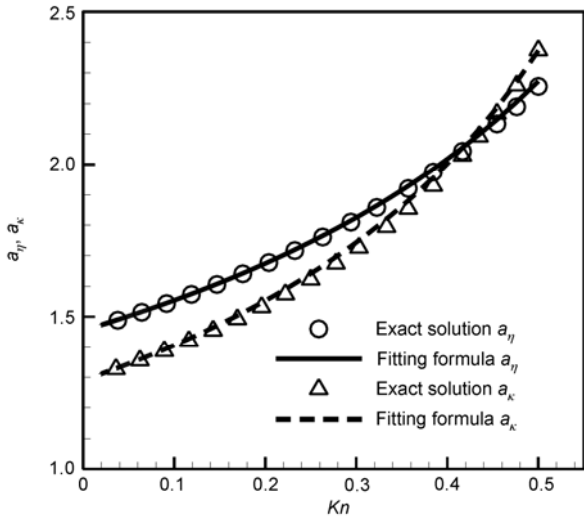


Figure 1 Relations of α_η and α_κ to the Knudsen number.

Kn can be fitted as:

$$\alpha_\eta = \frac{1}{1 - 0.9Kn} + 0.46, \tag{22}$$

$$\alpha_\kappa = \frac{1}{1 - 1.04Kn} + 0.29. \tag{23}$$

2 Results and discussion

The theoretical relations (17), (18) and (19) take into account the effects of the two parallel solid walls on the transport coefficients of gases between them. The first examination employs the case shown in Table 2, which are compared with the present theory in Figure 2. They are in good agreement. They demonstrate that the solid walls result in the nonlinear decrease of transport coefficients as the Knudsen number increases.

Another examination comes from Couette flows and thermal Couette flows. According to eq. (1), the viscosity coefficient is equal to the ratio of the wall shear stress τ_w to $\Delta U_w/L$ in the Couette flow, and the thermal conductivity coefficient is equal to the ratio of the wall heat flux q_w to $\Delta T_w/L$ in the thermal Couette flow, where ΔU_w and ΔT_w are the velocity and temperature differences between the upper and lower plates in these flows, respectively. More computational details on them were described in refs. [10,11], and are not repeated here. As shown in Figures 2(b) and (c), our theories (18) and (19) are in good agreement with the DSMC results based on eq. (1).

Briefly speaking, the physical mechanism for the transport coefficients of gases near a solid wall to decrease lies in the irrelevance of the velocities of a molecules before and

