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A HIERARCHY OF MODELS RELATED TO NANOFLOWS AND SURFACE DIFFUSION

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Abstract. **In last years a great interest was brought to molecular transport problems at nanoscales, such as surface diffusion or molecular flows in nano or sub-nano-channels. In a series of papers V. D. Borman, S. Y. Krylov, A. V. Prosyanov and J. J. M. Beenakker proposed to use kinetic theory in order to analyze the mechanisms that determine mobility of molecules in nanoscale channels. This approach proved to be remarkably useful to give new insight on these issues, such as density dependence of the diffusion coefficient. In this paper we revisit these works to derive the kinetic and diffusion models introduced by V. D. Borman, S. Y. Krylov, A. V. Prosyanov and J. J. M. Beenakker by using classical tools of kinetic theory such as scaling and systematic asymptotic analysis. Some results are extended to less restrictive hypothesis.**

to the memory of Carlo Cercignani

1. Introduction.

In last years a great interest was brought to micro and nanoflows, in part driven by applications such as MEMS, micropumps, lab-on-the-chip systems, carbon nanotubes, molecular sieves, etc. Such flows through micro or nanogeometries (micro- or nano-channels or micro or nano-porous materials) exhibit unusual behavior and therefore create the need for new or more precise models for

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numerical simulations.

The gas flows in micro-geometries are often characterized by rather large Knudsen number but small Reynolds and Mach number. Moreover some phenomena which are usually neglected in classical fluid dynamics may take importance, such as thermal creep flow, thermal stress slip flow or thermal edge flow. The main tool at this scale is the kinetic theory used either for direct numerical simulations or for deriving correct fluid limit models able to take into account the main characteristics of the flow. A survey of this approach and a complete bibliography can be found in ([17]) and ([18]) and for diffusion models on specific geometries and applications the reader can refer to ([1]), ([9]) and ([2]). When considering flows through smaller geometries, down to nanoscale, new issues must be addressed (see [3], [14]). The first one occurs when the size of the channel is comparable with the range of interaction of the gas molecules with the wall, i.e., for a diameter of a few nanometers. Then surface-dominated effects become predominant, and in the vicinity of the surface, the gas flow loses its three-dimensional character and becomes two- and, in the limit, one-dimensional, and the mass flux can dramatically exceeds predictions of the Knudsen diffusion model ([13]). Therefore these effects must be included in the models. Finally, more complicated effects occur when the size of the pore is still smaller (around 0.5 nanometer or smaller), and becomes comparable to the de Broglie wavelength and quantum effects must be considered at this scale.

In this paper we focus on gas flows through geometries with characteristic size of some nanometers so that the gas molecule-surface interaction is important but the quantum effects of zero-point energy can be neglected. Traditionally, at this scale, for the numerical simulation, one uses molecular dynamics ([14]), or for surface diffusion, lattice gas hopping models. Unfortunately molecular dynamics leads to expensive computations and is limited to short space and time simulations. A different approach is proposed in a series of papers ([7],[8],[4],[15],[5],[16],[6]). The authors proposed to use kinetic theory in order to analyze the mechanisms that determine mobility of molecules in nanoscale channels. This approach proved to be remarkably useful to give new insight on these issues and, in particular, it was proved that this new kinetic theory of surface diffusion is able to explain in a rather natural way the density dependence of the diffusion coefficient which has been observed for instance in zeolites. Those articles are not enough known in the community of applied mathematics and kinetic theory and it seems interesting to revisit them from a mathematical point of view and to derive the kinetic and diffusion models by using classical tools of kinetic theory such as scaling and systematic asymptotic analysis. In particular the rigorous approach for modelling molecules trapped by surface effects, introduced in ([10]) and ([11]), will be useful in this context. We consider here the simple case of molecules moving in a *2D plane*.

The molecule-surface interaction is located on a narrow layer (typically $L =$ 0.3 nanometers). On microscale geometries, for instance in a pipe with diameter around some micrometers the flow of molecules inside this layer need not to be described precisely and can simply be modelled by a classical boundary condition such as specular or diffuse reflection. For pipes with smaller diameter, about some nanometers, but rather long ($X =$ some micrometers or more), the effect of the molecule-surface interaction is too much important to be described by a simple boundary condition. So the starting point of our study is a kinetic model including the molecule-surface interaction through Vlasov terms which takes into account the potential interaction of the atoms on the surface and through a relaxation term of molecules by phonons which represents the effect of the thermal fluctuations. This is a crude representation of the very complex interaction between molecules and the surface but sufficient to include in the model much more information than the usual boundary conditions. Nevertheless such a model is still very expensive for simulation because of the smallness of the surface layer and the stiffness of the effect of the interaction potential. It is therefore useful to look for other models derived from this basic kinetic equation by asymptotic analysis. The main influence of the surface on the flow is the confinement of some molecules in a narrow zone close to the surface, the "surface layer". On the scale we consider here it is relevant to perform an asymptotic analysis when the ratio $L/X \to 0$. This leads to the second model of the hierarchy, which can be seen as a multi-phase model coupling the bulk flow of molecules outside the range of surface forces and a two energy group kinetic model describing the surface molecules, i.e., the molecules within the range of surface forces (see [7]).

However the kinetic equations for the surface molecules still contain several time scales that can be quite different and make its solution difficult. The first time scale is given by t_{fl} the "time of flight" over the potential well, the second one is given by τ_{ms} the molecule-phonon relaxation time and the last one is given by τ_z, the characteristic time for a molecule to cross the surface layer. These times must be compared with t_{max} the characteristic time of observation of the overall system. When $t_{fl} << t_{max}$, but $\tau_{ms} \approx t_{max}$, in so far as we are interested in the mass flow along the surface we do not need to get information on the variation of the distribution function on a short time scale ($\approx t_{fl}$) and it is useful to derive a kinetic model at a "mesoscopic" time scale comparable to τ_{ms} and t_{max}, by an asymptotic analysis when $t_{fl}/t_{max} \to 0$. If we consider a larger observation time such that $\tau_{ms} << t_{max}$, the system of surface molecules can be described by a diffusion model obtained by an asymptotic limit of the "multi-phase" kinetic model when $\tau_{ms}/t_{max} \to 0$. Thus various diffusion models are derived according to the respective size of τ_{ms} and τ_z. These successive rescalings and asymptotic limits lead to a hierarchy of models which is sketched on figure 2.

