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# Poiseuille and thermal transpiration flows of a dense 2 gas between two parallel plates

## 3 Masanari Hattori<sup>1,2</sup>†

<sup>1</sup>Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University, Kyoto

5 615-8540, Japan

<sup>6</sup> <sup>2</sup>Research Project of Fluid Science and Engineering, Advanced Engineering Research Center, Kyoto

7 University, Kyoto 615-8540, Japan

8 (Received xx; revised xx; accepted xx)

The Poiseuille and thermal transpiration flows of a dense gas between two parallel plates are 9 investigated on the basis of the Enskog kinetic equation under the diffuse reflection boundary 10 condition. In contrast to the case of an ideal gas, the density and the gradients of pressure 11 and normal stress component in the flow direction are not uniform in the direction normal 12 to the plates for a dense gas. The nonuniform normal stress gradient contributes also to the 13 acceleration or deceleration of the thermal transpiration flow for small Knudsen numbers. 14 The profiles of mass and heat flows as well as the net mass flows are obtained for various 15 Knudsen numbers and ratios of the molecular diameter to the distance of plates. In the 16 analysis of the Poiseuille flow, most characteristics of a force-driven flow with a small force 17 are recovered. However, for the case of a dense gas, differences between the force-driven and 18 the present pressure-driven flows are observed even within the linearized regime for small 19 force and pressure gradient, especially at the microscopic level. The behaviour of velocity 20 distribution functions, in particular, the way of their approach to ones for the Boltzmann 21 equation as the molecular diameter becomes smaller, is clarified. 22

## 23 Key words:

## 24 **1. Introduction**

25 Gases in small systems, such as porous media with small pores and micro and nanodevices,

26 cannot be described properly by conventional fluid dynamics. This is because the mean free

27 path of gas molecules can be comparable to the characteristic length of system so that the

underlying assumption that the gas is very close to the local equilibrium breaks down due

to insufficient intermolecular collisions. The kinetic theory of gases is required to describe their behaviour correctly.

Generally, solution of the Boltzmann equation, the governing equation in the kinetic theory, is a formidable task since besides a time and a position the molecular velocity also plays a role of independent variables and the term representing the effect of intermolecular

† Email address for correspondence: hattori.masanari.4r@kyoto-u.ac.jp

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collisions (the collision integral) is complicated. As for its numerical solution method, both 34 the stochastic direct simulation Monte Carlo (DSMC) method (see, e.g., Bird 1994) and 35 deterministic methods (see, e.g., Dimarco and Pareschi 2014, and the references therein) 36 have been developed continuously from earlier times. Owing to the continuous efforts of many 37 researchers, there is a huge accumulation of results for the flows of ideal gases these days (see, 38 e.g., Sone 2007; Cercignani 1988), which are described by the Boltzmann equation. There 39 40 are a large number of kinetic theory studies on classical problems in fluid dynamics such as the Poiseuille flow, the Couette flow, etc. and those on phenomena peculiar to nonequilibrium 41 gases such as the thermal transpiration flow, which is induced by a temperature gradient along 42 a channel wall in the absence of an external force and a pressure gradient. 43

Meanwhile, when gases become dense, they exhibit non-ideal gas effects. Kinetic theory 44 45 descriptions are available also for this case. The Enskog equation, which can describe effects owing to the finite size of molecules such as the excluded volume, and its extension, the 46 Enskog-Vlasov equation, in which long-range interactions are dealt with by a collective 47 mean field, have been widely accepted. Because the finite size of molecules is taken into 48 account in the Enskog collision integral, it is more complicated than the Boltzmann collision 49 integral. For these equations, the DSMC method was successfully constructed more than 50 two decades ago (Frezzotti 1997; Montanero and Santos 1996). Then, using this method 51 Frezzotti and his co-workers have conducted many studies on liquid-vapor systems based on 52 the Enskog-Vlasov equation (see, e.g., Frezzotti et al 2005, 2019). 53

Besides the liquid-vapor systems, the dense gas effects become relevant in small systems 54 such as nanoporous media, which has been activating the recent kinetic theory studies (see, 55 e.g., Wu et al 2016; Sheng et al 2020; Shan et al 2021). In these studies, the competition 56 of system characteristic length, mean free path and molecular diameter is focused on, and its 57 effect on the phenomena is investigated. This trend may be due to related applications such 58 as shale gas extraction where the pressure is high and the characteristic length is short, and 59 to the fact that deterministic numerical computations are becoming feasible thanks to the 60 extension of fast Fourier spectral method (Filbet et al 2006) to the Enskog equation (Wu et al 61 2015). However, all of the aforementioned works concentrate on the force-driven Poiseuille 62 flow, and currently, no other type of flow seems to be investigated at the same level. 63

Under these circumstances, a time-dependent heat transfer in a dense gas between two 64 parallel plates was investigated in Hattori et al (2022) and interesting features such as the 65 effect of the finite molecular size on the propagation of disturbance were demonstrated. In the 66 present work, we newly consider the thermal transpiration flow as well as the pressure-driven 67 Poiseuille flow of a dense gas between two parallel plates. Analysis of these flows for the case 68 of a rarefied gas is a fundamental problem in the kinetic theory (see, e.g., Cercignani and 69 Daneri 1963; Cercignani and Sernagiotto 1966; Niimi 1968; Sone and Yamamoto 1968; 70 Loyalka 1971; Niimi 1971; Hasegawa and Sone 1988; Ohwada et al 1989; Loyalka and 71 Hamoodi 1990; Kosuge et al 2005; Takata and Funagane 2011; Funagane and Takata 2012). 72 We investigate the counterpart problem for a dense gas. We clarify how finite-size effects of 73 molecules affect these flows, thereby aiming to contribute to increased understanding of the 74 dense gas flow characteristics. 75

The paper is organized as follows. In Section 2, the problem is stated and formulated. 76 The problem is reduced to the spatially one-dimensional boundary-value problems of the 77 linearized Enskog equation for the Poiseuille and thermal transpiration flows, in which the 78 ratio of the mean free path and that of the molecular diameter to the distance of plates 79 are included as nondimensional parameters characterizing the smallness of the system and 80 denseness of the gas. Then, the numerical method is briefly explained in Section 3. The 81 82 method is the iteration based on the integral formulation of the Enskog equation combined with the fast Fourier spectral method for the computation of the collision integral. Section 4 83

- <sup>84</sup> presents the numerical results, where we show the behaviour of the macroscopic quantities
- 85 (gradients of pressure and stress and profiles of density and mass/heat flow) as well as the
- 86 velocity distribution functions (VDFs). Comparison between the force-driven and the present
- 87 pressure-driven Poiseuille flows is also carried out. Section 5 concludes the paper.

## 88 2. Formulation

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## 2.1. Problem and assumptions

Consider a dense gas between two parallel plates at rest located respectively at  $X_1 = \pm D/2$ , 90 where  $X_i$  are the Cartesian coordinates. The two plates are kept at the temperature  $T_w(X_2) =$ 91  $T_0(1 + c_T X_2/D)$  [ $c_T = (D/T_0)(dT_w/dX_2)$  is a constant], and the gas is subject to some 92 pressure gradient in the  $X_2$  direction. We will find a solution that has a pressure gradient 93 constant in the  $X_2$  direction (but nonconstant in the  $X_1$  direction). There is no external force 94 acting on the gas. The average density of the gas over the cross section  $X_2 = 0$  is given by 95  $\rho_0$ . We will investigate the steady behaviour of the gas under the assumptions that (i) the 96 behaviour of the gas can be described by the Enskog equation for hard-sphere molecules 97 with a common diameter  $\sigma$  and mass m with the factor of pair correlation being given 98 according to the Carnahan–Starling equation of state (Carnahan and Starling 1969); (ii) the 99 gas molecules are diffusely reflected on the surface of the plates; (iii) the magnitudes of the 100 applied temperature gradient  $|c_{\rm T}|$  and the pressure gradient  $(D/p_0)|\partial p/\partial X_2|$  are so small 101 that the equation and boundary condition can be linearized around the state that is achieved 102 when both gradients are absent (p is the pressure,  $p_0 = \rho_0 R T_0$  and R is the specific gas 103 constant). 104

105 Some comments on the appropriateness of the linearization assumption (iii) may be in order. At a glance, the assumption might look restrictive to describe the flows well. However, 106 107 (1) the pressure and temperature gradients can in fact be small in small system like micro/nano channels and porous media with small pores; (2) the assumption is actually employed also 108 109 in literatures (see, e.g., any references cited in the third sentence of the fifth paragraph in Section 1); (3) it is reported (see, e.g., Ohwada et al 1989; Sharipov 2003; Ewart et 110 al 2007) that the results for rarefied gases obtained based on the linearized Boltzmann 111 or model kinetic equations agree well with experimental results for a wide range of the 112 Knudsen number. Based on these facts, the assumption is also employed here for the Enskog 113 equation. Phenomena due to nonlinear effects, expected to be significant when the applied 114 pressure or temperature gradient is not small, e.g., nonuniformity of temperature profile in 115 116 pressure-driven flow (Zheng et al 2002), are outside of the scope of the present work.

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## 2.2. Basic equation and boundary condition

Let us denote by X = Dx the position, by  $(2RT_0)^{1/2}\zeta$  the molecular velocity, by  $\rho_0(2RT_0)^{-3/2}\hat{f}$  the VDF of gas molecules, by  $\sigma = D\hat{\sigma}$  the molecular diameter, by  $\rho_0\hat{\rho}$  the density of the gas and by  $T_w = T_0\hat{T}_w$  the temperature of the plates. Then, from assumptions (i) and (ii), the behaviour of the gas is described by the following boundary-value problem for  $\hat{f}$ :

$$\zeta_{1}\frac{\partial \hat{f}}{\partial x_{1}} + \zeta_{2}\frac{\partial \hat{f}}{\partial x_{2}} = \frac{1}{k}\hat{Q}(\hat{f}) \quad \left(-\frac{1-\hat{\sigma}}{2} < x_{1} < \frac{1-\hat{\sigma}}{2}\right), \tag{2.1a}$$
$$\hat{Q}(\hat{f}) = \frac{1}{2\sqrt{2\pi}}\int \left[\hat{Y}\left(\hat{\rho}\left(\boldsymbol{x} + \frac{1}{2}\hat{\sigma}\boldsymbol{k}\right);\eta_{0}\right)\hat{f}(\boldsymbol{x} + \hat{\sigma}\boldsymbol{k},\boldsymbol{\zeta}_{*}')\hat{f}(\boldsymbol{x},\boldsymbol{\zeta}')\right]$$

$$-\hat{Y}\left(\hat{\rho}\left(\boldsymbol{x}-\frac{1}{2}\hat{\sigma}\boldsymbol{k}\right);\eta_{0}\right)\hat{f}(\boldsymbol{x}-\hat{\sigma}\boldsymbol{k},\boldsymbol{\zeta}_{*})\hat{f}(\boldsymbol{x},\boldsymbol{\zeta})\right]$$
$$\times(\hat{\boldsymbol{V}}\cdot\boldsymbol{k})H(\hat{\boldsymbol{V}}\cdot\boldsymbol{k})\mathrm{d}\boldsymbol{k}\mathrm{d}\boldsymbol{\zeta}_{*},\qquad(2.1b)$$

(2.1i)

$$\hat{Y}(\hat{\rho};\eta_0) = \frac{Y(\hat{\rho}\eta_0)}{Y(\eta_0)}, \quad Y(\eta) = \frac{1}{2} \frac{2-\eta}{(1-\eta)^3}, \quad \eta_0 = \frac{(\rho_0/m)\pi\sigma^3}{6}, \tag{2.1c}$$

$$\hat{\rho} = \int \hat{f} d\zeta, \qquad (2.1d)$$

$$\zeta' = \zeta + (\hat{V} \cdot \boldsymbol{k})\boldsymbol{k}, \quad \zeta'_* = \zeta_* - (\hat{V} \cdot \boldsymbol{k})\boldsymbol{k}, \quad \hat{V} = \zeta_* - \zeta, \quad (2.1e)$$

$$k = \frac{\sqrt{\pi}}{2}$$
Kn, Kn  $= \frac{\ell_0}{D}$ ,  $\ell_0 = \left[\sqrt{2\pi\sigma^2}(\rho_0/m)Y(\eta_0)\right]^{-1}$ , (2.1f)

b.c: 
$$\hat{f} = \frac{\hat{\rho}_w}{(\pi \hat{T}_w(x_2))^{3/2}} \exp\left(-\frac{\zeta^2}{\hat{T}_w(x_2)}\right) \quad (\zeta_1 \ge 0, \ x_1 = \mp \frac{1 - \hat{\sigma}}{2}),$$
 (2.1g)

$$\hat{\rho}_w = \mp 2 \sqrt{\frac{\pi}{\hat{T}_w(x_2)}} \int_{\zeta_1 \leq 0} \zeta_1 \hat{f} \mathrm{d}\zeta, \qquad (2.1h)$$

$$\hat{T}_{w}(x_{2}) = 1 + c_{\mathrm{T}}x_{2},$$

with 
$$\frac{1}{1-\hat{\sigma}} \left( \int_{-(1-\hat{\sigma})/2}^{(1-\hat{\sigma})/2} \int \hat{f} d\zeta dx_1 \right) \Big|_{x_2=0} = 1.$$
 (2.1*j*)

Here, k is the unit vector in the direction joining centres of the colliding molecules, H is 118 119 the Heaviside function,  $\eta_0$  and  $\hat{\rho}\eta_0$  are the volume fractions of molecules corresponding to the average and local densities which indicate denseness of the gas and  $\zeta = |\zeta|$ , respectively. 120 The  $\ell_0$  is the mean free path of gas molecules at the equilibrium state at rest with density 121  $\rho_0$  and temperature  $T_0$ . We shall use k in place of the Knudsen number Kn to indicate the 122 degree of gas rarefaction (or smallness of the system). The  $\hat{Q}$  is the Enskog collision integral, 123 and it includes the parts which are quadratic in  $\hat{f}$  like the Boltzmann collision integral. 124 125 However, colliding molecules occupy different positions due to the finite molecular size, and the collision frequency is increased by the function  $\hat{Y}$  that represents an approximate pair 126 correlation function. Hence  $\hat{Q}$  is a five-fold integral that is nonlocal in the position x as well 127 as  $\zeta$  and it is more complicated than the Boltzmann collision integral which is local in x. The 128 integration in  $\hat{Q}$  is carried out over the whole space of  $\zeta_*$  and over the whole direction of k. 129 In the integral, quantities, here the VDF  $\hat{f}(\mathbf{x} \pm \hat{\sigma} \mathbf{k}, \cdot)$  and the density  $\hat{\rho}(\mathbf{x} \pm (1/2)\hat{\sigma} \mathbf{k})$ , are 130 read as zero if their arguments are outside of the domain  $\{z = (z_1, z_2, z_3) ||z_1| \leq (1 - \hat{\sigma})/2\}$ . 131 This rule is also applied to various integrals appearing later. The functional form (2.1c) of 132  $\hat{Y}$  (or Y) corresponds to the Carnahan–Starling equation of state. The centre of a molecule 133 is able to move in the domain with a width  $D - \sigma$ , which is narrower than the gap width 134 D by the molecular diameter  $\sigma$ . This fact is reflected to the collision integral (2.1b) and the 135 condition (2.1i) as well as the equation (2.1a) and the boundary condition (2.1g). 136

Note that the nondimensional numbers k,  $\hat{\sigma}$  and  $\eta_0$  in (2.1) are not independent but are related as (Sheng et al 2020)

$$k = \frac{\sqrt{\pi}}{2}\hat{\sigma}\frac{1}{6\sqrt{2}\eta_0 Y(\eta_0)}.$$
(2.2)

In the present paper, k and  $\hat{\sigma}$ , the degree of gas rarefaction and the molecular size, are considered as the parameters of the problem. We regard the volume fraction of molecules  $\eta_0$ as a function of k and  $\hat{\sigma}$  determined by (2.2). Its plot is shown in figure 1, which implies that

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Figure 1: Plot of the volume fraction of molecules  $\eta_0$  as a function of k for  $\hat{\sigma} = 0.001$ , 0.01, 0.05, 0.1 and 0.15.

the gas becomes more dense with the decrease of k and the increase of  $\hat{\sigma}$  and that it becomes less dense with the increase of k and the decrease of  $\hat{\sigma}$ .