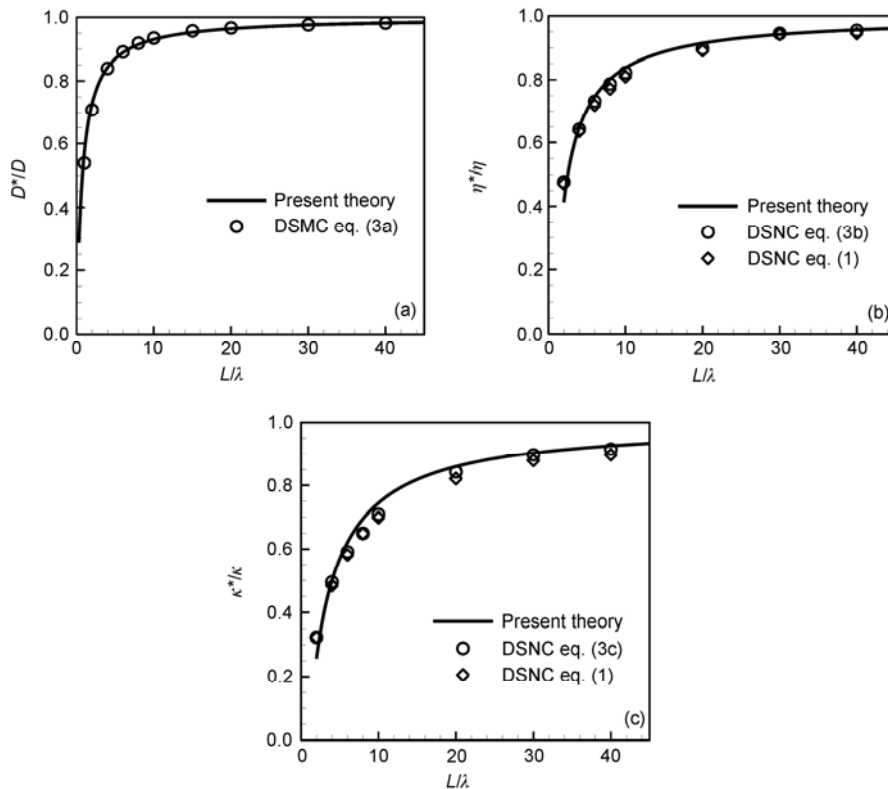


Figure 2 Transport coefficients of argon gas in the standard conditions between two parallel solid walls versus the wall distance. (a) Diffusion; (b) viscosity; (c) thermal conductivity.

after striking the solid wall. For a typical case of gases between two parallel solid walls, our analysis has established a quantitative relationship between the transport coefficients of gases and the Knudsen number, which is helpful to understanding various transport phenomena of gases around solid walls.

Appendix Viscosity and thermal conductivity coefficients of gases between two parallel solid walls

The autocorrelation functions of viscosity and thermal conductivity of gases in a system can be written as:

$$C^\eta(t) = \langle J_{xy}^\eta(0) J_{xy}^\eta(t) \rangle = \left\langle \sum_{i=1}^N m v_{ix} v_{iy}(0) \sum_{i=1}^N m v_{ix} v_{iy}(t) \right\rangle, \quad (a1)$$

$$\begin{aligned} C^\kappa(t) &= \langle J_y^\kappa(0) J_y^\kappa(t) \rangle \\ &= \left\langle \sum_{i=1}^N \left[\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right] v_{iy}(0) \right. \\ &\quad \left. \times \sum_{i=1}^N \left[\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right] v_{iy}(t) \right\rangle, \end{aligned} \quad (a2)$$

with the initial values

$$C^\eta(0) = \left\langle \sum_{i=1}^N m v_{ix} v_{iy}(0) \sum_{i=1}^N m v_{ix} v_{iy}(0) \right\rangle = \frac{1}{4} N m^2 c_m^4, \quad (a3)$$

$$\begin{aligned} C^\kappa(0) &= \left\langle \sum_{i=1}^N \left[\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right] v_{iy}(0) \right. \\ &\quad \left. \times \sum_{i=1}^N \left[\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right] v_{iy}(0) \right\rangle \\ &= \frac{5}{16} N m^2 c_m^6. \end{aligned} \quad (a4)$$

Similar to eq. (6), the autocorrelation functions of viscosity and thermal conductivity changed owing to the two different mechanisms, that is

$$\Delta C^\eta(t_0) = C^\eta(t_0 + \Delta t) - C^\eta(t_0) = \Delta C_{\text{bulk}}^\eta(t_0) + \Delta C_{\text{wall}}^\eta(t_0), \quad (a5)$$

$$\Delta C^\kappa(t_0) = C^\kappa(t_0 + \Delta t) - C^\kappa(t_0) = \Delta C_{\text{bulk}}^\kappa(t_0) + \Delta C_{\text{wall}}^\kappa(t_0). \quad (a6)$$

The first part due to the collisions between molecules themselves decays exponentially [6],

$$\Delta C_{\text{bulk}}^\eta(t_0) = -C^\eta(t_0) \xi \Delta t, \quad (a7)$$

$$\Delta C_{\text{bulk}}^\kappa(t_0) = -C^\kappa(t_0) \chi \Delta t, \quad (a8)$$

where $\xi = \frac{\rho c_m^2}{2\eta}$ and $\chi = \frac{5\rho c_m^4}{8T\kappa}$.

The second part due to the interaction between the gaseous molecules and solid walls can be treated in analogy to the derivations of eqs. (8)–(12), which gives

$$\Delta C_{\text{wall}}^\eta(t_0) = - \left\langle \sum_{i=1}^N m v_{ix} v_{iy}(0) \sum_{j=1}^{N_{\text{wall}}} m v_{jx} v_{jy}(t_0) \right\rangle, \quad (a9)$$

$$\begin{aligned} \Delta C_{\text{wall}}^\kappa(t_0) &= - \left\langle \sum_{i=1}^N \left[\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right] v_{iy}(0) \right. \\ &\quad \left. \times \sum_{j=1}^{N_{\text{wall}}} \left[\frac{1}{2} m v_j^2 - \frac{5}{2} kT \right] v_{jy}(t_0) \right\rangle. \end{aligned} \quad (a10)$$