This paper is organized as follows. The hierarchy of models indicated above is derived in section 2 to 4 under a simplifying hypothesis on the surface potential and for low density flows for which intermolecular collisions are negligible. In Section 2 we derive a multiphase kinetic model where the equations for the molecules in the range of interaction of the surface reduce from two space-dimension to one-space dimension. Section 3 is devoted to the derivation, when $t_{fl}/t_{max} \to 0$, of a mesoscopic kinetic model for the flow of molecules inside the surface layer assuming that the surface potential is rapidly oscillating in the x-direction parallel to the surface. This homogenized model is derived under the assumption that surface molecules can be described by a one energy group of molecules trapped in the surface layer. In section 4 we study the diffusion limit,when $\tau_{ms}/t_{max} \to 0$, of the kinetic model for surface molecules derived in section 2. In a first step we consider that surface molecules can be described by a one energy group of molecules trapped in the surface layer and we derive the diffusion limit in the isothermal case and afterwards

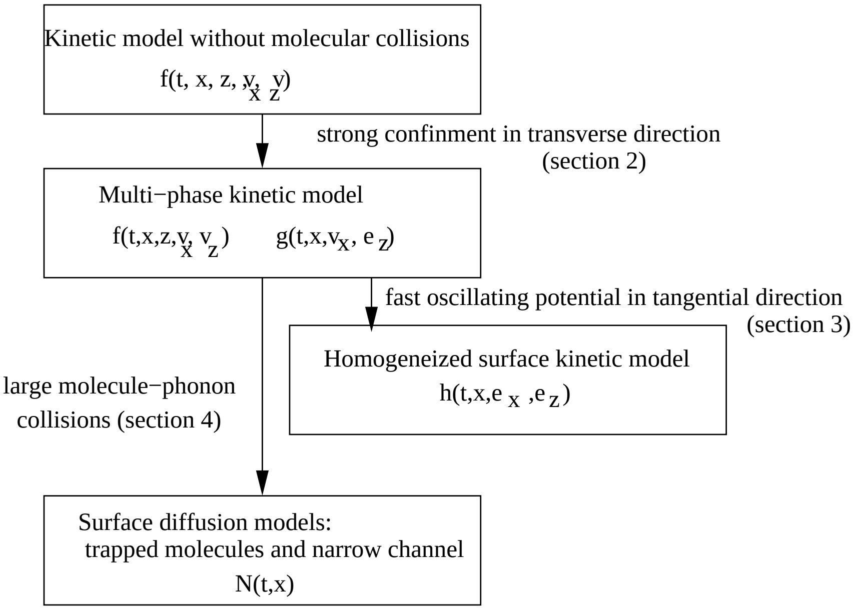

Figure 1. *hierarchy of models.*

in the non-isothermal case. In a second step the diffusion limit is obtained for the two energy group model in the configuration of a narrow channel with two surface layers and no bulk flow and we consider several regimes according to the ratio of τ_{ms} and τ_z.

2. Kinetic model for a gas flow with local interaction with the surface of a solid.

2.1. **Introduction.** In this section we address the issue of modeling a flow of molecules at the vicinity of a solid wall, for instance in a narrow channel. The influence of the interaction of molecules with the surface induces a change in the behavior of the gas flow. It has been noticed in previous works ([3], [6]) that the flow loses its three dimensional character and becomes two- and, in the limit, one-dimensional and the transport is modified by this phenomenon. The same mechanism has been studied in a more rigorous way in ([11]). Here, since we assume that the molecules are moving in a 2D (x, z) plane, the flow near the surface will be a one dimensional flow. Following the ideas presented in ([7]) and ([3]), and the mathematical approach proposed in ([11]), we set up kinetic models that take into account the effect of the molecule-solid interaction and describe the motion of molecules within the range of surface forces in lower dimension space.

For the sake of simplicity we consider that the molecules move in a plane (x, z) (see remark 1 for the case of a 3D-flow near a plane wall) and we consider a solid occupying the half-space $z < 0$, and a set of molecules of a gas moving in the region $z > 0$. The state of the gas is described by the distribution function $F =$

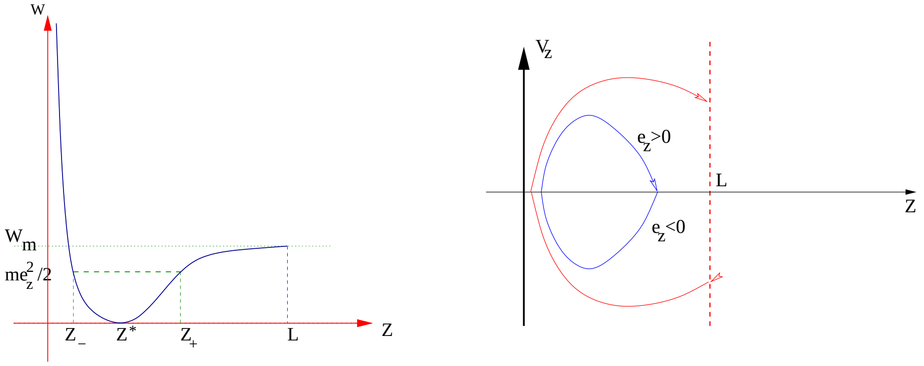

FIGURE 2. *Repulsive-attractive potential (left) and trajectories of molecules in the phase plane (right)*

$F(t,x,z,v_x,v_z)$ and its evolution is modeled by the following kinetic equation

$$\partial_t F + v_x\partial_x F + v_z\partial_z F - \frac{1}{m}\partial_x\mathcal{V}\ \partial_{v_x}F - \frac{1}{m}\partial_z\mathcal{V}\ \partial_{v_z}F = I_{ph} + Q_m, \qquad (1)$$

where $\mathcal{V} = \mathcal{V}(x,z)$ is the the interaction potential of the molecules with the solid, I_{ph} is the molecule-phonon collision integral describing the interaction of the gas molecules with the thermal fluctuations of the solid and Q_m describes the interaction of the gas molecules with each other.

We assume that the potential $\mathcal{V}$ satisfies

1. $0 \le \mathcal{V}$,
2. $\forall x,\ \lim_{z\to 0}\mathcal{V}(x,z) = +\infty$,
3. the normal part of the potential is a repulsive-attractive potential, i.e. for every fixed x the potential $z \to \mathcal{V}(x,z)$ is repulsive (i.e. $\partial_z\mathcal{V}(x,z) < 0$) for $0 \le z < z_m(x)$ and is attractive $(\partial_z\mathcal{V}(z) > 0)$ for $z_m(x) < z$.
4. The range of the surface forces is finite and thus, the potential satisfies $\mathcal{V}(x,z) = \mathcal{V}_m$ for $z \ge L$.