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(k)

## 2.3. Macroscopic quantities

For later convenience, here we introduce the macroscopic variables besides the density given by (2.1*d*). The flow velocity, temperature, pressure, stress tensor and heat-flow vector are given by  $(2RT_0)^{1/2}\hat{v}_i$ ,  $T_0\hat{T}$ ,  $p = p_0\hat{p}$ ,  $p_0\hat{p}_{ij}$  and  $p_0(2RT_0)^{1/2}\hat{q}_i$ , respectively, where  $\hat{v}_i$ ,  $\hat{T}$ ,  $\hat{p}$ ,  $\hat{p}_{ij}$  and  $\hat{q}_i$  are defined as the following moments of the VDF  $\hat{f}$ :

$$\hat{v}_i = \frac{1}{\hat{\rho}} \int \zeta_i \hat{f} d\zeta, \qquad (2.3a)$$

$$\hat{T} = \frac{2}{3\hat{\rho}} \int (\zeta_k - \hat{v}_k)^2 \hat{f} d\zeta, \qquad (2.3b)$$

$$\hat{p} = \hat{\rho}\hat{T} \times \frac{1 + \eta + \eta^2 - \eta^3}{(1 - \eta)^3}, \quad \eta = \hat{\rho}\eta_0,$$
(2.3c)

$$\hat{p}_{ij} = \hat{p}_{ij}^{(k)} + \hat{p}_{ij}^{(v)}, \qquad (2.3d)$$

$$\hat{p}_{ij}^{(k)} = 2 \int (\zeta_i - \hat{v}_i)(\zeta_j - \hat{v}_j)\hat{f} d\zeta,$$
(2.3e)

$$\hat{p}_{ij}^{(\mathbf{v})} = \frac{1}{2\sqrt{2\pi}k} \int \int_0^{\hat{\sigma}} k_i k_j \hat{Y} \left( \hat{\rho} \left( \mathbf{x} + \left( \frac{1}{2} \hat{\sigma} - \hat{\alpha} \right) \mathbf{k} \right); \eta_0 \right) \hat{f}(\mathbf{x} - \hat{\alpha} \mathbf{k}, \boldsymbol{\zeta}_*) \hat{f}(\mathbf{x} + (\hat{\sigma} - \hat{\alpha}) \mathbf{k}, \boldsymbol{\zeta})$$

$$\times (\hat{Y} + \mathbf{k})^2 H(\hat{Y} + \mathbf{k}) d\hat{\alpha} d\mathbf{k} d\boldsymbol{\zeta} d\boldsymbol{\zeta}$$
(2.36)

$$\chi(\mathbf{v} \cdot \mathbf{k}) \Pi(\mathbf{v} \cdot \mathbf{k}) \mathrm{d} \mathbf{u} \mathrm{d} \mathbf{k} \mathrm{d} \boldsymbol{\zeta} \mathrm{d} \boldsymbol{\zeta}_*, \qquad (2.5)$$

$$\hat{q}_{i} = \hat{q}_{i}^{(k)} + \hat{q}_{i}^{(v)}, \qquad (2.3g)$$

$$\hat{q}_{i}^{(k)} = \int (x_{i} - \hat{q}_{i}) \langle x_{i} - \hat{q}_{i} \rangle^{2} \hat{q}_{i} x_{i} \qquad (2.3g)$$

$$\hat{q}_{i}^{(k)} = \int (\zeta_{i} - \hat{v}_{i})(\zeta_{k} - \hat{v}_{k})^{2} \hat{f} d\zeta, \qquad (2.3h)$$

$$\hat{q}_{i}^{(\mathbf{v})} = \frac{1}{4\sqrt{2\pi}k} \int \int_{0}^{\hat{\sigma}} k_{i} \left[ (\zeta_{\ell}' - \hat{v}_{\ell})^{2} - (\zeta_{\ell} - \hat{v}_{\ell})^{2} \right] \\ \times \hat{Y} \left( \hat{\rho} \left( \mathbf{x} + \left( \frac{1}{2} \hat{\sigma} - \hat{\alpha} \right) \mathbf{k} \right); \eta_{0} \right) \hat{f} (\mathbf{x} - \hat{\alpha} \mathbf{k}, \zeta_{*}) \hat{f} (\mathbf{x} + (\hat{\sigma} - \hat{\alpha}) \mathbf{k}, \zeta) \\ \times (\hat{V} \cdot \mathbf{k}) H (\hat{V} \cdot \mathbf{k}) d\hat{\alpha} d\mathbf{k} d\zeta d\zeta_{*}.$$

$$(2.3i)$$

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Equation (2.3*c*) is the Carnahan–Starling equation of state. The stress tensor  $\hat{p}_{ij}$  and the heat-flow vector  $\hat{q}_i$  are given by a sum of two parts respectively. The first part,  $\hat{p}_{ij}^{(k)}$  and  $\hat{q}_i^{(k)}$ , is called the kinetic part and has a familiar form. The second part,  $\hat{p}_{ij}^{(v)}$  and  $\hat{q}_i^{(v)}$ , is called the potential part (Cercignani and Lampis 1988), and it represents the contribution of instantaneous transfers of momentum and energy in binary collisions.

## 2.4. Linearization

Recalling that we consider the situation where the applied temperature and pressure gradients are small [see the assumption (iii) in Section 2.1], within the linearized regime, we can seek the solution  $\hat{f}$  of problem (2.1) as a sum of reference state and perturbation, as follows:

$$\hat{f} = \hat{M}(x_1, \zeta) + \Phi(x_1, x_2, \zeta) + O(\Phi^2) \quad (|\Phi| \ll \hat{M}),$$
(2.4a)

$$\hat{M} = \hat{\rho}_M(x_1)E(\zeta), \quad E(\zeta) = \pi^{-3/2}e^{-\zeta^2},$$
(2.4b)

$$\Phi = c_{\rm T} \left\{ x_2 E(\zeta) \left[ \hat{\omega}_{\rm T}(x_1) + (\zeta^2 - \frac{3}{2}) \hat{\rho}_M(x_1) \right] + \Psi_{\rm T}(x_1, \zeta) \right\} + c_{\rm P} \left[ x_2 E(\zeta) \hat{\omega}_{\rm P}(x_1) + \Psi_{\rm P}(x_1, \zeta) \right].$$
(2.4c)

152 Here, some notes may be in order:

(1) The  $\hat{M}$  is the reference state of the gas that is achieved when both the temperature and 153 pressure gradients are absent, i.e., when there is no driving factor in the system. While for an 154 ideal gas (the case of the Boltzmann equation) this state is a uniform equilibrium state at rest, 155 for a dense gas it is an equilibrium state at rest with a density distribution  $\hat{\rho}_M(x_1)$  varying in 156 the direction normal to the plates [Frezzotti (1997); see also figure 2(a) shown later]. The 157 nonuniformity of the reference density is attributed to the fact that some of intermolecular 158 collisions which detach the molecules from the plates are forbidden near the boundary due 159 to their finite size and accordingly they are pushed to the plates. 160

(2) The  $\Phi$  is a perturbation around the reference state  $\hat{M}$ . In its expression, the subscripts 161 T and P are attached to discriminate the quantities related to the thermal transpiration 162 and Poiseuille flows, respectively. The  $O(\Phi^2)$ -term in (2.4*a*) is the negligible error in the 163 linearized regime. As will be seen later in Section 4, when the molecular size  $\hat{\sigma}$  is finite, the 164 pressure gradient  $\partial_{x_2} \hat{p}$  and the stress gradient  $\partial_{x_2} \hat{p}_{22}$  are not identical, and moreover they are 165 nonuniform in  $x_1$ . Here, the latter is regarded as the driving force for the Poiseuille flow since 166 it is the stress rather than the pressure that has a role of the mechanical surface force. Thus, we 167 require that its average in the  $x_1$  direction to be normalized and zero, in accordance with the 168 nature of the Poiseuille and thermal transpiration flows, respectively. To be more precise, with  $\hat{p}_{22}$  being evaluated with  $\hat{f} = \hat{M} + \Phi$ , we require that  $(1 - \hat{\sigma})^{-1} \int_{-(1 - \hat{\sigma})/2}^{(1 - \hat{\sigma})/2} \partial_{x_2} \hat{p}_{22}|_{c_T = 0} dx_1 = c_P$ 169 170 and  $(1 - \hat{\sigma})^{-1} \int_{-(1 - \hat{\sigma})/2}^{(1 - \hat{\sigma})/2} \partial_{x_2} \hat{p}_{22}|_{c_p=0} dx_1 = 0$  for respective flows, where the constant  $c_p$ 171 represents the magnitude of the averaged stress gradient in the Poiseuille flow  $[|c_P| \ll 1]$ 172 by assumption (iii)]. Since  $\partial_{x_2}\hat{p}_{22} = \partial_{x_2}\hat{p} = \text{const.}$  for the Boltzmann equation,  $c_P$  also corresponds to the magnitude of pressure gradient  $(D/p_0)|dp/dX_2|$  in this case. The parts  $c_P x_2 E(\zeta)\hat{\omega}_P(x_1)$  and  $c_T x_2 E(\zeta)[\hat{\omega}_T(x_1) + (\zeta^2 - \frac{3}{2})\hat{\rho}_M(x_1)]$  are the perturbed Maxwellians 173 174 175 representing the pressure (or stress) and temperature gradients, respectively. Recall that the 176 magnitude of the latter is represented by the coefficient  $c_{\rm T} [= (D/T_0)(dT_w/dX_2)]$ . The  $\Psi_{\rm T}$ 177 and  $\Psi_{\rm P}$ , which are considered to be odd in  $\zeta_2$ , represent the respective flows. 178

(3) The expression (2.4) might look like an arbitrary assumption at a glance, however,
it turns out to be an appropriate form of the solution. It is an extension of the similarity
solution for a rarefied gas [see also, e.g., (2.8) in Takata and Funagane (2011) or (1) in
Ohwada et al (1989)] to the case of the dense gas, where the nonuniformity of densities

(2.6b)

in  $x_1$  is taken into account here due to the finite molecular size both for the reference part 183  $\hat{\rho}_M$  and the perturbed parts  $\hat{\omega}_{T,P}$  [the case of Boltzmann equation corresponds to the case 184  $\hat{\rho}_M(x_1) \equiv 1, \, \hat{\omega}_T(x_1) \equiv -1 \text{ and } \hat{\omega}_P(x_1) \equiv 1].$  To confirm the consistency of (2.4), actually 185 we can proceed in the following way, which is detailed in Appendix A. First, substitute 186  $\hat{f} = \hat{M} = \hat{\rho}_M E$  into the equation (2.1*a*) and the condition for average density (2.1*j*). Then, 187 we reach the system which determines the reference density  $\hat{\rho}_M$  (and  $\hat{M}$  accordingly) with 188 189 no inconsistency. Second, introduce the perturbation  $\Phi$  and substitute  $\hat{f} = \hat{M} + \Phi$  [see also (2.4a) into the equation (2.1a), the boundary condition (2.1g) and the condition for average 190 density (2.1*i*), and neglect the second and higher-order terms of perturbation  $\Phi$  according 191 to the assumption (iii). Then, we are left with the linearized system for the perturbation  $\Phi$ , 192 without any inconsistency. Third, substitute the expression (2.4c) into the system for  $\Phi$  and 193 194 closely examine the resulting expressions, in particular those of the collision integral. Then, we find that the form (2.4c) introduces no inconsistency, and the systems for the perturbed 195 densities  $\hat{\omega}_{T,P}$  and the VDFs  $\Psi_{T,P}$  are accordingly obtained. 196

#### 197 2.4.1. Problems of $\hat{\rho}_M$ , $\hat{\omega}_{T,P}$ and $\Psi_{T,P}$

In (2.4),  $\hat{\rho}_M$ ,  $\hat{\omega}_{T,P}$  and  $\Psi_{T,P}$  are the functions to be determined. Following the above steps explained in the item (3) or Appendix A, we find that the densities  $\hat{\rho}_M$ ,  $\hat{\omega}_T$  and  $\hat{\omega}_P$  satisfy the following integro-differential equations, while the VDFs  $\Psi_T$  and  $\Psi_P$  are the solutions of the following boundary-value problems of the linearized Enskog equation:

$$\frac{d\hat{\rho}_M(x_1)}{dx_1} = J_1[\hat{\rho}_M](x_1) \quad \left(-\frac{1-\hat{\sigma}}{2} < x_1 < \frac{1-\hat{\sigma}}{2}\right), \tag{2.5a}$$

with 
$$\frac{1}{1-\hat{\sigma}} \int_{-(1-\hat{\sigma})/2}^{(1-\hat{\sigma})/2} \hat{\rho}_M(x_1) dx_1 = 1,$$
 (2.5b)

$$\frac{\mathrm{d}\hat{\omega}_{\beta}(x_{1})}{\mathrm{d}x_{1}} = K_{1}[\hat{\omega}_{\beta}, \hat{\rho}_{M}](x_{1}) \quad (-\frac{1-\hat{\sigma}}{2} < x_{1} < \frac{1-\hat{\sigma}}{2}), \tag{2.6a}$$

with

$$K_{2}[\hat{\omega}_{\mathrm{T}}, \hat{\rho}_{M}] = J_{2}[\hat{\rho}_{M}] - 1, \qquad (2.6b)$$
  

$$K_{2}[\hat{\omega}_{\mathrm{P}}, \hat{\rho}_{M}] = 1, \qquad (2.6c)$$

$$\zeta_1 \frac{\partial \Psi_\beta}{\partial x_1} = \frac{1}{k} L(\Psi_\beta) + I_\beta \quad \left(-\frac{1-\hat{\sigma}}{2} < x_1 < \frac{1-\hat{\sigma}}{2}\right), \tag{2.7a}$$

b.c. 
$$\Psi_{\beta} = 0 \quad (\zeta_1 \ge 0, \ x_1 = \mp \frac{1 - \hat{\sigma}}{2}).$$
 (2.7b)