Eqs. (a9) and (a10) show that there are two factors to affect the autocorrelation functions of viscosity and thermal conductivity. One is the number of molecules striking the walls N_{wall} , and the other is the velocity component normal to the walls. Assume that $\Delta C_{\text{wall}}^\eta(t_0)$ and $\Delta C_{\text{wall}}^\kappa(t_0)$ are both proportional to the autocorrelation functions of the molecules colliding with the walls, that is

$$\frac{\Delta C_{\text{wall}}^\eta(t_0)}{C^\eta(t_0)} = - \frac{N_{\text{wall}} \langle m^2 v_{ix}^2 v_{iy}^2 \rangle_{\text{wall}}}{N \langle m^2 v_{ix}^2 v_{iy}^2 \rangle}, \quad (a11)$$

$$\frac{\Delta C_{\text{wall}}^\kappa(t_0)}{C^\kappa(t_0)} = - \frac{N_{\text{wall}} \left\langle \left(\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right)^2 v_{iy}^2 \right\rangle_{\text{wall}}}{N \left\langle \left(\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right)^2 v_{iy}^2 \right\rangle}. \quad (a12)$$

It is known that the normal velocity distribution of gaseous molecules colliding with a wall [2,7],

$$f_{\text{wall}} = \frac{2v_y}{\pi c_m^4} \exp[-(v_x^2 + v_y^2 + v_z^2)/c_m^2] \quad (a13)$$

and therefore

$$\langle m^2 v_{ix}^2 v_{iy}^2 \rangle_{\text{wall}} = \frac{1}{2} m^2 c_m^4, \quad (a14a)$$

$$\langle m^2 v_{ix}^2 v_{iy}^2 \rangle = \frac{1}{4} m^2 c_m^4, \quad (a14b)$$

$$\left\langle \left(\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right)^2 v_{iy}^2 \right\rangle_{\text{wall}} = \frac{13}{16} m^2 c_m^6, \quad (a14c)$$

$$\left\langle \left(\frac{1}{2} m v_i^2 - \frac{5}{2} kT \right)^2 v_{iy}^2 \right\rangle = \frac{5}{16} m^2 c_m^6. \quad (a14d)$$

Substitution of eqs. (a13) and (a14) into eqs. (a11) and (a12) yields

$$\Delta C_{\text{wall}}^\eta(t_0) = - \frac{2c_m \Delta t}{\sqrt{\pi} L} C^\eta(t_0), \quad (a15)$$

$$\Delta C_{\text{wall}}^\kappa(t_0) = - \frac{13c_m \Delta t}{5\sqrt{\pi} L} C^\kappa(t_0). \quad (a16)$$

Contrary to the present analysis that employs a continuous view to treat the autocorrelation, gaseous molecules always collide with a solid wall discretely. To match the

difference, a modified factor should be introduced:

$$\Delta C_{\text{wall}}^{\eta}(t_0) = -\alpha_{\eta} \frac{2c_m \Delta t}{\sqrt{\pi L}} C^{\eta}(t_0), \tag{a17}$$

$$\Delta C_{\text{wall}}^{\kappa}(t_0) = -\alpha_{\kappa} \frac{13c_m \Delta t}{5\sqrt{\pi L}} C^{\kappa}(t_0). \tag{a18}$$

Similar to the derivations of eq. (14), the autocorrelation functions of viscosity are obtained from eqs. (a5), (a7) and (a17), and eqs. (a6), (a8) and (a18), respectively,

$$C^{\eta}(t) = C^{\eta}(0) \exp[-(1 + \alpha_{\eta} \phi_{\eta}) \xi t], \tag{a19}$$

$$C^{\kappa}(t) = C^{\kappa}(0) \exp[-(1 + \alpha_{\kappa} \phi_{\kappa}) \chi t], \tag{a20}$$

with

$$\phi_{\eta} = \frac{2c_m}{\sqrt{\pi L} \xi} = \frac{2c_m}{\sqrt{\pi L}} \times \frac{2\eta}{\rho c_m^2} = \frac{5}{4} Kn, \tag{a21}$$

$$\phi_{\kappa} = \frac{13c_m}{5\sqrt{\pi L} \chi} = \frac{2c_m}{\sqrt{\pi L}} \times \frac{8\kappa T}{5\rho c_m^4} = \frac{39}{16} Kn. \tag{a22}$$