Following ([15]), we assume a simplified form of the collision term describing the interaction between molecules and phonons. This is a crude approximation but sufficient to include in the model new physical effects. More precisely we define

$$\text{for } z < L,\ I_{ph}[F] \quad = \quad \frac{1}{\tau_{ms}}\left(\frac{m\ n[F]}{2k\pi T}M - F\right), \qquad (2)$$

where τ_{ms} is the molecule-phonon relaxation time, M is the dimensionless equilibrium distribution function

$$M(v_x,v_z) = \exp\left(-\frac{m(v_x^2+v_z^2)}{2kT}\right),$$

$$n[F](t,x,z) \quad = \quad \int_{v_z}\int_{v_x} F(t,x,z,v_x,v_z)\ dv_x\ dv_z\ .$$

Let us remark that the right-hand-side in equation (1) satisfies the relation

$$\int \left(\frac{m\ n[F]}{2k\pi T}M - F\right)\ dv = 0,$$

which insures the mass conservation.

Let us notice that the range of the surface forces L is small (typically $L \approx 0.3nm$) and in most cases much smaller than the mean free path of the molecules in the gas phase. Finally, since the interaction of molecules with phonons is important only on a part $[0, L^*]$ of the range L of surface forces ($0 \leq z \leq L^*$, with $L^* < L$), we can assume that $I_{ph} = 0$, for $z \geq L$.
Those assumptions imply that in the bulk flow the motion of the gas molecules is given by the Boltzmann equation

$$\partial_t F + v_x \partial_x F + v_z \partial_z F = Q_m, \tag{3}$$

which is consistent with the classical kinetic theory.

The main goal in our modeling is to take into account the confinement of some gas molecules in the surface layer ($0 \leq z \leq L$) due to the interaction with the surface. But since the width of this surface layer is very small, as indicated above, it is useful to derive by asymptotic analysis a model by assuming that the ratio L/X tends to zero (where X is the characteristic length of observation). The phenomenon of confinement is mainly transverse to the boundary, but since the interaction potential works in both x and z-directions the analysis is rather technically complicated. We suggest to simplify once more the configuration to make easier the analysis while keeping in the model enough important features to put in evidence new phenomena near the surface at the nanoscale. So we assume that the motion of the gas molecules inside the bulk flow is given by (3) and that the motion of the gas molecule inside the range of the surface forces can be separated into two independent components, the tangential and the transverse ones. This can be achieved by assuming that

$$\partial_x \mathcal{V}(x, z) = \varphi(x) \text{ and } \partial_z \mathcal{V}(x, z) = \psi(z),$$

which can be obtained by assuming that the interaction potential writes, for $z < L$

$$\mathcal{V}(x, z) = U(x) + W(z), \tag{4}$$

where W is a repulsive attractive potential with $W(z) = W_m$ for $z \geq L$. Then if $W_m >> U_m$ the well depth of the tangential component of the potential, then we can assume that

$$\text{for} \quad z > L, \quad \mathcal{V}(x, z) = U(x) + W_m \approx W_m, \tag{5}$$

which is consistent with the assumption that the range of the surface forces is smaller than L (see figure (2)).

Another simplification is related to the intermolecular collisions. The study of the influence of the surface layer on the flow is relevant only in geometries with one characteristic dimension (for instance the size of the pore in a porous medium or the diameter of a pipe) about some nanometers. Thus in a first step it is reasonable to assume that we are working at a scale where the intermolecular collisions can be neglected so that

$$Q_m = 0. \tag{6}$$

These assumptions (4-5-6) are used to derive a hierarchy of models describing a gas flow in the vicinity of the surface.

Remark 1. It should be noted that, under the assumptions (2) and (6), we can assume that the molecules are moving in the original 3D space $(x, y, z)(z > 0)$. More specifically, if we assume the 3D version of (2) originally for the molecule-phonon interaction, then F corresponds to the marginal velocity distribution function, i.e., the integral of the original velocity distribution function with respect to v_y from $-\infty$ to ∞.

2.2. **Motion of molecules in a repulsive-attractive potential.**

Before all we need to introduce some notations associated with the motion of a molecule in a one-dimensional repulsive-attractive potential. Let us denote by ε_z the total energy of the normal motion

$$\varepsilon_z = \frac{1}{2} m v_z^2 + W(z),$$

and let us introduce the "equivalent velocity"

$$\text{for } v_z \neq 0,\ e_z = e_z(z, v_z) = sgn(v_z)\sqrt{v_z^2 + \frac{2}{m} W(z)},$$

so that e_z is an odd function of v_z and

$$lim_{v_z \to 0+}\ e_z(z, v_z) = \sqrt{\frac{2}{m} W(z)} \neq lim_{v_z \to 0-}\ e_z(z, v_z) = -\sqrt{\frac{2}{m} W(z)}.$$

We define $z_-(e_z)$ and $z_+(e_z)$ in the following way:

- for $e_z \neq 0$

$$\begin{array}{ll} 0 < z_-(e_z) < z_m < z_+(e_z), & \\ \quad \text{for } 0 < \sqrt{2W_m/m} < |e_z|, & z_+(e_z) = L, \\ & W(z_-(e_z)) = \frac{m}{2} e_z^2, \\ \quad \text{for } 0 < |e_z| < \sqrt{2W_m/m}, & W(z_+(e_z)) = \frac{m}{2} e_z^2, \\ & W(z_-(e_z)) = \frac{m}{2} e_z^2. \end{array}$$

- for $e_z = 0$,

$$z_-(0) = z_m = z_+(0)$$

We notice that the particles with equivalent velocity $|e_z| < \sqrt{2W_m/m}$ are *trapped* (i.e. cannot leave the "surface layer" $0 < z < L$) and move between $z_-(e_z)$ and $z_+(e_z)$, but the particles with $|e_z| > \sqrt{2W_m/m}$ are *free* and move between $z_-(e_z)$ and $z_+(e_z) = L$ and can go out the surface layer and go into the gas (see fig 2). The velocity of a particle with equivalent velocity e_z located at position z, $z_-(e_z) \leq z \leq z_+(e_z)$, is given by

$$v_z(z, e_z) = sgn(e_z)\sqrt{e_z^2 - \frac{2}{m} W(z)}, \quad \text{for } z \in [z_-(e_z), z_+(e_z)], \tag{7}$$

and

$$v_z(z_-(e_z), e_z) = v_z(z_-(-e_z), -e_z) = 0. \tag{8}$$

Moreover, for trapped molecules we have also

$$v_z(z_+(e_z), e_z) = v_z(z_+(-e_z), -e_z) = 0. \tag{9}$$

Let us define

$$\sigma_z(z, e_z) = (e_z^2 - \frac{2}{m} W(z))^{-1/2} \text{ for } |e_z| > \sqrt{2W(z)/m},$$

so that $\sigma_z(z,e_z)\ v_z(z,e_z) = sgn(e_z)$, and

$$\begin{aligned}\tau_z(e_z) &= \int_{z_-(e_z)}^{z_+(e_z)} \sigma_z(z,e_z)dz = \int_{z_-(e_z)}^{z_+(e_z)} (e_z^2 - \frac{2}{m}W(z))^{-1/2}dz,\\ l(e_z) &= |e_z|\ \tau_z(e_z).\end{aligned}$$