Here,  $\beta = T, P$  in (2.6*a*) and (2.7). The  $J_1, J_2$  and  $J_3$  appearing in (2.5*a*), (2.6*b*) and the definition (2.11a) of the source term  $I_{\rm T}$  shown later are integrals of  $\hat{\rho}_M$  given by (B1) in Appendix B. The  $K_1$ ,  $K_2$  and  $K_3$  appearing in (2.6) and the definition (2.11) of  $I_\beta$  are integrals that are linear with respect to  $\hat{\omega}_{\beta}$  given by (B 3) in Appendix B. The integrals  $J_1$ and  $K_1$  represent the contribution coming from the collision integral  $\hat{Q}$  to the densities  $\hat{\rho}_M$ and  $\hat{\omega}_{\beta}$ . Equations (2.6c) and (2.6b) are the reduced form of aforementioned conditions on the stress gradient  $\partial_{x_2} \hat{p}_{22}$  explained in the item (2) of Section 2.4 (see also the last paragraph in Appendix A.3). By these conditions (2.6c) and (2.6b),  $\hat{\omega}_P$  and  $\hat{\omega}_T$ , which satisfy the same linear equation (2.6a) and are thus equal up to a multiplicative constant, are distinguished each other. The L appearing in (2.7a) is the following Enskog collision operator linearized

around the reference local equilibrium state  $\hat{M}(x_1, \zeta)$ :

$$L(\psi)(\mathbf{x},\boldsymbol{\zeta}) = C(\psi)(\mathbf{x},\boldsymbol{\zeta}) - v(x_{1},\boldsymbol{\zeta})\psi(\mathbf{x},\boldsymbol{\zeta}), \qquad (2.8a)$$

$$C(\psi)(\mathbf{x},\boldsymbol{\zeta}) = \frac{1}{2\sqrt{2\pi}} \int \left\{ \hat{Y} \left( \hat{\rho}_{M} \left( x_{1} + \frac{1}{2} \hat{\sigma} k_{1} \right); \eta_{0} \right) \times \left[ \hat{M}(x_{1} + \hat{\sigma} k_{1},\boldsymbol{\zeta}'_{*})\psi(\mathbf{x},\boldsymbol{\zeta}') + \psi(\mathbf{x} + \hat{\sigma} \mathbf{k},\boldsymbol{\zeta}'_{*})\hat{M}(x_{1},\boldsymbol{\zeta}') \right] \right. \\ \left. - \hat{Y} \left( \hat{\rho}_{M} \left( x_{1} - \frac{1}{2} \hat{\sigma} k_{1} \right); \eta_{0} \right) \psi(\mathbf{x} - \hat{\sigma} \mathbf{k},\boldsymbol{\zeta}_{*})\hat{M}(x_{1},\boldsymbol{\zeta}) + \hat{Y}_{1} \left( \hat{\rho}_{M} \left( x_{1} + \frac{\hat{\sigma}}{2} k_{1} \right); \eta_{0} \right) \langle \psi \rangle \left( \mathbf{x} + \frac{\hat{\sigma}}{2} \mathbf{k} \right) \hat{M}(x_{1} + \hat{\sigma} k_{1},\boldsymbol{\zeta}'_{*}) \hat{M}(x_{1},\boldsymbol{\zeta}') - \hat{Y}_{1} \left( \hat{\rho}_{M} \left( x_{1} - \frac{\hat{\sigma}}{2} k_{1} \right); \eta_{0} \right) \langle \psi \rangle \left( \mathbf{x} - \frac{\hat{\sigma}}{2} \mathbf{k} \right) \hat{M}(x_{1} - \hat{\sigma} k_{1},\boldsymbol{\zeta}_{*}) \hat{M}(x_{1},\boldsymbol{\zeta}) \right] \right\} \\ \left. \times (\hat{\mathbf{V}} \cdot \mathbf{k}) H(\hat{\mathbf{V}} \cdot \mathbf{k}) d\mathbf{k} d\boldsymbol{\zeta}_{*}, \qquad (2.8b)$$

$$v(x_{1},\boldsymbol{\zeta}) = \frac{1}{2\sqrt{2\pi}} \int \hat{Y} \left( \hat{\rho}_{M} \left( x_{1} - \frac{1}{2} \hat{\sigma} k_{1} \right); \eta_{0} \right) d\mathbf{k} d\mathbf{k} \right) \left. \left. \left( \hat{Y} - \hat{Y}_{1} \left( \hat{\varphi}_{M} \left( x_{1} - \frac{1}{2} \hat{\sigma} k_{1} \right); \eta_{0} \right) d\mathbf{k} \right) \right] \right\}$$

$$\times \hat{M}(x_1 - \hat{\sigma}k_1, \boldsymbol{\zeta}_*)(\hat{\boldsymbol{V}} \cdot \boldsymbol{k}) H(\hat{\boldsymbol{V}} \cdot \boldsymbol{k}) \mathrm{d}\boldsymbol{k} \mathrm{d}\boldsymbol{\zeta}_*, \qquad (2.8c)$$

where

$$\hat{Y}_1(r;\eta_0) = \frac{1}{Y(\eta_0)} \frac{\eta_0(5 - 2r\eta_0)}{2(1 - r\eta_0)^4},$$
(2.9a)

$$\langle \psi \rangle (\mathbf{x}) = \int \psi(\mathbf{x}, \zeta) \mathrm{d}\zeta.$$
 (2.9b)

In the decomposition (2.8*a*) of *L*, *C* is the integral operator with some smoothing property in the molecular velocity  $\zeta$  and  $\nu$  is the collision frequency for the reference equilibrium state  $\hat{M}(x_1, \zeta)$ . The  $\hat{Y}_1$  given in (2.9*a*) is just a perturbed part of  $\hat{Y}$  such that

201 
$$\hat{Y}(\hat{\rho}_M + c \langle \psi \rangle; \eta_0) = \hat{Y}(\hat{\rho}_M; \eta_0) + c \langle \psi \rangle \hat{Y}_1(\hat{\rho}_M; \eta_0) + O(c^2) (|c| \ll 1).$$
(2.10)

The source term  $I_{\beta}$  in (2.7*a*) is given in terms of the densities  $\hat{\rho}_M$  and  $\hat{\omega}_{T,P}$  as

$$I_{\rm T}(x_1,\zeta) = -\zeta_2 E(\zeta) \left[ \hat{\rho}_M(x_1)(\zeta^2 - \frac{3}{2}) + \hat{\omega}_{\rm T}(x_1) \right] \\ - \frac{\hat{\sigma} E(\zeta)}{k2\sqrt{2\pi}} \Big\{ \zeta_2 K_3[\hat{\omega}_{\rm T},\hat{\rho}_M](x_1) + J_3[\hat{\rho}_M](x_1,\zeta) \Big\},$$
(2.11*a*)

$$I_{\rm P}(x_1,\zeta) = -\zeta_2 E(\zeta)\hat{\omega}_{\rm P}(x_1) - \frac{\hat{\sigma}}{k2\sqrt{2\pi}}\zeta_2 E(\zeta)K_3[\hat{\omega}_{\rm P},\hat{\rho}_M](x_1).$$
(2.11b)

Thanks to the symmetry of the present problem with respect to the middle of the gap  $x_1 = 0$ , we can seek the VDF  $\Psi_\beta$  with the following property:

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$$\Psi_{\beta}(x_1, \zeta_1, \zeta_2, \zeta_3) = \Psi_{\beta}(-x_1, -\zeta_1, \zeta_2, \zeta_3) \quad (0 < x_1 < \frac{1 - \hat{\sigma}}{2}; \beta = T, P).$$
(2.12)

205 Thus, hereafter, we impose the following condition

206 
$$\Psi_{\beta}(0,\zeta_1,\zeta_2,\zeta_3) = \Psi_{\beta}(0,-\zeta_1,\zeta_2,\zeta_3)$$
(2.13)

on  $\Psi_{\beta}$ , which is obtained by substituting  $x_1 = 0$  into (2.12), and we consider the problem of  $\Psi_{\beta}$  on  $-(1 - \hat{\sigma})/2 < x_1 < 0$ .

## 209 2.4.2. Expressions of macroscopic quantities

Substituting the solution (2.4) into (2.1*d*), (2.3*a*)–(2.3*c*), (2.3*e*), (2.3*f*), (2.3*h*) and (2.3*i*), within negligible error  $O(c_p^2, c_T^2)$  in the linearized regime, we have the following expressions for the macroscopic quantities  $\hat{\rho}$ ,  $\hat{v}_i$ ,  $\hat{T}$ ,  $\hat{p}$ ,  $\hat{p}_{ij}^{(k)}$ ,  $\hat{p}_{ij}^{(v)}$ ,  $\hat{q}_i^{(k)}$  and  $\hat{q}_i^{(v)}$ :

$$\hat{\rho} = \hat{\rho}_M(x_1) + c_T x_2 \hat{\omega}_T(x_1) + c_P x_2 \hat{\omega}_P(x_1) + O(c_P^2, c_T^2),$$
(2.14a)

$$\hat{v}_2 = c_{\rm T} u[\Psi_{\rm T}](x_1) + c_{\rm P} u[\Psi_{\rm P}](x_1) + O(c_{\rm P}^2, c_{\rm T}^2), \qquad (2.14b)$$

$$\hat{v}_1 = O(c_P^2, c_T^2), \quad \hat{v}_3 = O(c_P^2, c_T^2),$$
(2.14c)

$$\hat{T} = 1 + c_{\rm T} x_2 + O(c_{\rm P}^2, c_{\rm T}^2), \qquad (2.14d)$$

$$\hat{p} = \hat{\rho}_M(x_1)S_1(\hat{\rho}_M(x_1)\eta_0) + c_T x_2 G_T(x_1) + c_P x_2 G_P(x_1) + O(c_P^2, c_T^2), \qquad (2.14e)$$

$$\hat{p}_{22}^{(k)} = \hat{\rho}_M(x_1) + c_T x_2 G_{22,T}^{(k)}(x_1) + c_P x_2 G_{22,P}^{(k)}(x_1) + O(c_P^2, c_T^2), \qquad (2.14f)$$

$$\hat{p}_{12}^{(k)} = c_{\rm T} P_{12}^{(k)} [\Psi_{\rm T}](x_1) + c_{\rm P} P_{12}^{(k)} [\Psi_{\rm P}](x_1) + O(c_{\rm P}^2, c_{\rm T}^2), \qquad (2.14g)$$

$$\hat{p}_{11}^{(k)} = \hat{p}_{22}^{(k)} + O(c_{\rm P}^2, c_{\rm T}^2), \qquad \hat{p}_{33}^{(k)} = \hat{p}_{22}^{(k)} + O(c_{\rm P}^2, c_{\rm T}^2),$$

$$\hat{p}_{13}^{(k)} = O(c_{\rm P}^2, c_{\rm T}^2), \quad \hat{p}_{23}^{(k)} = O(c_{\rm P}^2, c_{\rm T}^2),$$
(2.14*h*)

$$\hat{p}_{11}^{(v)} = P_{11,M}^{(v)}(x_1) + c_T x_2 G_{11,T}^{(v)}(x_1) + c_P x_2 G_{11,P}^{(v)}(x_1) + O(c_P^2, c_T^2), \qquad (2.14i)$$

$$\hat{p}_{22}^{(v)} = P_{22,M}^{(v)}(x_1) + c_T x_2 G_{22,T}^{(v)}(x_1) + c_P x_2 G_{22,P}^{(v)}(x_1) + O(c_P^2, c_T^2), \qquad (2.14j)$$

$$\hat{p}_{12}^{(v)} = c_{\rm T} P_{12,\rm T}^{(v)}(x_1) + c_{\rm P} P_{12,\rm P}^{(v)}(x_1) + O(c_{\rm P}^2, c_{\rm T}^2), \qquad (2.14k)$$

$$\hat{p}_{33}^{(v)} = \hat{p}_{22}^{(v)} + O(c_{\rm P}^2, c_{\rm T}^2), \quad \hat{p}_{13}^{(v)} = O(c_{\rm P}^2, c_{\rm T}^2), \quad \hat{p}_{23}^{(v)} = O(c_{\rm P}^2, c_{\rm T}^2), \quad (2.14l)$$

$$\hat{z}_{33}^{(k)} = \hat{z}_{33} O(c_{\rm P}^{(k)}, c_{\rm T}^{(k)}) + \hat{z}_{33} O(c_{\rm P}^2, c_{\rm T}^2), \quad (2.14l)$$

$$\hat{q}_{2}^{(\mathbf{x})} = c_{\mathrm{T}}Q^{(\mathbf{x})}[\Psi_{\mathrm{T}}](x_{1}) + c_{\mathrm{P}}Q^{(\mathbf{x})}[\Psi_{\mathrm{P}}](x_{1}) + O(c_{\mathrm{P}}^{2}, c_{\mathrm{T}}^{2}), \qquad (2.14m)$$

$$\hat{q}_{2}^{(v)} = c_{\rm T} Q_{\rm T}^{(v)}(x_1) + c_{\rm P} Q_{\rm P}^{(v)}(x_1) + O(c_{\rm P}^2, c_{\rm T}^2), \qquad (2.14n)$$

$$\hat{q}_1^{(k)} = O(c_{\rm P}^2, c_{\rm T}^2), \ \hat{q}_3^{(k)} = O(c_{\rm P}^2, c_{\rm T}^2), \ \hat{q}_1^{(v)} = O(c_{\rm P}^2, c_{\rm T}^2), \ \hat{q}_3^{(v)} = O(c_{\rm P}^2, c_{\rm T}^2).$$
 (2.14*o*)