Substitution of eq. (a19) and (a20) into the G-K relation (3b) and (3c) yields the viscosity coefficient and thermal conductivity of gases between the parallel solids walls as follows:

$$\eta^* = \frac{1}{k_B VT} \int_0^{\infty} C^{\eta}(t) dt = \frac{1}{k_B VT} \frac{C^{\eta}(0)}{(1 + \alpha_{\eta} \phi_{\eta}) \xi} = \frac{\eta}{1 + \alpha_{\eta} \phi_{\eta}}, \tag{a23}$$

$$\begin{aligned} \kappa^* &= \frac{1}{k_B VT^2} \int_0^{\infty} C^{\kappa}(t) dt \\ &= \frac{1}{k_B VT^2} \frac{C^{\kappa}(0)}{(1 + \alpha_{\kappa} \phi_{\kappa}) \chi} = \frac{\kappa}{1 + \alpha_{\kappa} \phi_{\kappa}}, \end{aligned} \tag{a24}$$

or

$$\frac{\eta^*}{\eta} = \frac{1}{1 + 5\alpha_{\eta} Kn/4}, \tag{a25}$$

$$\frac{\kappa^*}{\kappa} = \frac{1}{1 + 39\alpha_{\kappa} Kn/16}. \tag{a26}$$

To determine α_{η} and α_{κ} , let us consider a small time interval $[t_0, t_0 + \tau_c]$, where τ_c is the mean collision time. For the small interval, approximately,

$$\begin{aligned} \Delta C_{\text{wall}}^{\eta}(\tau_c) &= \int_{t_0}^{t_0 + \tau_c} \Delta C_{\text{wall}}^{\eta}(t) dt = \int_{t_0}^{t_0 + \tau_c} -\frac{2c_m}{\sqrt{\pi L}} C^{\eta}(t) dt \\ &\approx \int_{t_0}^{t_0 + \tau_c} -\frac{2c_m}{\sqrt{\pi L}} C^{\eta}(t_0) dt = -\frac{2c_m \tau_c}{\sqrt{\pi L}} C^{\eta}(t_0). \end{aligned} \tag{a27}$$

Meanwhile, according to the continuous model (a17), we have

$$\begin{aligned} \Delta C_{\text{wall}}^{\eta}(\tau_c) &= \int_{t_0}^{t_0 + \tau_c} \Delta C_{\text{wall}}^{\eta}(t) dt = \int_{t_0}^{t_0 + \tau_c} -\frac{2\alpha_{\eta} c_m}{\sqrt{\pi L}} C^{\eta}(t) dt \\ &= \int_{t_0}^{t_0 + \tau_c} -\frac{2\alpha_{\eta} c_m}{\sqrt{\pi L}} C^{\eta}(0) \exp[-(1 + \alpha_{\eta} \phi_{\eta}) \xi t] dt \\ &= -\frac{2\alpha_{\eta} c_m}{\sqrt{\pi L}} \times \frac{C^{\eta}(t_0)}{(1 + \alpha_{\eta} \phi_{\eta}) \xi} \\ &\quad \times \left\{ 1 - \exp[-(1 + \alpha_{\eta} \phi_{\eta}) \xi \tau_c] \right\}. \end{aligned} \tag{a28}$$

Let the right side of eq. (a27) equal that of eq. (a28). Then

$$\frac{4}{5\alpha_{\eta}} + \exp\left[-\frac{4}{5}(1 + \alpha_{\eta} \phi_{\eta})\right] = 1 - \frac{4}{5} \phi_{\eta}. \tag{a29}$$

Substituting eq. (a21) into eq. (a29), we have

$$\frac{4}{5\alpha_{\eta}} + \exp\left[-\left(\frac{4}{5} + Kn\alpha_{\eta}\right)\right] = 1 - Kn. \tag{a30}$$

The equation to determine α_{κ} can be obtained similarly, which is

$$\frac{8}{15\alpha_{\kappa}} + \exp\left[-\left(\frac{8}{15} + \frac{13}{10} Kn\alpha_{\kappa}\right)\right] = 1 - \frac{13}{10} Kn. \tag{a31}$$

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