As in ([11]), $\tau_z(e_z)$ can be interpreted as the time for a trapped molecule to cross the surface layer and $l(e_z)$ is a length. Moreover, for every fixed $z \in]0, L]$ the application $v_z \to e_z$ is a one-to-one application from $[0, +\infty[$ onto $[\sqrt{\frac{2}{m}W(z)}, +\infty[$ and from (7) we have

$$dv_z = |e_z|\sigma_z(z,e_z)de_z \text{ for } v_z > 0,\ e_z > 0.$$

On the same way, for every fixed $z \in]0, L]$ the application $v_z \to e_z$ is a one-to-one application from $]-\infty, 0]$ onto $]-\infty, -\sqrt{\frac{2}{m}W(z)}]$ and

$$dv_z = |e_z|\sigma_z(z,e_z)de_z \text{ for } v_z < 0,\ e_z < 0.$$

Thus if we denote $\mathcal{E}_z(z) = \{e_z,\ |e_z| > (2W(z)/m)^{1/2}\}$, then for a given function $\psi(z, v_z)$ we have

$$\begin{aligned}\int_{v_z} \psi(z,v_z)\ dv_z &= \int_{v_z>0} \psi(z,v_z)\ dv_z + \int_{v_z<0} \psi(z,v_z)\ dv_z,\\ &= \int_{\sqrt{\frac{2}{m}W(z)}}^{+\infty} \psi(z,v_z(z,e_z))\ |e_z|\sigma_z(z,e_z)de_z\\ &\quad + \int_{-\infty}^{-\sqrt{\frac{2}{m}W(z)}} \psi(z,v_z(z,e_z))\ |e_z|\sigma_z(z,e_z)de_z\\ &= \int_{|e_z|>\sqrt{\frac{2}{m}W(z)}} \psi(z,v_z(z,e_z))\ |e_z|\sigma_z(z,e_z)de_z,\\ &= \int_{\mathcal{E}_z(z)} \psi(z,v_z(z,e_z))\ |e_z|\sigma_z(z,e_z)de_z,\end{aligned}$$

and

$$\begin{aligned}&\int_0^L \int_{\mathcal{E}_z(z)} \psi(z,v_z(z,e_z))|e_z|\sigma_z(z,e_z)\ de_z\ dz\\ &= \int_{e_z} \int_{z_-(e_z)}^{z_+(e_z)} \psi(z,v_z(z,e_z))|e_z|\sigma_z(z,e_z)\ dz\ de_z.\end{aligned}$$

To take into account the molecule-solid interaction we split the flow in two parts, the *surface flow* (for $0 \leq z < L$) and the *bulk flow* (for $L < z$). Since the intermolecular collisions are neglected, the state of the molecules in the bulk flow is described by the distribution function

$$f(t,x,z,v_x,v_z) = F(t,x,z,v_x,v_z),$$

which satisfies the following equation

$$\partial_t f + v_x\partial_x f + v_z\partial_z f = 0.$$

2.3. **Kinetic model for the molecules inside the surface layer.** We consider now the population of molecules inside the surface layer and we split it into two groups. The group of "trapped molecules", with $\mid e_z \mid < \sqrt{2W_m/m}$ and the group of "free molecules" with $\mid e_z \mid > \sqrt{2W_m/m}$. We introduce for $z_-(e_z) \leq z \leq z_+(e_z)$,

$$\begin{aligned} \phi^t(t,x,z,v_x,e_z) &= F(t,x,z,v_x,v_z(z,e_z)), \text{ for } \mid e_z \mid < \sqrt{\frac{2W_m}{m}}, \\ \phi^f(t,x,z,v_x,e_z) &= F(t,x,z,v_x,v_z(z,e_z)), \text{ for } \mid e_z \mid > \sqrt{\frac{2W_m}{m}}, \end{aligned}$$

and

$$\phi(e_z) = \phi^t(e_z)\chi^t(e_z) + \phi^f(e_z)\chi^f(e_z),$$

where $\chi^t(e_z)$ is the characteristic function of the set $\{e_z, |e_z| \leq \sqrt{2W_m/m}\}$ and $\chi^f(e_z)$ is the characteristic function of the set $\{e_z, |e_z| > \sqrt{2W_m/m}\}$. Let us notice that at the boundary of the surface layer ($z = L$) we have

$$\begin{aligned} \phi^f(t,x,L,v_x,e_z) &= f(t,x,L,v_x,v_z(L,e_z)), \text{ for } e_z < 0, \quad (10) \\ f(t,x,L,v_x,v_z) &= \phi^f(t,x,L,v_x,e_z(L,v_z)), \text{ for } v_z > 0. \quad (11) \end{aligned}$$

Then $\phi^a,\ a = t, f$ satisfy

$$\partial_t\phi^a + v_x\partial_x\phi^a - \frac{1}{m}U'(x)\partial_{v_x}\phi^a + v_z(z,e_z)\partial_z\phi^a = \frac{1}{\tau_{ms}}(\frac{n[\phi]}{\gamma_0}M - \phi^a), \quad (12)$$

where τ_{ms} is the molecule-phonon relaxation time, M is the dimensionless equilibrium distribution function

$$M(v_x,e_z) = \exp\left(-\frac{m(v_x^2+e_z^2)}{2kT}\right),$$

$n[\phi]$ is the expression of $n[F]$ in term of the new variables

$$n[\phi] = \int_{v_x}\int_{\mathcal{E}_z(z)} \phi(t,x,z,v_x,e_z)|e_z|\sigma_z(z,e_z)\ de_z\ dv_x,$$

and

$$\gamma_0(z) = \int_{v_x}\int_{\mathcal{E}_z(z)} M(v_x,e_z)|e_z|\sigma_z(z,e_z)\ de_z\ dv_x = \frac{2k\pi T}{m}\exp\left(-\frac{W(z)}{kT}\right).$$

Multiplying (12) by $|e_z|\sigma_z(z,e_z)$, we get

$$\partial_t(|e_z|\sigma_z\phi^a) + v_x\partial_x(|e_z|\sigma_z\phi^a) - \frac{1}{m}U'(x)\partial_{v_x}(|e_z|\sigma_z\phi^a) + e_z\partial_z\phi^a = |e_z|\sigma_z I^a_{ph}[\phi], \quad (13)$$

where

$$I^a_{ph}[\phi] = \frac{1}{\tau_{ms}}\left(\frac{n[\phi]}{\gamma_0}M - \phi^a\right).$$

Let us notice that, from (8-9), we have

$$\phi^t(t,x,z_\pm,v_x,e_z) = \phi^t(t,x,z_\pm,v_x,-e_z) = F(t,x,z_\pm,v_x,0). \quad (14)$$