Here,

$$u[\Psi_{\beta}] = \frac{1}{\hat{\rho}_M} \int \zeta_2 \Psi_{\beta} d\zeta, \qquad (2.15a)$$

$$G_{\rm T} = \hat{\rho}_M(x_1)S_1(\hat{\rho}_M(x_1)\eta_0) + \hat{\omega}_{\rm T}(x_1)[S_1(\hat{\rho}_M(x_1)\eta_0) + S_2(\hat{\rho}_M(x_1)\eta_0)], \quad (2.15b)$$
  

$$G_{\rm P} = \hat{\omega}_{\rm P}(x_1)[S_1(\hat{\rho}_M(x_1)\eta_0) + S_2(\hat{\rho}_M(x_1)\eta_0)], \quad (2.15c)$$

$$S_1(r) = \frac{1+r+r^2-r^3}{(1-r)^3}, \quad S_2(r) = \frac{2r(2+2r-r^2)}{(1-r)^4}, \tag{2.15d}$$

$$G_{22,T}^{(k)} = \hat{\rho}_M(x_1) + \hat{\omega}_T(x_1), \quad G_{22,P}^{(k)} = \hat{\omega}_P(x_1), \tag{2.15e}$$

$$P_{12}^{(k)}[\Psi_{\beta}] = 2 \int \zeta_1 \zeta_2 \Psi_{\beta} d\zeta, \qquad (2.15f)$$

$$P_{12,\beta}^{(v)}(x_1) = P_{12,\omega_\beta}^{(v)}(x_1) + P_{12}^{(v)}[\Psi_\beta](x_1), \qquad (2.15g)$$

$$Q^{(k)}[\Psi_{\beta}] = \int \zeta_2 \left(\zeta^2 - \frac{5}{2}\right) \Psi_{\beta} d\zeta, \qquad (2.15h)$$

$$Q_{\rm T}^{(\rm v)} = Q^{(\rm v)}[\Psi_{\rm T}](x_1) - \left\{ u[\Psi_{\rm T}](x_1) + \frac{\hat{\sigma}}{\sqrt{2\pi}} \right\} P_{22,M}^{(\rm v)}(x_1), \tag{2.15i}$$

$$Q_{\rm P}^{(\rm v)} = Q^{(\rm v)}[\Psi_{\rm P}](x_1) - u[\Psi_{\rm P}](x_1)P_{22,M}^{(\rm v)}(x_1).$$
(2.15*j*)

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The expressions of the stress contributions  $P_{11,M}^{(v)}$ ,  $P_{22,M}^{(v)}$ ,  $P_{12,\omega_{\rm T}}^{(v)}$  and  $P_{12,\omega_{\rm P}}^{(v)}$  and the gradients  $G_{11,{\rm T}}^{(v)}$ ,  $G_{11,{\rm P}}^{(v)}$ ,  $G_{22,{\rm T}}^{(v)}$  and  $G_{22,{\rm P}}^{(v)}$ , which are all defined as the integrals of the densities  $\hat{\rho}_M$ ,  $\hat{\omega}_{\rm T}$ 210 211 and  $\hat{\omega}_{\rm P}$ , and those of  $P_{12}^{(v)}[\Psi_{\beta}]$  and  $Q^{(v)}[\Psi_{\beta}]$ , are given in Appendix C. Note that  $c_{\rm T}G_{\rm T}$ ,  $c_{\rm T}(G_{22,\rm T}^{(\rm k)} + G_{22,\rm T}^{(\rm v)})$  and  $c_{\rm T}(Q^{(\rm k)}[\Psi_{\rm T}] + Q_{\rm T}^{(\rm v)})$  [or  $c_{\rm P}G_{\rm P}$ ,  $c_{\rm P}(G_{22,\rm P}^{(\rm k)} + G_{22,\rm P}^{(\rm v)})$  and  $c_{\rm P}(Q^{(\rm k)}[\Psi_{\rm P}] + Q_{\rm T}^{(\rm v)})$  [or  $c_{\rm P}G_{\rm P}$ ,  $c_{\rm P}(G_{22,\rm P}^{(\rm k)} + G_{22,\rm P}^{(\rm v)})$  and  $c_{\rm P}(Q^{(\rm k)}[\Psi_{\rm P}] + Q_{\rm T}^{(\rm v)})$  [or  $c_{\rm P}G_{\rm P}$ ,  $c_{\rm P}(G_{22,\rm P}^{(\rm k)} + G_{22,\rm P}^{(\rm v)})$  and  $c_{\rm P}(Q^{(\rm k)}[\Psi_{\rm P}] + Q_{\rm T}^{(\rm v)})$  [or  $c_{\rm P}G_{\rm P}$ ,  $c_{\rm P}(G_{22,\rm P}^{(\rm k)} + G_{22,\rm P}^{(\rm v)})$  and  $c_{\rm P}(Q^{(\rm k)}[\Psi_{\rm P}] + Q_{\rm T}^{(\rm v)})$  [or  $c_{\rm P}G_{\rm P}$ ,  $c_{\rm P}(G_{22,\rm P}^{(\rm k)} + G_{22,\rm P}^{(\rm v)})$ ] 212 213  $Q_{\rm P}^{(\rm v)}$ ] are the gradient of pressure  $\partial_{x_2}\hat{p}$ , that of (2, 2) component of stress  $\partial_{x_2}\hat{p}_{22}$  and the heat flow  $\hat{q}_2$  for the thermal transpiration (or Poiseuille) flow, respectively within the linearized 214 215 regime [see (2.14e), (2.3d), (2.14f), (2.14j), (2.3g), (2.14m) and (2.14n)]. 216 It is better to mention again the expression (2.14) is obtained within the linearized regime. 217 At a glance, it might look strange that the temperature  $\hat{T}$  is uniform for the Poiseuille flow 218 and that the diagonal kinetic-part stress components are equal to each other [see (2.14d) with 219  $c_{\rm T} = 0$  and (2.14h)]. However, they are justified in the linearized regime, and deviations 220 from them are attributed to nonlinear effects of  $O(c_{\rm P}^2, c_{\rm T}^2)$ , which are neglected here due to 221 the smallness (see also the last sentence in Section 2.1). The  $c_{P,T}$  need to be sufficiently 222 223 small compared to 1, and in addition, compared to the degree of gas rarefaction k when we consider the flow with small k. [Some of the quantities of interest in the present paper are of 224 O(k) rather than O(1).] Although there is no definite threshold, e.g., when  $c_{P,T} \leq 0.001$  or 225  $c_{\rm PT} \lesssim 0.0001$ , the nonlinear effects would likely not be significant for the cases presented 226

in Section 4, where k is in the range [0.05, 10].

228 Also, as in other works based on the linearization assumption, flows between two infinitely wide parallel plates are considered in the present work. Thus, when flows in a finite-length 229 channel with moderate pressure and temperature differences is considered, its length (and 230 the lateral width when a rectangular channel is considered as in experiments) needs to be 231 sufficiently long compared to both its gap width D and the mean free path so that the results 232 for infinitely wide plates give a good description of the flow (Sharipov 1999). Note that, 233 for the case of a rarefied gas, there is an experiment of pressure-driven flow (Ewart et al 234 235 2007) taking this condition carefully into consideration (the channel length and lateral width are respectively about 1000 and 52 times the gap width). There, it is reported that the 236 237 experimental results agree well with numerical results for infinitely wide plates (Loyalka 238 1975) based on a model kinetic equation for a wide range of the Knudsen number about up 239 to 10.

## 240 2.4.3. Net mass flow and conservation law

Denoting by  $\rho_0(2RT_0)^{1/2}D\mathcal{M}$  the net mass flow through the gap per unit time and unit length in  $X_3$ ,  $\mathcal{M}$  is given as

$$\mathcal{M} = c_{\rm T} \mathcal{M}_{\rm T} + c_{\rm P} \mathcal{M}_{\rm P} + O(c_{\rm P}^2, c_{\rm T}^2),$$
 (2.16)

244 where

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$$\mathcal{M}_{\beta} = \int_{-(1-\hat{\sigma})/2}^{(1-\sigma)/2} \hat{\rho}_{M}(s) u[\Psi_{\beta}](s) \mathrm{d}s.$$
(2.17)

Multiplying (2.1a) by  $\zeta_2$  and integrating the result over the whole space of  $\zeta$ , we have the following conservation equation for the momentum in the  $x_2$  direction within the negligible error in the linearized regime:

$$\frac{\partial \hat{p}_{12}}{\partial x_1} + \frac{\partial \hat{p}_{22}}{\partial x_2} = O(c_{\rm P}^2, c_{\rm T}^2).$$
(2.18)

Substituting the expression of  $\hat{p}_{12}$  and  $\hat{p}_{22}$  [see (2.3*d*), (2.14*f*), (2.14*g*), (2.14*j*) and (2.14*k*)] into (2.18) and integrating the result over  $[-(1 - \hat{\sigma})/2, x_1]$  with respect to  $x_1$ , we obtain

$$c_{\rm T}S_{\rm T}(x_1) + c_{\rm P}S_{\rm P}(x_1) = O(c_{\rm P}^2, c_{\rm T}^2),$$
 (2.19)

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253 where

 $S_{\beta}(x_{1}) = P_{12}^{(k)} [\Psi_{\beta}](x_{1}) + P_{12,\beta}^{(v)}(x_{1}) - P_{12}^{(k)} [\Psi_{\beta}](-\frac{1-\hat{\sigma}}{2})$  $+ \int_{-(1-\hat{\sigma})/2}^{x_{1}} \left[ G_{22,\beta}^{(k)}(s) + G_{22,\beta}^{(v)}(s) \right] ds.$ (2.20)

In obtaining (2.20), we have used the fact that the potential part of the stress  $P_{12,\beta}^{(v)}$  vanishes on the boundary  $x_1 = -(1 - \hat{\sigma})/2$ . The relation (2.19) will be used for the accuracy test of our computation.

## 258 3. Numerical method

The densities  $\hat{\rho}_M$ ,  $\hat{\omega}_T$  and  $\hat{\omega}_P$ , which are defined by (2.5) and (2.6), can be obtained numerically by the method in Frezzotti (1997). Thus, the problem is reduced to (2.7) with (2.13) for the VDFs  $\Psi_T$  and  $\Psi_P$ .

Let us explain the numerical solution method for the problems of  $\Psi_T$  and  $\Psi_P$ . We solve them by using the iteration based on the integral formulation (Takata and Funagane 2011; Hattori and Takata 2015) of the Enskog equation combined with the fast Fourier spectral method (Filbet et al 2006) for the computation of the collision integral. Taking into account (2.8*a*) and (2.13) and formally integrating the equation (2.7*a*) with respect to  $x_1$ , we have

$$\Psi_{\beta}(x_{1},\boldsymbol{\zeta}) = \int_{-(1-\hat{\sigma})/2}^{x_{1}} \left[ \frac{1}{k\zeta_{1}} C(\Psi_{\beta})(s,\boldsymbol{\zeta}) + \frac{1}{\zeta_{1}} I_{\beta}(s,\boldsymbol{\zeta}) \right] \exp\left(-\frac{1}{k\zeta_{1}} \int_{s}^{x_{1}} \nu(p,\boldsymbol{\zeta}) dp\right) ds,$$

$$(-\frac{1-\hat{\sigma}}{2} < x_{1} < 0, \ \zeta_{1} > 0), \quad (3.1a)$$

$$\begin{split} \Psi_{\beta}(x_{1},\boldsymbol{\zeta}) &= \Psi_{\beta}(0,\boldsymbol{\zeta}^{-}) \exp\left(-\frac{1}{k\zeta_{1}} \int_{0}^{x_{1}} \nu(p,\boldsymbol{\zeta}) \mathrm{d}p\right) \\ &+ \int_{0}^{x_{1}} \left[\frac{1}{k\zeta_{1}} C(\Psi_{\beta})(s,\boldsymbol{\zeta}) + \frac{1}{\zeta_{1}} I_{\beta}(s,\boldsymbol{\zeta})\right] \exp\left(-\frac{1}{k\zeta_{1}} \int_{s}^{x_{1}} \nu(p,\boldsymbol{\zeta}) \mathrm{d}p\right) \mathrm{d}s, \\ &\quad (-\frac{1-\hat{\sigma}}{2} < x_{1} < 0, \ \zeta_{1} < 0), \quad (3.1b) \end{split}$$

where  $\zeta^- = (-\zeta_1, \zeta_2, \zeta_3)$  and  $\beta = T, P$ . Since C is an integral operator,  $C(\Psi_\beta)$  is mild in  $\zeta$ 262 even if its argument function  $\Psi_{\beta}$  is not. Thus, the factor of steep variation of  $\Psi_{\beta}$  in  $\zeta$  (or 263 264  $\zeta_1$ ) is explicit in this formulation, which will be advantageous in accurately capturing the structure of the solution. The solution  $\Psi_{\beta}$  is constructed by iteration based on (3.1) from 265 its initial guess. The data of  $C(\Psi_{\beta})$  are computed by the fast Fourier spectral method from 266 the given data of  $\Psi_{\beta}$ . The fast Fourier spectral method for the nonlinear Enskog collision 267 integral is explained in Wu et al (2015). Following the reference, we can prepare the method 268 for the linearized Enskog collision operator C in the present work. The spatial integration 269 with respect to p and that with respect to s in (3.1) are performed analytically after v and 270  $(C(\Psi_{\beta}), I_{\beta})$  are interpolated respectively with piecewise linear and quadratic functions from 271 their data on the lattice points for position  $x_1$ . 272

273 Information of lattice systems and accuracy is briefly given in Appendix D.

## **4. Numerical results and discussions**

Figure 2 shows the quantities related to the density and the gradients of the pressure and the (2, 2) component of stress in the x<sub>2</sub>-direction, namely  $\hat{\rho}_M$ ,  $\hat{\omega}_T$  and  $\hat{\omega}_P$ ,  $G_T$ ,  $G_{22,T}^{(k)} + G_{22,T}^{(v)}$ ,



Figure 2: Profiles of quantities related to the density and the gradients of the pressure and the (2, 2) component of stress. (a)  $\hat{\rho}_M$ , (b)  $\hat{\omega}_T$  and  $\hat{\omega}_P$ , (c)  $G_T$ , (d)  $G_{22,T}^{(k)} + G_{22,T}^{(v)}$ , (e)  $G_P$  and (f)  $G_{22,P}^{(k)} + G_{22,P}^{(v)}$ .

*G*<sub>P</sub> and  $G_{22,P}^{(k)} + G_{22,P}^{(v)}$ , for the molecular-size parameter  $\hat{\sigma} = 0.01$  and 0.1 and the degree of gas rarefaction k = 0.1, 1 and 10 (see also the last sentence in Section 2.4.2). The profiles for small  $\hat{\sigma}$  and large k (e.g., for  $\hat{\sigma} = 0.01$  and k = 10) are almost uniform and close to the counterparts for the Boltzmann equation. On the other hand, for large  $\hat{\sigma}$  and small k (e.g., for  $\hat{\sigma} = 0.1$  and k = 0.1), or when the gas is dense, they vary significantly near the boundary and are nonuniform in the  $x_1$  direction. As for the origin of nonuniformity of densities  $\hat{\rho}_M$ 

and  $\hat{\omega}_{TP}$  [figures 2(a) and 2(b)], see also the item (1) in Section 2.4. The gradient of the 283 pressure actually differs from that of the (2, 2) component of stress [compare figures 2(c) 284 and 2(d), and figures 2(e) and 2(f)], even if their averages over  $x_1$  are taken. This is in marked 285 contrast to the case of an ideal gas (or the Boltzmann equation), in which the gradients of 286 the pressure and the normal stress components are uniform and identical for each of the two 287 flows considered here. The stress gradient for the thermal transpiration flow is negative near 288 289 the boundary and positive in the central part of the gap [figure 2(d)]. That for the Poiseuille flow is smaller in the central part of the gap than near the boundary [figure 2(f)]. 290

The densities  $\hat{\rho}_M(x_1)$  and  $\hat{\omega}_P(x_1)$  shown in figures 2 seem to variate significantly only 291 near the boundary within the distance  $O(\hat{\sigma})$  and approach to their values  $\hat{\rho}_M(0)$  and  $\hat{\omega}_P(0)$  at 292 the middle of the gap. By using the rescaled distance from the boundary  $(x_1 + (1 - \hat{\sigma})/2)/\hat{\sigma}$ 293 and semilog plot, figures 3(a)-(d) demonstrate the observation. The approach to the values 294  $\hat{\rho}_M(0)$  and  $\hat{\omega}_P(0)$  in the uniform region is actually sufficiently fast in the scale of  $O(\hat{\sigma})$ . 295 Moreover, the magnitude of the deviation between the density on the boundary and that at 296 the middle of the gap is of the order of the volume fraction of molecules  $\eta_0$  [figures 3(e)–(f)]. 297 From these results, when  $\hat{\sigma}$  and k are decreased simultaneously so that  $\eta_0$  is finite, a thin 298 layer with the thickness of  $O(\hat{\sigma})$  adjacent to the boundary, where the densities deviate up to 299  $O(\eta_0)$  from their values in the uniform region outside the layer, is expected to appear. 300

In figure 4, the profiles of the mass flow  $\hat{\rho}_M u[\Psi_T]$  for the thermal transpiration flow are 301 shown for various values of the degree of gas rarefaction k and the molecular-size parameter 302  $\hat{\sigma}$ . When k is not small, the flow is smaller for larger  $\hat{\sigma}$  [see panel (a)]. Its main reason is 303 simply that the increase of the temperature along the plate in the units of the effective width 304  $D - \sigma$  where the centre of a molecule can move, which becomes shorter for larger  $\sigma$ , is 305 small, so that the flow is less driven. This effect is more significant than the enhancement 306 of the flow due to the increase of the effective Knudsen number defined with the length 307  $D - \sigma$ , which should be taken into account too. Related observation will be done for the 308 net mass flow shown later. When k is relatively small, in turn, as  $\hat{\sigma}$  increases, the flow is 309 enhanced over the whole gap including near the boundary. Indeed, for k = 0.1, the mass flow 310 is larger for larger  $\hat{\sigma}$  [see panel (b)]. This is expected to be associated with the increase of the 311 thermal conductivity of the gas accompanied by the increase of  $\hat{\sigma}$ , which is explained by the 312 Chapman–Enskog theory for a dense gas (Chapman and Cowling 1991) for small Knudsen 313 numbers, because the thermal slip coefficient, which approximately represents the magnitude 314 315 of the induced flow, is likely larger for the gas with larger thermal conductivity, judging from the relation between them for monoatomic rarefied gases. The negative gradient of stress near 316 the boundary also contributes to the increase of the mass flow there [see figure 2(d)]. With 317 further decrease of k, we observe considerable decrease of the mass flow in the central part 318 of the gap [see figures 4(c) and 4(d)]. Figure 2(d) implies that this is due to the deceleration 319 by the positive gradient of stress there. Incidentally, when k is small and  $\hat{\sigma}$  is large, although 320 the profile of the flow velocity  $u[\Psi_T]$  differs quantitatively from the mass flow  $\hat{\rho}_M u[\Psi_T]$ 321 due to the nonuniformity of  $\hat{\rho}_M$ , the qualitative features mentioned above is common with 322  $u[\Psi_{\rm T}].$ 323

The profiles of the mass flow  $\hat{\rho}_M u[\Psi_P]$  for the Poiseuille flow are shown in figure 5 for various values of the degree of gas rarefaction k and the molecular-size parameter  $\hat{\sigma}$ . The profile is flatter and the flow is smaller for larger  $\hat{\sigma}$ , which is consistent with that the magnitude of the Poiseuille flow is roughly inversely proportional to the viscosity for small k and its increase accompanied by the increase of  $\hat{\sigma}$ .

Figure 6 shows the profiles of the heat flow for the thermal transpiration flow. When *k* is small, the heat flow is enhanced for larger  $\hat{\sigma}$ , which is consistent with the aforementioned increase of the thermal conductivity. It changes steeply near the boundary for large  $\hat{\sigma}$  as in the mass flow. The profile of the heat flow for the Poiseuille flow is shown in figure 7. This



Figure 3: Deviation of densities  $\hat{\rho}_M$  and  $\hat{\omega}_P$  from their values at the middle of the gap. (a)  $|\hat{\rho}_M(x_1) - \hat{\rho}_M(0)|$  for k = 0.1, (b)  $|\hat{\rho}_M(x_1) - \hat{\rho}_M(0)|$  for k = 1, (c)  $|\hat{\omega}_P(x_1) - \hat{\omega}_P(0)|$ for k = 0.1, (d)  $|\hat{\omega}_P(x_1) - \hat{\omega}_P(0)|$  for k = 1, (e)  $|\hat{\rho}_M(-(1 - \hat{\sigma})/2) - \hat{\rho}_M(0)|/(4\eta_0)$  and (f)  $|\hat{\omega}_P(-(1 - \hat{\sigma})/2) - \hat{\omega}_P(0)|/(8\eta_0)$ . In (a)–(d), the quantities are plotted as functions of  $(x_1 + (1 - \hat{\sigma})/2)/\hat{\sigma}$ , the distance from the boundary scaled by the molecular diameter  $\hat{\sigma}$ . In (e) and (f), the quantities are scaled by the volume fraction of molecules  $\eta_0$  and plotted as functions of k.



Figure 4: Profiles of the mass flow of the thermal transpiration flow.  $\hat{\rho}_M u[\Psi_T]$  versus  $x_1$ . (a) k = 10, 1 and 0.3, (b) k = 0.1, (c) k = 0.07 and (d) k = 0.05.

heat flow is known to be owing to the effect of gas rarefaction in the case of an ideal gas since it occurs under the isothermal condition and it has no direct relation to the thermal conductivity and viscosity. Our result shows that heat flow of this kind is also enhanced with the increase of  $\hat{\sigma}$ .

Let us consider the force-driven flow, a flow driven by a uniform external force in the 337 direction parallel to the plates. This flow has been studied in the framework of kinetic theory 338 with an interest in non-Navier–Stokes effects such as the heat flow along the force direction, 339 the temperature bimodality and the anisotropy of normal stress components (see, e.g., Tij 340 and Santos 1994; Malek Mansour et al 1997). Note that these are nonlinear effects, i.e., 341 they manifest themselves in second order in the magnitude of the normalized force. The 342 behaviour of the mass flow of the Poiseuille flow observed in figure 5 is similar to those of 343 the force-driven flow within the linearized regime for small force (Wu et al 2016; Sheng et 344 al 2020), where the aforementioned effects are suppressed sufficiently. Thus, we have also 345 carried out the computations of the latter case, which is described by the solution of the 346 problem (2.7) of  $\Psi_{\rm P}$  with the source term  $I_{\rm P}$  being replaced by 347

$$-\zeta_2 \hat{\rho}_M E \equiv I_{\rm F}.\tag{4.1}$$

Since  $I_P$  and  $I_F$  are identical for the Boltzmann equation (both are given by  $-\zeta_2 E$ ), so are the VDFs ( $\Psi_P$  and its counterpart) and the flow velocities, heat flows and shear stresses obtained as their moments. On the other hand, for the case of a dense gas, there are differences for the profiles of mass and heat flows between two cases although the differences are very slight



Figure 5: Profiles of the mass flow of the Poiseuille flow.  $\hat{\rho}_M u[\Psi_P]$  versus  $x_1$ . (a) k = 10 and 1, (b) k = 0.3, (c) k = 0.1, (d) k = 0.07 and (e) k = 0.05.

[see figures 8(a) and 8(b), in particular, the curves for  $\hat{\sigma} = 0.15$ ]. Recall that the expressions of  $I_P$  and  $I_F$  [see (2.11*b*) and (4.1)] differ for the case of a dense gas. Actually, there is a difference between their marginal functions

356 
$$\int_{-\infty}^{\infty} \int_{0}^{\infty} (I_{\rm P}(x_1,\zeta), I_{\rm F}(x_1,\zeta)) d\zeta_2 d\zeta_3 \equiv (I_{\rm P}^{\dagger}(x_1,\zeta_1), I_{\rm F}^{\dagger}(x_1,\zeta_1))$$
(4.2)

near the boundary for large  $\hat{\sigma}$  as shown in figures 8(c) and 8(d). For  $\hat{\sigma} = 0.1$  and  $x_1 = -0.45$ , their difference normalized by maximum,  $\max_{\zeta_1} |I_P^{\dagger} - I_F^{\dagger}| / \max_{\zeta_1} |I_F^{\dagger}|$ , is larger than 0.051



Figure 6: Profiles of the heat flow of the thermal transpiration flow.  $Q^{(k)}[\Psi_T] + Q_T^{(v)}$  versus  $x_1$ . (a) k = 10, 1 and 0.3, (b) k = 0.1, (c) k = 0.07 and (d) k = 0.05.

(5.1%). This demonstrates that, for the case of the Enskog equation, there are differences
between the force-driven and the pressure-driven flows even within the linearized regime,
especially at the microscopic level.

In figure 9, we show the net mass flows for the thermal transpiration and Poiseuille flows. 362 In panels (a) and (b),  $\mathcal{M}_{\rm T}$  and  $\mathcal{M}_{\rm P}$  given by (2.17) are shown respectively, while in panels 363 (c) and (d), their ratios to the net mass flows for the case of the Boltzmann equation, say 364  $\mathcal{M}_{T,B}$  and  $\mathcal{M}_{P,B}$ , are shown. The  $\mathcal{M}_{T}$  exhibits the behaviour corresponding to that for the 365 mass flow profile observed in figure 4. Namely, as k becomes smaller, the enhancement of 366 the flow with the increase of  $\hat{\sigma}$  compensates the decrease of the effective gap width, and 367 consequently the values of the net mass flows are close to each other for different  $\hat{\sigma}$ 's (e.g., 368 for k = 0.1 and 0.07). With further decrease of k, the mass flow rate is smaller for larger  $\hat{\sigma}$ 369 again because the flow decreases in the central part of the gap. For the Poiseuille flow, when 370  $\hat{\sigma}$  is small, the Knudsen minimum is clearly observed [see panel (b)], which is attributed to 371 that the braking effect due to the plate becomes smaller both as  $k \to 0$  and  $k \to \infty$  (more 372 thorough explanation is found in the literature). On the other hand, as is also pointed out in 373 Wu et al (2016) and Sheng et al (2020) for the force-driven flows, the plot becomes flatter 374 for larger  $\hat{\sigma}$  and the Knudsen minimum becomes more invisible. This is because the flow 375 376 is not enhanced in the central part of the gap as k becomes smaller; see the plot curves for  $\hat{\sigma} = 0.1$  or 0.15 in figures 5(c)-5(e), which are almost unchanged. In figures 9(e) and 9(f), 377



Figure 7: Profiles of the heat flow of the Poiseuille flow.  $Q^{(k)}[\Psi_P] + Q_P^{(v)}$  versus  $x_1$ . (a) k = 10, 1 and 0.3, (b) k = 0.1, (c) k = 0.07 and (d) k = 0.05.

#### 378 we show the following quantities

$$k_* = \frac{k}{1 - \hat{\sigma}}, \quad \mathcal{M}_{\beta,*} = \frac{\mathcal{M}_{\beta}}{(1 - \hat{\sigma})^2} \quad (\beta = \mathrm{T}, \mathrm{P})$$
(4.3)

introduced by the conversion which corresponds to the replacement of the reference length *D* by  $D - \sigma$ . As  $k_*$  becomes larger, the plots for different  $\hat{\sigma}$ 's exhibit the common trend, which implies that the behaviour of the gas for large Knudsen numbers can be characterized well in terms of the length  $D - \sigma$ . This is consistent with the explanation of the mass flow for the thermal transpiration flow given in the third paragraph of this section.

Figures 10–12 show the VDF  $\Psi_T$  for the degree of gas rarefaction k = 0.1, 1 and 10 at three spatial points  $x_1 = -(1 - \hat{\sigma})/2$ , -0.25 and 0 as functions of the normal velocity component  $\zeta_1$  with ( $\zeta_2, \zeta_3$ ) being fixed at (1.106, 0). In the figures, the close-ups of the VDFs at the boundary near  $\zeta_1 = 0$  are also shown in panel (b) of each figure. First, the following overall behaviour similar to the case of the Boltzmann equation is observed:

• There is a jump discontinuity at  $\zeta_1 = 0$  on the boundary  $x_1 = -(1 - \hat{\sigma})/2$ .

- When *k* is small, the discontinuity is small and the VDFs behave moderately in the gas.
- When k is large, the VDFs are localized around  $\zeta_1 = 0$  including in the gas.

However, for the finite molecular size  $\hat{\sigma} \neq 0$ , the VDFs deviate considerably from those for the Boltzmann equation for  $\zeta_1 < 0$  near the origin on the boundary even when  $\hat{\sigma}$  is small [see panel (b) of each figure]. As  $\hat{\sigma}$  is decreased, while the values of macroscopic quantities approach those for the Boltzmann equation uniformly in  $x_1$  (see, e.g., figures 4 and 5), the



Figure 8: Comparison between the pressure-driven and force-driven Poiseuille flows for the mass flow, heat flow and marginal source term. k = 0.1. (a) ρ̂<sub>M</sub>u[Ψ<sub>P</sub>],
(b) Q<sup>(k)</sup>[Ψ<sub>P</sub>] + Q<sup>(v)</sup><sub>P</sub>, (c) I<sup>†</sup><sub>P</sub> and I<sup>†</sup><sub>F</sub> for σ̂ = 0.1 and (d) I<sup>†</sup><sub>P</sub> and I<sup>†</sup><sub>P</sub> for σ̂ = 0.001. In (a) and (b), the symbols indicate the pressure-driven case, while the solid lines the force-driven case. In (c) and (d), the solid lines indicate the pressure-driven case.