We introduce the following dimensionless quantities

$$\tilde{t} = \frac{t}{t^*},\ \tilde{\tau}_{ms} = \frac{\tau_{ms}}{\tau^*_{ms}},\ \tilde{x} = \frac{x}{x^*},\ \tilde{z} = \frac{z}{z^*},\ \tilde{e}_{x/z} = \frac{e_{x/z}}{v^*},\ \ \tilde{v}_x = \frac{v_x}{v^*},\ \tilde{v}_z = \frac{v_z}{v^*}. \quad (15)$$

$$\tilde{f} = \frac{f}{\phi^*},\ \ \tilde{\phi} = \frac{\phi}{\phi^*},\ \ \tilde{\sigma}_z = \frac{\sigma_z}{\sigma^*},\ \ \tilde{U} = \frac{U}{U^*}, \tilde{W} = \frac{W}{U^*} \quad (16)$$

where τ^*_{ms} is a reference relaxation time, $t^* = \tau^*_{ms}$, $v^* = \sqrt{(2kT)/m}$ a reference velocity, $x^* = v^*\tau^*_{ms}$ and $z^* = L$ are reference lengths, $\phi^* = n^*/{v^*}^2$, where n^* is a reference number density, $U^* = (m/2){v^*}^2$, $\sigma^* = 1/v^*$. Moreover we introduce

$$\tilde n[\tilde\phi](\tilde t,\tilde x,\tilde z) = \int_{\tilde v_x}\int_{\tilde{\mathcal{E}}_z(\tilde z)} \tilde\phi(\tilde t,\tilde x,\tilde z,\tilde v_x,\tilde e_z)|\tilde e_z|\tilde\sigma_z(\tilde z,\tilde e_z)\, d\tilde e_z\, d\tilde v_x,$$

(where $\tilde{\mathcal{E}}_z(\tilde z) = \{\tilde e_z,\ |\tilde e_z| > \sqrt{\tilde W(\tilde z)}\}$) so that $\tilde n[\tilde\phi] = n[\phi]/n^*$, and

$$\tilde M = \exp\left(-\tilde v_x^2 - \tilde e_z^2\right), \quad \tilde\gamma_0 = \frac{\gamma_0}{{v^*}^2} = \pi\exp\left(-\tilde W\right).$$

Finally we assume that

$$\varepsilon = \frac{z^*}{x^*} << 1,$$

is a small parameter. Inserting (15-16) in equation (13) for $a = t, f$, we get

$$\partial_{\tilde t}(|\tilde e_z|\tilde\sigma_z\tilde\phi^a) + \tilde v_x\partial_{\tilde x}(|\tilde e_z|\tilde\sigma_z\tilde\phi^a) - \frac{1}{2}\tilde U'(\tilde x)\partial_{\tilde v_x}(|\tilde e_z|\tilde\sigma_z\tilde\phi^a) + \frac{1}{\varepsilon}\tilde e_z\partial_{\tilde z}\tilde\phi^a = |\tilde e_z|\tilde\sigma_z\tilde I^a_{ph}[\tilde\phi], \quad (17)$$

where

$$\tilde I^a_{ph}[\tilde\phi] = \frac{1}{\tilde\tau_{ms}}\left(\frac{\tilde n[\tilde\phi]}{\tilde\gamma_0}\tilde M - \tilde\phi^a\right).$$

To derive a "surface equation" we look for a solution of (17) in the following form

$$\tilde\phi^a = \tilde\phi^{a,0} + \varepsilon\tilde\phi^{a,1} + \varepsilon^2\tilde\phi^{a,2} + \ldots, \quad (18)$$

where the function $\tilde\phi^{a,i}$ are taken so that (see (14))

$$\tilde\phi^{t,i}(\tilde t,\tilde x,\tilde z_\pm,\tilde v_x,\tilde e_z) = \tilde\phi^{t,i}(\tilde t,\tilde x,\tilde z_\pm,\tilde v_x,-\tilde e_z), \quad (19)$$

$$\tilde\phi^{f,i}(\tilde t,\tilde x,\tilde z_-,\tilde v_x,\tilde e_z) = \tilde\phi^{f,i}(\tilde t,\tilde x,\tilde z_-,\tilde v_x,-\tilde e_z). \quad (20)$$

Inserting (18) in (17), we get

at leading order

$$\tilde e_z\partial_{\tilde z}\tilde\phi^{a,0} = 0,$$

and thus $\tilde\phi^{a,0}$ does not depend on $\tilde z$, i.e.

$$\tilde\phi^{a,0} = \tilde\phi^{a,0}(\tilde t,\tilde x,\tilde v_x,\tilde e_z). \quad (21)$$

This property together with (19-20) implies that

$$\tilde\phi^{a,0}(\tilde t,\tilde x,\tilde v_x,\tilde e_z) - \tilde\phi^{a,0}(\tilde t,\tilde x,\tilde v_x,-\tilde e_z) = 0,$$

i.e. implies that $\tilde\phi^{a,0}$ is an even function of $\tilde e_z$.

at order + 1

$$\partial_{\tilde t}(|\tilde e_z|\tilde\sigma_z\tilde\phi^{a,0}) + \tilde v_x\partial_{\tilde x}(|\tilde e_z|\tilde\sigma_z\tilde\phi^{a,0}) - \frac{1}{2}\tilde U'(\tilde x)\partial_{\tilde v_x}(|\tilde e_z|\tilde\sigma_z\tilde\phi^{a,0}) + \tilde e_z\partial_{\tilde z}\tilde\phi^{a,1} = |\tilde e_z|\tilde\sigma_z\tilde I^a_{ph}[\tilde{\phi^0}],$$

and since $\tilde\phi^{a,0}$ (and also $|\tilde e_z|\tilde\sigma^z\tilde\phi^{a,0}$) is an even function in $\tilde e_z$ we can take the even part and we obtain

$$\begin{aligned}\partial_{\tilde t}(|\tilde e_z|\tilde\sigma_z\tilde\phi^{a,0}) + \tilde v_x\partial_{\tilde x}(|\tilde e_z|\tilde\sigma_z\tilde\phi^{a,0}) - \frac{1}{2}\tilde U'(\tilde x)\partial_{\tilde v_x}(|\tilde e_z|\tilde\sigma_z\tilde\phi^{a,0})& \\ +\frac{\tilde e_z}{2}[\partial_{\tilde z}\tilde\phi^{a,1}(\tilde e_z) - \partial_{\tilde z}\tilde\phi^{a,1}(-\tilde e_z)] &= |\tilde e_z|\tilde\sigma_z\tilde I^a_{ph}[\tilde{\phi^0}].\end{aligned}$$

Then we integrate with respect to $\tilde{z}$ and denoting $\tilde{l} = \tilde{l}(\tilde{e}_z) = |\tilde{e}_z|\tilde{\tau}_z(\tilde{e}_z)$ where $\tilde{\tau}_z(\tilde{e}_z) = \int_{\tilde{z}_-}^{\tilde{z}_+} \tilde{\sigma}_z(\tilde{z}, \tilde{e}_z)\, d\tilde{z}$, we get,

$$
\begin{aligned}
&\partial_{\tilde{t}}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{a,0}) + \tilde{v}_x\partial_{\tilde{x}}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{a,0}) - \frac{1}{2}\tilde{U}'(x)\partial_{\tilde{v}_x}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{a,0}) \\
&+\frac{\tilde{e}_z}{2}\,[\int_{\tilde{z}_-}^{\tilde{z}_+} \partial_{\tilde{z}}\tilde{\phi}^{a,1}(\tilde{z},\tilde{e}_z)d\tilde{z} - \int_{\tilde{z}_-}^{\tilde{z}_+} \partial_{\tilde{z}}\tilde{\phi}^{a,1}(\tilde{z},-\tilde{e}_z)d\tilde{z}] \quad = \quad \tilde{Q}^{a,*}_{ph}[\tilde{\phi}^0],
\end{aligned}
$$

where

$$
\begin{aligned}
\tilde{Q}^{a,*}_{ph}[\tilde{\phi}^0] &= \frac{\tilde{l}(\tilde{e}_z)}{\tilde{\tau}_{ms}}\left(\tilde{\Theta}^*[\tilde{\phi}^0]\tilde{M} - \tilde{\phi}^{a,0}\right), \\
\tilde{\Theta}^*[\tilde{\phi}^0](\tilde{t},\tilde{x},\tilde{e}_z) &= \frac{1}{\tilde{\tau}_z}\int_{\tilde{z}_-}^{\tilde{z}_+} (\tilde{n}[\tilde{\phi}^0](\tilde{t},\tilde{x},\tilde{z})\tilde{\sigma}_z(\tilde{z},\tilde{e}_z)/\tilde{\gamma}_0(\tilde{z}))\, d\tilde{z}
\end{aligned}
$$

But we remark that

$$
\begin{aligned}
\frac{\tilde{e}_z}{2}\int_{\tilde{z}_-}^{\tilde{z}_+} \partial_{\tilde{z}}(\tilde{\phi}^{a,1}(\tilde{z},\tilde{e}_z) - \tilde{\phi}^{a,1}(\tilde{z},-\tilde{e}_z))d\tilde{z} \quad &= \quad \frac{\tilde{e}_z}{2}([\tilde{\phi}^{a,1}(\tilde{z}_+,\tilde{e}_z) - \tilde{\phi}^{a,1}(\tilde{z}_+,-\tilde{e}_z)] - \\
&[\tilde{\phi}^{a,1}(\tilde{z}_-,\tilde{e}_z) - \tilde{\phi}^{a,1}(\tilde{z}_-,-\tilde{e}_z)]), \quad (22)
\end{aligned}
$$

Let us first consider the trapped molecules (i.e. $a = t$). From (19) we can conclude that this term vanishes. Thus, we obtain the following equation (in dimensionless form) for the trapped molecules

$$
\partial_{\tilde{t}}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{t,0}) + \tilde{v}_x\partial_{\tilde{x}}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{t,0}) - \frac{1}{2}\tilde{U}'(x)\partial_{\tilde{v}_x}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{t,0}) \quad = \quad \tilde{Q}^{t,*}_{ph}[\tilde{\phi}^0].
$$

We introduce the dimensionless 1D distribution function $\tilde{g}$ which is a density number of molecules per x-unit

$$
\begin{aligned}
\tilde{g}^t(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z) &= \tilde{l}(\tilde{e}_z)\tilde{\phi}^{t,0}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z), \\
\tilde{g}^0(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z) &= \tilde{l}(\tilde{e}_z)\tilde{\phi}^{t,0}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z)\tilde{\chi}^t(\tilde{e}_z) + \tilde{l}(\tilde{e}_z)\tilde{\phi}^{f,0}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z)\tilde{\chi}^f(\tilde{e}_z),
\end{aligned}
$$

where $\tilde{\chi}^t(\tilde{e}_z)$ is the characteristic function of the set $\{\tilde{e}_z, |\tilde{e}_z| \leq \sqrt{\tilde{W}_m}\}$ and $\tilde{\chi}^f(\tilde{e}_z)$ is the characteristic function of the set $\{\tilde{e}_z, |\tilde{e}_z| > \tilde{W}_m\}$. Then the above equation writes

$$
\partial_{\tilde{t}}\tilde{g}^t + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}^t - \frac{1}{2}\tilde{U}'(x)\partial_{\tilde{v}_x}\tilde{g}^t \quad = \quad \tilde{Q}^t_{ph}[\tilde{g}^0],
$$

where

$$
\begin{aligned}
\tilde{Q}^t_{ph}[\tilde{g}^0] &= \frac{1}{\tilde{\tau}_{ms}}\left(\tilde{\Theta}[\tilde{g}^0]\tilde{l}(\tilde{e}_z)\tilde{M} - \tilde{g}^t\right), \\
\tilde{\Theta}[\tilde{g}^0](\tilde{t},\tilde{x},\tilde{e}_z) &= \frac{1}{\tilde{\tau}_z(\tilde{e}_z)}\int_{\tilde{z}_-}^{\tilde{z}_+} (\tilde{n}[\tilde{g}^0/\tilde{l}](\tilde{t},\tilde{x},\tilde{z})\tilde{\sigma}_z(\tilde{z},\tilde{e}_z)/\tilde{\gamma}_0(\tilde{z}))\, d\tilde{z}.
\end{aligned}
$$

Let us now consider the "free molecules". We first remark that (from (18) and (21))

$$
\tilde{l}(\tilde{e}_z)\tilde{\phi}^{f,0} = \tilde{l}(\tilde{e}_z)\tilde{\phi}^f(1,\tilde{e}_z) + \mathcal{O}(\varepsilon).
$$

Moreover the flux term is given by (22), with $a = f$ and $\tilde{z}_+ = 1$ in dimensionless variables. As previously the term in $\tilde{z}_-$ vanishes because of (20) but the term in $\tilde{z}_+ = 1$ does not vanish and represents the flux of molecules between the surface

layer and the bulk flow (see figure 2).
Then (22) for free molecules writes

$$\frac{\tilde{e}_z}{2}[\tilde{\phi}^{f,1}(1,\tilde{e}_z)-\tilde{\phi}^{f,1}(1,-\tilde{e}_z)]$$

which can be equivalently written (since $\tilde{\phi}^{f,0}(1,\tilde{e}_z)-\tilde{\phi}^{f,0}(1,-\tilde{e}_z)$=0)

$$\frac{\tilde{e}_z}{2\varepsilon}[\tilde{\phi}^{f,0}(1,\tilde{e}_z)+\varepsilon\tilde{\phi}^{f,1}(1,\tilde{e}_z)-(\tilde{\phi}^{f,0}(1,-\tilde{e}_z)+\varepsilon\tilde{\phi}^{f,1}(1,-\tilde{e}_z))].$$