397 VDFs exhibit nonuniform approach in  $(x_1, \zeta_1)$ . In the following, we consider the cause of this behaviour of the VDFs with the aid of the expression (3.1b). Since the first term in the 398 right-hand side of (3.1b) is exponentially small for  $|\zeta_1| \ll 1$ , we only have to examine the 399 second term. As in the case of the Boltzmann equation, the integral  $C(\Psi_{\rm T})$ , the collision 400 frequency v and the source term  $I_{\rm T}$  are smooth in velocity  $\zeta$  (or  $\zeta_1$ ) also for finite  $\hat{\sigma}$ , which 401 402 can be confirmed actually from the numerical results. Thus it is the exponential function that induces the steep variation of  $\Psi_T$  in  $\zeta_1 < 0$  near the origin. Taking into account the 403 expression of the argument of the exponential function, we see that only the integrand in the 404 range  $|s + (1 - \hat{\sigma})/2| \leq k |\zeta_1|$  actually contributes to the integral with respect to s. In the 405 meantime,  $C(\Psi_{\rm T})$  and v vary significantly in  $x_1$  in the region within  $O(\hat{\sigma})$  from the boundary 406 as figure 13 implies. Thus, for  $|\zeta_1| \leq \hat{\sigma}/k$ ,  $\Psi_\beta$  is determined from  $C(\Psi_\beta)$  and v substantially 407 affected by the boundary and accordingly its value may deviate largely from that for the case 408 of the Boltzmann equation. To confirm the estimate, we show the deviation of the VDF  $\Psi_T$ 409 from that for the case of the Boltzmann equation  $\Psi_{T,B}$ , say  $\Delta \Psi_T = \Psi_T - \Psi_{T,B}$ , normalized by 410 its value at  $\zeta_1 = -0$  in figure 14. When they are plotted as functions of  $k\zeta_1/\hat{\sigma}$ , they overlap 411 well each other for large k and small  $\hat{\sigma}$ . This supports the above estimate. Note that  $\Psi_{\rm P}$  also 412 413 has the features described in this paragraph although their figures are omitted. The comparison of the results shown in this section with other approaches like molecular 414



Figure 9: Quantities related to the net mass flows for the thermal transpiration and Poiseuille flows. (a)  $\mathcal{M}_T$ , (b)  $\mathcal{M}_P$ , (c)  $\mathcal{M}_T/\mathcal{M}_{T,B}$ , (d)  $\mathcal{M}_P/\mathcal{M}_{P,B}$ , (e)  $\mathcal{M}_{T,*}$  and (f)  $\mathcal{M}_{P,*}$ .

415 dynamics (MD) simulation is not carried out here since unfortunately it is difficult to find the 416 simulation result of a corresponding system such as molecules under the dense gas condition 417 confined in the channel joined to two reservoirs maintained at different temperature and 418 pressure. However, instead, let us mention some known correspondences between results 419 obtained by the Enskog equation and molecular dynamics, which supports the description of 420 phenomena in dense gases based on the kinetic theory:

(1) It is known that the profile of reference density obtained from the Enskog equation,  $\hat{\rho}_M(x_1)$  in the present paper, agrees well with that obtained by the MD simulation [see, e.g., Fig. 6 in Frezzotti (1997)].

20



Figure 10: The VDF  $\Psi_{T}$  at  $(\zeta_{2}, \zeta_{3}) = (1.106, 0)$  for k = 0.1. (a)  $x_{1} = -(1 - \hat{\sigma})/2$ , (b) close-up of (a), (c)  $x_{1} = -0.25$  and (d)  $x_{1} = 0$ .

424 (2) For the force-driven flow, it is demonstrated in Sheng et al (2020) that the velocity
425 profile obtained from the Enskog equation agrees well with that obtained by the MD
426 simulation (see Figs. 5 and 6 in the reference).

427 (3) As for the thermal response, heat flow as well as the profiles of stress, density and
428 temperature between two parallel plates kept at different constant temperatures obtained from
429 the Enskog equation agrees well with that obtained by the MD simulation [see Frezzotti
430 (1999)].

## 431 5. Concluding remarks

We have investigated the thermal transpiration and Poiseuille flows of a dense gas between two parallel plates based on the Enskog equation under the diffuse reflection boundary condition. The problem was linearized around the local equilibrium state that is achieved in the absence of driving sources. Then, the reduced spatially one-dimensional problems were solved numerically by a method based on the integral formulation combined with the fast Fourier spectral method for the computation of the Enskog collision integral. Our findings in the present work are summarized as follows:

(i) In contrast to the case of an ideal gas, the density and the gradients of pressure and
 normal stress component in the flow direction are not uniform in the direction normal to the
 plates for a dense gas. The nonuniformity or significant variation has been observed near
 the boundary within the distance of the order of molecular diameter for various quantities



Figure 11: The VDF  $\Psi_T$  at  $(\zeta_2, \zeta_3) = (1.106, 0)$  for k = 1. (a)  $x_1 = -(1 - \hat{\sigma})/2$ , (b) close-up of (a), (c)  $x_1 = -0.25$  and (d)  $x_1 = 0$ .

for a dense gas. The nonuniform normal stress gradient contributes to the acceleration or deceleration of the thermal transpiration flow for small Knudsen numbers.

(ii) The behaviour of mass and heat flows as well as net mass flows has been clarified forvarious Knudsen numbers and ratios of the molecular diameter to the distance of plates.

(iii) In the analysis of the Poiseuille flow, most characteristics of the force-driven flow with
a small force are recovered. However, for the case of a dense gas, differences between the
force-driven and the present pressure-driven flows are observed even within the linearized
regime for small force and pressure gradient, especially at the microscopic level.

(iv) The behaviour of VDFs, in particular, the way of their approach to ones for theBoltzmann equation as the molecular diameter becomes smaller, has been clarified.

Acknowledgements. The author expresses his sincere thanks to Professor Shigeru Takata for his encourage ment and helpful discussions.

Funding. This work was supported in part by JSPS KAKENHI grant no. 21K14076 and the HPCI System
 Research Project hp220077.

- 457 Declaration of interests. The author reports no conflict of interest.
- 458 Author ORCID. Masanari Hattori https://orcid.org/0000-0002-5482-0210.



Figure 12: The VDF  $\Psi_T$  at  $(\zeta_2, \zeta_3) = (1.106, 0)$  for k = 10. (a)  $x_1 = -(1 - \hat{\sigma})/2$ , (b) close-up of (a), (c)  $x_1 = -0.25$  and (d)  $x_1 = 0$ .

## 459 Appendix A. Outline of linearization procedure

In this Appendix, we summarize the outline of the linearization procedure for the Enskogequation.

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#### A.1. reference equilibrium state

First, substitute  $\hat{f} = \hat{M} = \hat{\rho}_M(x_1)E(\zeta)$  into equation (2.1*a*). Then, the left hand side (LHS) of (2.1*a*) is recast as

466 On the other hand, the right hand side (RHS) of (2.1a) is transformed as

$$[\operatorname{RHS of} (2.1a)] = \frac{1}{k2\sqrt{2\pi}} \int \left[ \hat{Y}\left( \hat{\rho}_M\left( x_1 + \frac{1}{2}\hat{\sigma}k_1 \right); \eta_0 \right) \hat{\rho}_M(x_1 + \hat{\sigma}k_1) E(\zeta'_*) \hat{\rho}_M(x_1) E(\zeta') \right] \\ - \hat{Y}\left( \hat{\rho}_M\left( x_1 - \frac{1}{2}\hat{\sigma}k_1 \right); \eta_0 \right) \hat{\rho}_M(x_1 - \hat{\sigma}k_1) E(\zeta_*) \hat{\rho}_M(x_1) E(\zeta) \right] (\hat{V} \cdot \boldsymbol{k}) H(\hat{V} \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{\zeta}_* \\ = -\frac{1}{k2\sqrt{2\pi}} \int \hat{Y}\left( \hat{\rho}_M\left( x_1 - \frac{1}{2}\hat{\sigma}k_1 \right); \eta_0 \right) \hat{\rho}_M(x_1 - \hat{\sigma}k_1) \hat{\rho}_M(x_1)$$



Figure 13: Plots of the collision integral  $C(\Psi_T)$  and the collision frequency  $\nu$  at  $(\zeta_2, \zeta_3) = (1.106, 0)$  for k = 1. (a)  $C(\Psi_T)$  at  $x_1 = -(1 - \hat{\sigma})/2$ , (b)  $C(\Psi_T)$  at  $x_1 = -0.25$ , (c)  $\nu$  at  $x_1 = -(1 - \hat{\sigma})/2$ , (d)  $\nu$  at  $x_1 = -0.25$ , and (e)  $\nu$  at  $\zeta_1 = 0$ .

$$\times (\hat{\boldsymbol{V}} \cdot \boldsymbol{k}) [H(-\hat{\boldsymbol{V}} \cdot \boldsymbol{k}) + H(\hat{\boldsymbol{V}} \cdot \boldsymbol{k})] E(\zeta_*) E(\zeta) d\boldsymbol{k} d\zeta_*$$

$$= \frac{1}{k2\sqrt{2\pi}} \int \hat{Y} \left( \hat{\rho}_M \left( x_1 - \frac{1}{2} \hat{\sigma} k_1 \right); \eta_0 \right) \hat{\rho}_M (x_1 - \hat{\sigma} k_1) \hat{\rho}_M (x_1)$$

$$\times (\zeta_1 k_1 + \zeta_2 k_2 + \zeta_3 k_3) E(\zeta) d\boldsymbol{k}$$

$$= \frac{2\pi}{k2\sqrt{2\pi}} \hat{\rho}_M (x_1) \zeta_1 E(\zeta) \int_{-1}^{-1} \hat{Y} \left( \hat{\rho}_M \left( x_1 - \frac{1}{2} \hat{\sigma} z \right); \eta_0 \right) \hat{\rho}_M (x_1 - \hat{\sigma} z) z dz$$



Figure 14: Plots of the normalized deviation of the VDF for the Enskog equation from that for the Boltzmann equation.  $\Delta \Psi_{\rm T}/(\Delta \Psi_{\rm T})|_{\zeta_1=-0}$  at  $(\zeta_2, \zeta_3) = (1.106, 0)$ . (a) versus  $\zeta_1$  and (b) versus  $k\zeta_1/\hat{\sigma}$ .

467 = 
$$\zeta_1 E(\zeta) J_1[\hat{\rho}_M](x_1),$$
 (A2)

where  $J_1$  is given in Appendix **B**. Note that (1) at the second equality,  $E(\zeta'_*)E(\zeta') = E(\zeta_*)E(\zeta)$  is used and change of a variable  $\mathbf{k} \to -\mathbf{k}$  is applied for the first term in the integrand; (2) at the third equality,  $H(-\hat{\mathbf{V}} \cdot \mathbf{k}) + H(\hat{\mathbf{V}} \cdot \mathbf{k}) = 1$  is used and the integration over  $\zeta_*$  is carried out; (3) at the fourth equality, with the  $x_1$  direction as the polar direction, the integration with respect to the azimuthal angle of  $\mathbf{k}$  is carried out (then the contribution from the parts multiplied by  $\zeta_2 k_2$  and  $\zeta_3 k_3$  vanish) and that with respect to the polar angle of  $\mathbf{k}$  is expressed as the integral with respect to the variable z.

Equating (A 1) and (A 2), we have the equation (2.5*a*) for the density  $\hat{\rho}_M(x_1)$ . Since  $\hat{M}$ is a Maxwellian, it satisfies the diffuse reflection boundary condition (2.1*g*) with the plate temperature  $\hat{T}_w(x_2)$  being replaced by the reference temperature 1. Substituting  $\hat{f} = \hat{M} =$  $\hat{\rho}_M(x_1)E(\zeta)$  into the condition (2.1*j*) for average density, immediately we have (2.5*b*). When the density  $\hat{\rho}_M(x_1)$  satisfies (2.5), the local equilibrium state  $\hat{M} = \hat{\rho}_M(x_1)E(\zeta)$  satisfies the Enskog equation (2.1*a*) in the domain  $-\frac{1-\hat{\sigma}}{2} < x_1 < \frac{1-\hat{\sigma}}{2}$ .

481 A.2. perturbation

Now, let us introduce the perturbation,  $\Phi$ , and express  $\hat{f}$  as  $\hat{f} = \hat{M} + \Phi$ . Then, subtracting Enskog equation (2.1*a*) for  $\hat{f} = M$  from that for  $\hat{f} = \hat{M} + \Phi$ , we have

484 
$$\zeta_1 \frac{\partial \Phi}{\partial x_1} + \zeta_2 \frac{\partial \Phi}{\partial x_2} = \frac{1}{k} [\hat{Q}(\hat{M} + \Phi) - \hat{Q}(\hat{M})] = \frac{1}{k} L(\Phi) + O(\Phi^2), \quad (A3)$$

where *L* is the collision operator linearized around the reference local equilibrium state  $\hat{M}(x_1, \zeta)$ . The expression (2.8) of *L* is obtained in a straightforward way by using the transformation  $\hat{Y}(\hat{\rho}) \hat{f} \hat{f} = [\hat{Y}(\hat{\rho}_M) + \langle \Phi \rangle \hat{Y}_1(\hat{\rho}_M) + O(\Phi^2)](\hat{M} + \Phi)(\hat{M} + \Phi) = \hat{Y}(\hat{\rho}_M)\hat{M}\hat{M} +$  $\{\hat{Y}(\hat{\rho}_M)(\hat{M}\Phi + \Phi\hat{M}) + \langle \Phi \rangle \hat{Y}_1(\hat{\rho}_M)\hat{M}\hat{M}\} + O(\Phi^2)$  [see also (2.10)].

Subtracting the boundary condition (2.1g) or the condition (2.1j) for average density for

 $\hat{f} = M$  from those for  $\hat{f} = \hat{M} + \Phi$ , respectively, we have

b.c. 
$$\Phi = \left[\check{\rho}_w + \hat{\rho}_M \left( \mp \frac{1 - \hat{\sigma}}{2} \right) \left( \zeta^2 - \frac{3}{2} \right) c_{\mathrm{T}} x_2 \right] E(\zeta) + O(c_{\mathrm{T}} \Phi, \Phi^2),$$
$$(\zeta_1 \ge 0, \ x_1 = \mp \frac{1 - \hat{\sigma}}{2}), \quad (A \, 4a)$$

$$\check{\rho}_w = -\frac{1}{2} c_{\mathrm{T}} x_2 \hat{\rho}_M \left( \mp \frac{1 - \hat{\sigma}}{2} \right) \mp 2\sqrt{\pi} \int_{\zeta_1 \le 0} \zeta_1 \Phi \mathrm{d}\zeta, \tag{A4b}$$

with 
$$\left(\int_{-(1-\hat{\sigma})/2}^{(1-\hat{\sigma})/2} \int \Phi d\zeta dx_1\right)\Big|_{x_2=0} = 0.$$
 (A4c)

489 Derivation of (A 4) is straightforward and parallel to the case of Boltzmann equation.

## A.3. form of perturbation

491 We need to find the appropriate form of the perturbation  $\Phi$  such that  $\Phi$  represents the gradients

of temperature and pressure (or stress) and satisfies its equation (A 3) and conditions (A 4)
within the linearized regime.

For the Boltzmann equation, it is known that such a solution  $\Phi$  can be sought in the form

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$$\Phi = c_{\rm T} \left[ x_2 E(\zeta) \left( -1 + (\zeta^2 - \frac{3}{2}) \right) + \bar{\Psi}_{\rm T}(x_1, \zeta) \right] + \bar{c}_{\rm P} \left[ x_2 E(\zeta) + \bar{\Psi}_{\rm P}(x_1, \zeta) \right], \quad (A5)$$

where  $\bar{c}_P$  is a small constant and  $\bar{\Psi}_T$  and  $\bar{\Psi}_P$  are odd in  $\zeta_2$ . The bar is attached to discriminate the quantities from those for the Enskog equation. Calculating the temperature  $\hat{T}$  and the stress  $\hat{p}_{22}$  with  $\hat{f} = \hat{M} + \Phi$  for the Boltzmann equation, we have  $\hat{T} = 1 + c_T x_2$  and  $\hat{p}_{22} = 1 + \bar{c}_P x_2 (= \hat{p})$ within the linearized regime [the negligible  $O(\bar{c}_P^2, c_T^2)$  error terms are dropped in these expressions]. We see that  $\bar{c}_P$  corresponds to the gradient of stress (or pressure) in the  $x_2$ direction. The problem for  $\Phi$  is rewritten to those for  $\bar{\Psi}_T$  and  $\bar{\Psi}_P$ .

Unfortunately, for the case of Enskog equation, the form (A 5) can not satisfy the equation 502 (A 3) and a modification is required. A clue for an appropriate modification is that the refer-503 ence state  $\hat{M}$  is a Maxwellian with uniform temperature but variable density profile in the  $x_1$ 504 direction for the case of Enskog equation. We attempt to make the perturbation have the corre-505 sponding properties too. Accordingly, we introduce perturbed density profile, say  $\hat{\omega}_{T}(x_1)$  and 506  $\hat{\omega}_{\rm P}(x_1)$ , as well while keeping the temperature is constant in  $x_1$ . This leads to the introduction 507 of the form (2.4c) of  $\Phi$ , i.e.,  $\Phi = c_T \{ x_2 E(\zeta) [\hat{\omega}_T(x_1) + (\zeta^2 - \frac{3}{2})\hat{\rho}_M(x_1)] + \Psi_T(x_1, \zeta) \} +$ 508  $c_{\rm P} \left[ x_2 E(\zeta) \hat{\omega}_{\rm P}(x_1) + \Psi_{\rm P}(x_1, \zeta) \right]$ . Note that the case of Boltzmann equation corresponds to 509 the case  $\hat{\rho}_M(x_1) \equiv 1$ ,  $\hat{\omega}_T(x_1) \equiv -1$  and  $\hat{\omega}_P(x_1) \equiv 1$ . 510

Calculating the temperature  $\hat{T}$  and the stress  $\hat{p}_{22}$  with  $\hat{f} = \hat{M} + \Phi$  for the Enskog equation, we have  $\hat{T} = 1 + c_T x_2$  and

$$\hat{p}_{22} = \hat{p}_{22}^{(k)} + \hat{p}_{22}^{(v)} \neq \hat{p}$$
  
=  $[\hat{\rho}_M(x_1) + P_{22,M}^{(v)}(x_1)]$   
+ $c_T x_2 [G_{22,T}^{(k)}(x_1) + G_{22,T}^{(v)}(x_1)] + c_P x_2 [G_{22,P}^{(k)}(x_1) + G_{22,P}^{(v)}(x_1)]$  (A 6)

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within the linearized regime [the negligible  $O(c_P^2, c_T^2)$  error terms are dropped in these expressions], where  $G_{22,T}^{(k)} = \hat{\rho}_M(x_1) + \hat{\omega}_T(x_1)$  and  $G_{22,P}^{(k)} = \hat{\omega}_P(x_1)$ , and the expressions of the stress contribution  $P_{22,M}^{(v)}$  and the gradients  $G_{22,T}^{(v)}$  and  $G_{22,P}^{(v)}$  are given in Appendix C. The calculation of  $\hat{p}_{22}^{(k)}$  is parallel to the case of Boltzmann equation. As for that of  $\hat{p}_{22}^{(v)}$  [(2.3f)],

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thanks to the explicit functional form of  $\Phi$  in  $\zeta$  except the parts of  $\Psi_{T,P}$ , the integration with respect to  $\zeta$  and  $\zeta_*$  can be carried out firstly with k and  $\hat{\alpha}$  being fixed and that with respect to the azimuthal angle of k can also be carried out subsequently. The contribution from  $\Psi_{T,P}$ vanishes due to their oddness in  $\zeta_2$ . Now, in accordance with the nature of the Poiseuille and thermal transpiration flows, we require that

$$\frac{1}{1-\hat{\sigma}} \int_{-(1-\hat{\sigma})/2}^{(1-\hat{\sigma})/2} [G_{22,\mathbf{P}}^{(\mathbf{k})}(x_1) + G_{22,\mathbf{P}}^{(\mathbf{v})}(x_1)] dx_1 = 1,$$
(A7*a*)

$$\frac{1}{1-\hat{\sigma}} \int_{-(1-\hat{\sigma})/2}^{(1-\hat{\sigma})/2} [G_{22,\mathrm{T}}^{(\mathrm{k})}(x_1) + G_{22,\mathrm{T}}^{(\mathrm{v})}(x_1)] \mathrm{d}x_1 = 0.$$
 (A7b)

See also the item (2) in Section 2.4. Under (A 7),  $c_P$  corresponds to the gradient of stress in the  $x_2$  direction averaged in the  $x_1$  direction [see (A 6)]. Substituting the expressions of  $G_{22,P}^{(k,v)}$  and  $G_{22,T}^{(k,v)}$  into (A 7*a*) and (A 7*b*), they reduce to the subsidiary conditions (2.6*c*) and (2.6*b*) for  $\hat{\omega}_P$  and  $\hat{\omega}_T$ . Their derivations are straightforward.

519 Finally, we have to check if the solution  $\Phi$  of the equation (A 3) under the conditions (A 4)

can be sought without any inconsistency in the form (2.4c) within the negligible error in the linearized regime.

Since  $\Phi|_{x_2=0} = c_T \Psi_T + c_P \Psi_P$  and  $\Psi_{T,P}$  is considered to be odd in  $\zeta_2$ , the condition (A 4c) for average density is satisfied automatically. Substituting (2.4c) into the boundary condition (A 4a) and (A 4b) leads to the homogeneous boundary condition (2.7b) for  $\Psi_{T,P}$ , whose derivation is parallel to the case of Boltzmann equation. The remaining is to check the compatibility to equation (A 3).

527 Substituting (2.4c) into equation (A 3) for  $\Phi$ , its LHS is recast as

$$\zeta_{1}\frac{\partial\Phi}{\partial x_{1}} + \zeta_{2}\frac{\partial\Phi}{\partial x_{2}} = c_{T}\left\{x_{2}\zeta_{1}E(\zeta)\left[\frac{d\hat{\omega}_{T}(x_{1})}{dx_{1}} + (\zeta^{2} - \frac{3}{2})\frac{d\hat{\rho}_{M}(x_{1})}{dx_{1}}\right] + \zeta_{1}\frac{\partial\Psi_{T}}{\partial x_{1}}(x_{1},\zeta) + \zeta_{2}E(\zeta)\left[\hat{\omega}_{T}(x_{1}) + (\zeta^{2} - \frac{3}{2})\hat{\rho}_{M}(x_{1})\right]\right\}$$

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$$+c_{\mathrm{P}}\left\{x_{2}\zeta_{1}E(\zeta)\frac{\mathrm{d}\hat{\omega}_{\mathrm{P}}(x_{1})}{\mathrm{d}x_{1}}+\zeta_{1}\frac{\partial\Psi_{\mathrm{P}}}{\partial x_{1}}(x_{1},\zeta)+\zeta_{2}E(\zeta)\hat{\omega}_{\mathrm{P}}(x_{1})\right\}.$$
 (A8)

530 We see that the terms in (A 8) can be classified into three different kinds of terms according

to their functional form with respect to  $x_2$  and  $\zeta$ : (1)  $c_T x_2 \zeta_1 E(\zeta) (\zeta^2 - 3/2) d\hat{\rho}_M(x_1)/dx_1$ ,

532 (2)  $c_{\mathrm{T},\mathrm{P}}x_2\zeta_1E(\zeta)d\hat{\omega}_{\mathrm{T},\mathrm{P}}(x_1)/dx_1$ , (3)  $c_{\mathrm{T}}\left\{\zeta_1\partial\Psi_{\mathrm{T}}(x_1,\zeta)/\partial x_1+\zeta_2E(\zeta)\left[\hat{\omega}_{\mathrm{T}}(x_1)+(\zeta^2-\frac{3}{2})\hat{\rho}_M(x_1)\right]\right\}$ 533 and  $c_{\mathrm{P}}\left\{\zeta_1\partial\Psi_{\mathrm{P}}(x_1,\zeta)/\partial x_1+\zeta_2E(\zeta)\hat{\omega}_{\mathrm{P}}(x_1)\right\}$ . The terms of third kind are odd in  $\zeta_2$  and do

not depend on  $x_2$ .

For RHS of (A 3), first let us rewrite the form (2.4c) as  $\Phi = (c_T \Psi_T + c_P \Psi_P) + c_T x_2 E(\zeta^2 - \frac{3}{2})\hat{\rho}_M + x_2 E(c_T \hat{\omega}_T + c_P \hat{\omega}_P)$ . Then substituting it into the RHS of (A 3) and making use of the linearity of the collision operator *L*, we have

$$\begin{aligned} \frac{1}{k}L(\Phi) &= \frac{1}{k}L(c_{\rm T}\Psi_{\rm T} + c_{\rm P}\Psi_{\rm P}) \\ &+ \frac{1}{k}L(c_{\rm T}x_2E(\zeta^2 - \frac{3}{2})\hat{\rho}_M) + \frac{1}{k}L(x_2E(c_{\rm T}\hat{\omega}_{\rm T} + c_{\rm P}\hat{\omega}_{\rm P})), \, (A\,9a) \end{aligned}$$

where

$$\frac{1}{k}L(c_{\rm T}\Psi_{\rm T} + c_{\rm P}\Psi_{\rm P}) = c_{\rm T}\frac{1}{k}L(\Psi_{\rm T}) + c_{\rm P}\frac{1}{k}L(\Psi_{\rm P}), \tag{A9b}$$

$$\frac{1}{k}L(c_{\mathrm{T}}x_{2}E(\zeta^{2}-\frac{3}{2})\hat{\rho}_{M}) = c_{\mathrm{T}}x_{2}\zeta_{1}E(\zeta)(\zeta^{2}-\frac{3}{2})J_{1}[\hat{\rho}_{M}](x_{1}) - c_{\mathrm{T}}\frac{\hat{\sigma}E(\zeta)}{k2\sqrt{2\pi}}J_{3}[\hat{\rho}_{M}](x_{1},\zeta), \quad (A\,9c) \\
\frac{1}{k}L(x_{2}E(c_{\mathrm{T}}\hat{\omega}_{\mathrm{T}}+c_{\mathrm{P}}\hat{\omega}_{\mathrm{P}})) = c_{\mathrm{T}}x_{2}\zeta_{1}E(\zeta)K_{1}[\hat{\omega}_{\mathrm{T}},\hat{\rho}_{M}](x_{1}) - c_{\mathrm{T}}\frac{\hat{\sigma}E(\zeta)}{k2\sqrt{2\pi}}\zeta_{2}K_{3}[\hat{\omega}_{\mathrm{T}},\hat{\rho}_{M}](x_{1}) \\
+ c_{\mathrm{P}}x_{2}\zeta_{1}E(\zeta)K_{1}[\hat{\omega}_{\mathrm{P}},\hat{\rho}_{M}](x_{1}) - c_{\mathrm{P}}\frac{\hat{\sigma}E(\zeta)}{k2\sqrt{2\pi}}\zeta_{2}K_{3}[\hat{\omega}_{\mathrm{P}},\hat{\rho}_{M}](x_{1}) \quad (A\,9d)$$

and the integrals 
$$J_1$$
,  $J_3$ ,  $K_1$  and  $K_3$  are given in Appendix B. Derivation of  $(A 9c)$  and  $(A 9d)$   
can be done straightforwardly in the similar way as  $(A 2)$ , where the same kind of operations  
[see the items (1)–(3) after (A 2)] can be used again. When the arguments proportional to  
 $x_2$  are substituted into the collision operator  $L(\psi)$  [(A 9c) and (A 9d)], due to the position  
displacements  $\mathbf{x} \pm \hat{\sigma} \mathbf{k}$  for  $\psi$  and  $\mathbf{x} \pm (\hat{\sigma}/2)\mathbf{k}$  for  $\langle \psi \rangle$  [see also (2.8)], factors with  $x_2 \pm \hat{\sigma} k_2$  and  
 $x_2 \pm (\hat{\sigma}/2)k_2$  occur in the integrand of  $L(\psi)$ . Then, the contribution from parts proportional  
to  $x_2$  gives the first term of RHS of (A 9c) and the first and third terms of RHS of (A 9d),  
and that from parts proportional to  $\pm \hat{\sigma} k_2$  and  $\pm (\hat{\sigma}/2)k_2$  gives the second term of RHS of  
(A 9c) and the second and fourth terms of RHS of (A 9d), respectively.

Corresponding to the classification after (A 8), the terms in RHS of (A 3),  $\frac{1}{k}L(\Phi)$ given in (A 9), can also be classified into: (1)  $c_{T}x_{2}\zeta_{1}E(\zeta)(\zeta^{2} - \frac{3}{2})J_{1}[\hat{\rho}_{M}](x_{1})$ , (2)  $c_{T,P}x_{2}\zeta_{1}E(\zeta)K_{1}[\hat{\omega}_{T,P},\hat{\rho}_{M}](x_{1})$  and (3)  $c_{T,P}(1/k)L(\Psi_{T,P})$ ,  $-c_{T}(\hat{\sigma}E(\zeta)/k2\sqrt{2\pi})J_{3}[\hat{\rho}_{M}](x_{1},\zeta)$ and  $-c_{T,P}(\hat{\sigma}E(\zeta)/k2\sqrt{2\pi})\zeta_{2}K_{3}[\hat{\omega}_{T,P},\hat{\rho}_{M}](x_{1})$ . The terms of third kind can be confirmed to be actually odd in  $\zeta_{2}$ .

Finally, we equate (A 8) and (A 9*a*) by taking into account the classification (1)–(3) of the terms. For the first kind of terms, because the equation for  $\hat{\rho}_M$ ,  $d\hat{\rho}_M(x_1)/dx_1 = J_1[\hat{\rho}_M](x_1)$ , holds, we find that they nicely cancel out. Equating the second kind of terms, we obtain the equation (2.6) for  $\hat{\omega}_{T,P}$ . Equating the third kind of terms, the equation (2.7) for  $\Psi_{T,P}$  with the source term (2.11) is obtained.