But from (18), we have $\tilde{\phi}^{f,0}+\varepsilon\tilde{\phi}^{f,1}=\tilde{\phi}^{f}+\mathcal{O}(\varepsilon^2)$, so that the flux term writes

$$\frac{\tilde{e}_z}{2\varepsilon}[\tilde{\phi}^{f}(1,\tilde{e}_z)-\tilde{\phi}^{f}(1,-\tilde{e}_z)]+\mathcal{O}(\varepsilon),$$

and since $\tilde{\phi}^{f,0}=\tilde{\phi}^{f}+\mathcal{O}(\varepsilon)$ we have

$$\begin{aligned}\partial_{\tilde{t}}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{f}(1,\tilde{e}_z))+\tilde{v}_x\partial_{\tilde{x}}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{f}(1,\tilde{e}_z))-\frac{1}{2}\tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{f}(1,\tilde{e}_z))&\\ +\frac{\tilde{e}_z}{2\varepsilon}[\tilde{\phi}^{f}(1,\tilde{e}_z)-\tilde{\phi}^{f}(1,-\tilde{e}_z)]&=\\ \frac{\tilde{l}(\tilde{e}_z)}{\tilde{\tau}_{ms}}\left(\tilde{\Theta}^*[\tilde{\phi}^{t,0}\tilde{\chi}^t+\tilde{\phi}^{f}\tilde{\chi}^{f}]\tilde{G}-\tilde{\phi}^{f}(1,\tilde{e}_z)\right)+\mathcal{O}(\varepsilon),&\end{aligned}$$

Using (10) and denoting (with some abuse of notation),

$$\tilde{\phi}^{f}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z)=\tilde{\phi}^{f}(\tilde{t},\tilde{x},1,\tilde{v}_x,\tilde{e}_z),$$

the equation of the free molecules finally writes

$$\begin{aligned}\partial_{\tilde{t}}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{f})+\tilde{v}_x\partial_{\tilde{x}}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{f})-\frac{1}{2}\tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}(\tilde{l}(\tilde{e}_z)\tilde{\phi}^{f})&\\ +\frac{|\tilde{e}_z|}{2\varepsilon}[\tilde{\phi}^{f}(|\tilde{e}_z|)-\tilde{f}(-|\tilde{v}_z(1,\tilde{e}_z)|)]&=\\ \frac{\tilde{l}(\tilde{e}_z)}{\tilde{\tau}_{ms}}\left(\tilde{\Theta}^*[\tilde{\phi}^{t,0}\tilde{\chi}^t+\tilde{\phi}^{f}\tilde{\chi}^{f}]\tilde{G}-\tilde{\phi}^{f}\right)+\mathcal{O}(\varepsilon).&\end{aligned}$$

Introducing as previously

$$\begin{aligned}\tilde{g}^{f}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z)&=\tilde{l}(\tilde{e}_z)\tilde{\phi}^{f}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z),\\ \tilde{g}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z)&=\tilde{g}^{t}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z)\tilde{\chi}^{t}(\tilde{e}_z)+\tilde{g}^{f}(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z)\tilde{\chi}^{f}(\tilde{e}_z),\end{aligned}$$

this equation writes

$$\partial_{\tilde{t}}\tilde{g}^{f}+\tilde{v}_x\partial_{\tilde{x}}\tilde{g}^{f}-\frac{1}{2}\tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}^{f}+\frac{1}{2\varepsilon\;\tilde{\tau}_z}[\tilde{g}^{f}(|\tilde{e}_z|)-\tilde{l}(\tilde{e}_z)\tilde{f}(-|\tilde{v}_z(1,\tilde{e}_z)|)]=\tilde{Q}^{f}_{ph}[\tilde{g}]+\mathcal{O}(\varepsilon),$$

where $\tilde{Q}^{f}_{ph}[\tilde{g}]=\frac{1}{\tilde{\tau}_{ms}}\left(\tilde{\Theta}[\tilde{g}]\tilde{l}(\tilde{e}_z)\tilde{M}-\tilde{g}^{f}\right)$. Let us remark that $\tilde{\Theta}[\tilde{g}^0]=\tilde{\Theta}[\tilde{g}]+\mathcal{O}(\varepsilon)$, so that the equation for trapped molecules writes

$$\partial_{\tilde{t}}\tilde{g}^{t}+\tilde{v}_x\partial_{\tilde{x}}\tilde{g}^{t}-\frac{1}{2}\tilde{U}'(x)\partial_{\tilde{v}_x}\tilde{g}^{t}\quad=\quad\tilde{Q}^{t}_{ph}[\tilde{g}]+\mathcal{O}(\varepsilon),$$

Denoting $\tilde{f}^{s}(\tilde{e}_z)=\tilde{f}(-|\tilde{v}_z(1,\tilde{e}_z)|)$ and neglecting $\mathcal{O}(\varepsilon)$ terms in the above equations for free and trapped molecules, we finally obtain the following system of coupled equations (in dimensionless form)

$$\begin{aligned}\partial_{\tilde{t}}\tilde{g}^{t}+\tilde{v}_x\partial_{\tilde{x}}\tilde{g}^{t}-\frac{1}{2}\tilde{U}'(x)\partial_{\tilde{v}_x}\tilde{g}^{t}&=\tilde{Q}^{t}_{ph}[\tilde{g}],\\ \partial_{\tilde{t}}\tilde{g}^{f}+\tilde{v}_x\partial_{\tilde{x}}\tilde{g}^{f}-\frac{1}{2}\tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}^{f}+\frac{1}{2\varepsilon\tilde{\tau}_z}[\tilde{g}^{f}(|\tilde{e}_z|)-\tilde{l}\tilde{f}^{s}]&=\tilde{Q}^{f}_{ph}[\tilde{g}].\end{aligned}$$

Now we come back to dimensional quantities, noticing that $\tau_z^* = z^*/v^* = \varepsilon\tau_{ms}^*$ and we define

$$
\begin{aligned}
g^t(t,x,v_x,e_z) &= \frac{n^*z^*}{{v^*}^2}\tilde{g}^t(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z),\\
g^f(t,x,v_x,e_z) &= \frac{n^*z^*}{{v^*}^2}\tilde{g}^f(\tilde{t},\tilde{x},\tilde{v}_x,\tilde{e}_z),\\
g(t,x,v_x,e_z) &= g^t(t,x,v_x,e_z)\chi^t(e_z) + g^f(t,x,v_x,e_z)\chi^f(e_z).
\end{aligned}
$$