#### 554 Appendix B. Definitions of $J_i$ and $K_i$

The integrals  $J_1$ ,  $J_2$  and  $J_3$  in (2.5*a*), (2.6*b*) and (2.11*a*) are given by

$$J_1[\hat{\rho}_M](x_1) = \frac{1}{k} \sqrt{\frac{\pi}{2}} \hat{\rho}_M(x_1) \int_{-1}^{1} \hat{Y}(\hat{\rho}_M(r_m);\eta_0) \hat{\rho}_M(r_o) z dz, \qquad (B\,1a)$$

$$J_{2}[\hat{\rho}_{M}] = -\frac{\sqrt{\pi}}{4\sqrt{2}k(1-\hat{\sigma})} \int_{-(1-\hat{\sigma})/2}^{(1-\hat{\sigma})/2} \int_{0}^{\hat{\sigma}} \int_{-1}^{1} (1-z^{2})\hat{Y}(\hat{\rho}_{M}(r_{c});\eta_{0}) \\ \times \hat{\rho}_{M}(r_{a})\hat{\rho}_{M}(r_{b})dzd\hat{\alpha}ds, \qquad (B\,1b)$$

$$J_{3}[\hat{\rho}_{M}](x_{1},\boldsymbol{\zeta}) = \frac{1}{\sqrt{\pi}} \int k_{2} \hat{Y} \left( \hat{\rho}_{M} \left( x_{1} + \frac{1}{2} \hat{\sigma} k_{1} \right); \eta_{0} \right)$$
$$\times \hat{\rho}_{M}(x_{1} + \hat{\sigma} k_{1}) \hat{\rho}_{M}(x_{1}) Z(\boldsymbol{\zeta} \cdot \boldsymbol{k}) \mathrm{d}\boldsymbol{k}, \tag{B1c}$$

where

$$r_o = x_1 - \hat{\sigma} z, \quad r_m = x_1 - \frac{1}{2}\hat{\sigma} z,$$
 (B 2*a*)

$$r_a = s - \hat{\alpha}z, \quad r_b = s + (\hat{\sigma} - \hat{\alpha})z, \quad r_c = s + (\frac{1}{2}\hat{\sigma} - \hat{\alpha})z, \tag{B2b}$$

$$Z(t) = \frac{1}{2}(1-t^2)e^{-t^2} + \frac{\sqrt{\pi}}{2}(t^3 - \frac{1}{2}t)\left(1 - \operatorname{erf}(t)\right), \quad \operatorname{erf}(t) = \frac{2}{\sqrt{\pi}}\int_0^t e^{-\tau^2} d\tau. \quad (B\,2c)$$

The integrals  $K_1$ ,  $K_2$  and  $K_3$  in (2.6) and (2.11) are given as follows:

$$K_{1}[\hat{\omega}_{\beta},\hat{\rho}_{M}](x_{1}) = \frac{1}{k}\sqrt{\frac{\pi}{2}} \bigg[ \int_{-1}^{1} \hat{Y}\left(\hat{\rho}_{M}\left(r_{m}\right);\eta_{0}\right) \left[\hat{\rho}_{M}(r_{o})\hat{\omega}_{\beta}(x_{1}) + \hat{\omega}_{\beta}(r_{o})\hat{\rho}_{M}(x_{1})\right] z dz \\ + \int_{-1}^{1} \hat{Y}_{1}\left(\hat{\rho}_{M}\left(r_{m}\right);\eta_{0}\right)\hat{\omega}_{\beta}(r_{m})\hat{\rho}_{M}(r_{o})\hat{\rho}_{M}(x_{1}) z dz \bigg], \quad (B \, 3a)$$

$$K_{2}[\hat{\omega}_{\beta},\hat{\rho}_{M}] = \frac{\sqrt{\pi}}{4\sqrt{2}k(1-\hat{\sigma})} \int_{-(1-\hat{\sigma})/2}^{(1-\hat{\sigma})/2} \int_{0}^{\hat{\sigma}} \int_{-1}^{1} (1-z^{2}) \\ \times \bigg\{\hat{Y}\left(\hat{\rho}_{M}\left(r_{c}\right);\eta_{0}\right) \left[\hat{\rho}_{M}(r_{a})\hat{\omega}_{\beta}(r_{b}) + \hat{\omega}_{\beta}(r_{a})\hat{\rho}_{M}(r_{b})\right] \\ + \hat{Y}_{1}\left(\hat{\rho}_{M}\left(r_{c}\right);\eta_{0}\right)\hat{\omega}_{\beta}\left(r_{c}\right)\hat{\rho}_{M}(r_{a})\hat{\rho}_{M}(r_{b})\bigg\} dz d\hat{\alpha} ds$$

$$+\frac{1}{1-\hat{\sigma}}\int_{-(1-\hat{\sigma})/2}^{(1-\sigma)/2}\hat{\omega}_{\beta}(s)ds,$$
(B 3b)  

$$K_{3}[\hat{\omega}_{\beta},\hat{\rho}_{M}](x_{1}) = \pi \int_{-1}^{1}(1-z^{2})\left[\hat{Y}\left(\hat{\rho}_{M}\left(r_{m}\right);\eta_{0}\right)\hat{\omega}_{\beta}(r_{o})\hat{\rho}_{M}(x_{1})\right.\right.$$

$$\left.+\frac{1}{2}\hat{Y}_{1}\left(\hat{\rho}_{M}\left(r_{m}\right);\eta_{0}\right)\hat{\omega}_{\beta}(r_{m})\hat{\rho}_{M}(r_{o})\hat{\rho}_{M}(x_{1})\right]dz.$$
(B 3c)

## 555 Appendix C. Definitions of several moments

The  $P_{11,M}^{(v)}$ ,  $P_{22,M}^{(v)}$ ,  $G_{11,T}^{(v)}$ ,  $G_{22,T}^{(v)}$ ,  $P_{12,\omega_T}^{(v)}$ ,  $P_{12}^{(v)}[\Psi_\beta]$  and  $Q^{(v)}[\Psi_\beta]$  in (2.14) and (2.15) are given by

$$\begin{bmatrix} P_{11,M}^{(v)} \\ P_{22,M}^{(v)} \end{bmatrix} = \frac{\sqrt{\pi}}{4\sqrt{2}k} \int_{-1}^{1} \int_{0}^{\hat{\sigma}} \begin{bmatrix} 2z^{2} \\ 1-z^{2} \end{bmatrix} \hat{Y} \left( \hat{\rho}_{M} \left( r_{C} \right); \eta_{0} \right) \hat{\rho}_{M}(r_{A}) \hat{\rho}_{M}(r_{B}) d\hat{\alpha} dz, \quad (C \, 1a) \\ \begin{bmatrix} G_{11,T}^{(v)} \\ G_{22,T}^{(v)} \end{bmatrix} = \frac{\sqrt{\pi}}{4\sqrt{2}k} \int_{-1}^{1} \int_{0}^{\hat{\sigma}} \begin{bmatrix} 2z^{2} \\ 1-z^{2} \end{bmatrix} \\ \times \left\{ \hat{Y} \left( \hat{\rho}_{M} \left( r_{C} \right); \eta_{0} \right) \left[ \hat{\rho}_{M}(r_{A}) \hat{\omega}_{T}(r_{B}) + \hat{\omega}_{T}(r_{A}) \hat{\rho}_{M}(r_{B}) \right] \\ + \hat{Y}_{1} \left( \hat{\rho}_{M} \left( r_{C} \right); \eta_{0} \right) \hat{\omega}_{T} \left( r_{C} \right) \hat{\rho}_{M}(r_{A}) \hat{\rho}_{M}(r_{B}) \\ + \hat{Y} \left( \hat{\rho}_{M} \left( r_{C} \right); \eta_{0} \right) \hat{\rho}_{M}(r_{A}) \hat{\rho}_{M}(r_{B}) \right\} d\hat{\alpha} dz, \quad (C \, 1b) \\ P^{(v)} = \sqrt{\pi} \int_{0}^{1} \int_{0}^{\hat{\sigma}} z(1-z^{2}) \end{bmatrix}$$

$$P_{12,\omega_{\mathrm{T}}}^{(\mathrm{v})} = \frac{\sqrt{\pi}}{4\sqrt{2}k} \int_{-1} \int_{0}^{+} z(1-z^{2}) \\ \times \left\{ \hat{Y}\left(\hat{\rho}_{M}\left(r_{C}\right);\eta_{0}\right) \left[ (\hat{\sigma}-\hat{\alpha})\hat{\rho}_{M}(r_{A})\hat{\omega}_{\mathrm{T}}(r_{B}) - \hat{\alpha}\hat{\omega}_{\mathrm{T}}(r_{A})\hat{\rho}_{M}(r_{B}) \right] \right\}$$

$$\begin{aligned} +(\frac{1}{2}\hat{\sigma}-\hat{\alpha})\hat{Y}_{1}\left(\hat{\rho}_{M}\left(r_{C}\right);\eta_{0}\right)\hat{\omega}_{T}\left(r_{C}\right)\hat{\rho}_{M}(r_{A})\hat{\rho}_{M}(r_{B})\\ +(\frac{1}{2}\hat{\sigma}-\hat{\alpha})\hat{Y}\left(\hat{\rho}_{M}\left(r_{C}\right);\eta_{0}\right)\hat{\rho}_{M}(r_{A})\hat{\rho}_{M}(r_{B})\bigg\}d\hat{\alpha}dz, \quad (C\,1c) \\ P_{12}^{(v)}[\Psi_{\beta}] &= \frac{1}{2\sqrt{2\pi}k}\int_{0}^{\hat{\sigma}}\int\int k_{1}k_{2}\hat{Y}\left(\hat{\rho}_{M}\left(x_{1}+(\frac{1}{2}\hat{\sigma}-\hat{\alpha})k_{1}\right);\eta_{0}\right)\\ \times\left[I_{P}^{(+)}(\zeta\cdot k)\hat{\rho}_{M}(x_{1}-\hat{\alpha}k_{1})\Psi_{\beta}(x_{1}+(\hat{\sigma}-\hat{\alpha})k_{1},\zeta)\right.\\ \left.+I_{P}^{(-)}(\zeta\cdot k)\hat{\rho}_{M}(x_{1}+(\hat{\sigma}-\hat{\alpha})k_{1})\Psi_{\beta}(x_{1}-\hat{\alpha}k_{1},\zeta)\right]d\zeta dk d\hat{\alpha}, (C\,1d) \\ Q^{(v)}[\Psi_{\beta}] &= \frac{1}{4\sqrt{2\pi}k}\int_{0}^{\hat{\sigma}}\int\int k_{2}\hat{Y}\left(\hat{\rho}_{M}\left(x_{1}+(\frac{1}{2}\hat{\sigma}-\hat{\alpha})k_{1}\right);\eta_{0}\right)\\ \times\left[I_{Q}^{(+)}(\zeta\cdot k)\hat{\rho}_{M}(x_{1}-\hat{\alpha}k_{1})\Psi_{\beta}(x_{1}+(\hat{\sigma}-\hat{\alpha})k_{1},\zeta)\right.\\ \left.+I_{Q}^{(-)}(\zeta\cdot k)\hat{\rho}_{M}(x_{1}+(\hat{\sigma}-\hat{\alpha})k_{1})\Psi_{\beta}(x_{1}-\hat{\alpha}k_{1},\zeta)\right]d\zeta dk d\hat{\alpha}, (C\,1e) \end{aligned}$$

where

$$r_A = x_1 - \hat{\alpha}z, \quad r_B = x_1 + (\hat{\sigma} - \hat{\alpha})z, \quad r_C = x_1 + (\frac{1}{2}\hat{\sigma} - \hat{\alpha})z, \quad (C\,2a)$$

$$I_P^{(\pm)}(t) = \pi^{-1/2} \int_{\pm t}^{\infty} (\tau \mp t)^2 e^{-\tau^2} \mathrm{d}\tau, \qquad (C\,2b)$$

$$I_Q^{(\pm)}(t) = \pm \pi^{-1/2} \int_{\pm t}^{\infty} (\tau \mp t)^2 (\tau \pm t) e^{-\tau^2} d\tau.$$
 (C2c)

The  $(G_{11,P}^{(v)}, G_{22,P}^{(v)})$  and  $P_{12,\omega_P}^{(v)}$  are respectively given by the definitions of  $(G_{11,T}^{(v)}, G_{22,T}^{(v)})$ and  $P_{12,\omega_T}^{(v)}$  with their respective last terms  $\hat{Y}(\hat{\rho}_M(r_C);\eta_0)\hat{\rho}_M(r_A)\hat{\rho}_M(r_B)$  and  $(\frac{1}{2}\hat{\sigma} - \hat{\alpha})\hat{Y}(\hat{\rho}_M(r_C);\eta_0)\hat{\rho}_M(r_A)\hat{\rho}_M(r_B)$  in the curly brackets being dropped and  $\hat{\omega}_T$  being replaced by  $\hat{\omega}_P$ .

## 560 Appendix D. Information of computations

In this Appendix, the information of computations is briefly described. The results shown 561 in Section 4 are those obtained with the molecular-velocity lattice system consisting of 562  $336 \times 64 \times 64$  points in  $\zeta_1 \zeta_2 \zeta_3$ -space and the spatial lattice system consisting of 181 points. For  $\zeta_1$ , the minimum lattice interval is  $1.243 \times 10^{-5}$  around  $\zeta_1 = 0$ , while the maximum interval is 0.0931 around  $\zeta_1 = \pm 4.5$ . For  $\zeta_2$  and  $\zeta_3$ , the lattice interval is uniformly 0.369. For  $x_1$ , the minimum lattice interval is  $5.242 \times 10^{-5}$  around  $x_1 = -1/2$ , while the maximum 563 564 565 566 interval is  $6.944 \times 10^{-3}$  around  $x_1 = 0$  in the case of  $\hat{\sigma} = 0$ . In the case of  $\hat{\sigma} \neq 0$ , this 567 arrangement is shrunk to the interval  $\left[-(1-\hat{\sigma})/2,0\right]$ . In the computation of the collision 568 integral,  $192 \times 64 \times 64$  modes in the frequency domain for  $\zeta_1 \zeta_2 \zeta_3$ -space and 32 and 16 569 Gauss-Legendre quadrature points for the polar and azimuthal angles of vector k (with the 570  $x_1$  direction as the polar direction) are used. The results shown in figures 2–14 are those 571 for which numerical convergence has been judged within the error invisible in the figures 572 through the comparison with the results obtained with other lattice systems and parameters. 573 574 The momentum conservation law (2.19) provides another measure of accuracy. The values of  $|S_{\rm T}|$  and  $|S_{\rm P}|$ , which should theoretically be zero within the linearized regime, are bounded 575

- respectively by  $6.0 \times 10^{-6}$  and  $3.0 \times 10^{-5}$  for all values of k and  $\hat{\sigma}$  chosen. This also supports the accuracy of the present computation.
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