We obtain finally the system governing the flow of molecules

Proposition 1. *Under hypothesis (4-5-6), in the limit of a small surface layer ($\varepsilon = \frac{L}{x^*} \to 0$), the flow of molecules can be described by the following multi-phase kinetic model*

$$
\begin{aligned}
\partial_t f + v_x\partial_x f + v_z\partial_z f &= 0, \qquad (23)\\
\partial_t g^t + v_x\partial_x g^t - \frac{1}{m}U'(x)\partial_{v_x} g^t &= Q_{ph}^t, \qquad (24)\\
\partial_t g^f + v_x\partial_x g^f - \frac{U'(x)}{m}\partial_{v_x} g^f - \frac{l\; f^s - g^f(|e_z|)}{2\tau_z} &= Q_{ph}^f, \qquad (25)\\
l(e_z)f(t,x,L,v_x,v_z)_{|v_z>0} &= g^f(t,x,v_x,e_z(L,v_z)), \qquad (26)
\end{aligned}
$$

where

$$
\begin{aligned}
Q_{ph}^a &= \frac{1}{\tau_{ms}}\left(\Theta[g]l(e_z)M - g^a\right), \quad a = t,f\\
\Theta[g](t,x,e_z) &= \frac{1}{\tau_z(e_z)}\int_{z_-(e_z)}^{z_+(e_z)} (n[g/l](t,x,z)\sigma_z(z,e_z)/\gamma_0(z))dz,\\
f^s(t,x,v_x,e_z) &= f(t,x,L,v_x,-|v_z(L,e_z)|),\\
l(e_z) &= |e_z|\;\tau_z(e_z).
\end{aligned}
$$

Remark 2.

1. This model can be interpreted as a multiphase model. The first phase, constituting of the bulk flow of molecules outside the range of the surface forces, is described by a usual kinetic equation (23). The molecules within the range of the surface forces are considered as a separate phase described by a two energy-group kinetic model, with the low energy "trapped molecules" (24) and the high energy "free molecules" (25). The two groups are coupled by the collision terms. The two phases are coupled by the relation (26) and the last term of the left-hand-side of equation (25). Let us notice that equations (24) and (25) do not give a precise description of the flow of the surface molecules with respect to the distance z to the surface, but give a relevant information of the flow parallel to the surface, and therefore will be useful for evaluating the transport flux in this direction.
2. The distribution function $f(t,x,z,v_x,e_z)$ describes the number density of gas molecules with velocity (v_x,v_z) in a unit (x,z)-area, but the distribution functions $g^t(t,x,v_x,e_z)$ and $g^f(t,x,v_x,e_z)$ describe a number density of surface molecules with velocity $(v_x,\ e_z)$ per unit x-length. As a consequence $\int_0^L n[\phi](t,x,z)dz$ is the number density of surface molecules per unit x-length. Moreover we can easily verify that

$$
\int_{e_z}\int_{v_x} Q_{ph}(v_x,e_z)\; dv_x\; de_z = 0,
$$

which ensures the local conservation of mass for surface molecules.

3. In this multiphase model, the "surface" of the solid part is identified to the interface $z = L$ between the surface layer and the bulk flow. Equation (23) describes the gas flow and equations (24-25) give a simplified description of what can be interpreted as a motion of molecules on the "surface". The condition (26) can be interpreted as a non local boundary condition for the bulk flow giving a description of the interaction between the gas molecules and the wall which is more detailed than usual local boundary conditions. More precisely, some molecules go from the bulk flow into the surface layer, are sent back by the repulsive interaction potential and immediately escape from the surface layer into the bulk flow, giving a specular reflexion. On the other hand, some molecules can go from the bulk flow into the surface layer, can have a collision with phonons and lose enough transverse energy so that they are trapped inside the boundary layer (where they are transported according to (24)) and, after some time, can gain in a collision with phonons enough energy to escape from the surface layer. Since τ_{ms} is small compared with the characteristic time of evolution of the bulk flow, this complicated interaction with the solid surface described by the multiphase model can be interpreted in a first approximation as a reflexion of the molecule by the boundary.

3. 1D-mesoscopic kinetic equation for surface molecules.

3.1. **Introduction.** In section 2 we derived a multiphase model describing the coupling of the bulk flow with the motion of molecules on the surface. This motion is given by a set of two coupled kinetic equations on variable x, including a Vlasov term due to the interaction potential parallel to the surface. In many applications this potential field is periodic with a small period 2δ that could be much smaller than the characteristic distance x^*, but nevertheless, for consistency with the asymptotic analysis leading to theorem 1, we assume that

$$L << \delta << x^*. \tag{27}$$

Some of the surface molecules have a small tangential energy so that they are *bound* in a potential well where they are oscillating very rapidly. At the scale x^* they can be considered as motionless. On the contrary surface molecules with a high tangential energy are *unbound* and can move across the potential wells, but their velocity strongly oscillate. In so far as we are interested in the mass flow along the surface over a domain much longer than δ we do not need to get information on the distribution function at the "microscopic" scale of a potential unit cell. Thus it is useful to derive a kinetic model at a "mesoscopic" scale larger than δ but comparable to l_{mp} the mean free path between two "collisions" with phonons. At this scale a kinetic model describing the motion of the unbound molecules by their average velocity over the potential cells is relevant. In this section we derive such a model in a simple configuration where we assume that the free molecules in the surface layer can be neglected so that all surface molecules are trapped. This is justified when $W_m >> kT$, which is true for some practical situations, and only very few molecules can escape from the interaction range of the normal interaction potential W so that $n[g^t + g^f] \approx n[g^t]$. In such situations it is reasonable to assume that

$$W_m = +\infty, \tag{28}$$

so that when a molecule enters the surface layer, it cannot escape. Moreover we neglect the flux of incoming molecules. This model is derived from the kinetic equation (24) by an asymptotic analysis when $\delta/x^* \to 0$. For this asymptotic analysis we consider the hypothesis (4-5-6), as above. Moreover we assume that the molecule-phonon relaxation time is constant i.e.

$$\tau_{ms} = const \tag{29}$$

and that U (the tangential part of the potential) is periodic with period 2δ. More precisely

$$U(x) = \hat{U}(x/\delta), \tag{30}$$

where $\hat{U}(y)$ is a periodic potential with period 2 defined on $[-1,+1]$ and such that $0 \le \hat{U}(y) \le U_m$ and $\hat{U}(\pm 1) = U_m$.

Before to derive such a model we need to introduce some notations related to the motion of a molecule in a periodic potential field. We denote

$$\text{for } v_x \neq 0,\ e_x = e_x(x, v_x) = sgn(v_x)\sqrt{v_x^2 + \frac{2}{m}U(x)}.$$

For any fixed x the application $v_x \to e_x$ is a one to one application from $[0,+\infty[$ onto $[\sqrt{2U(x)/m}, +\infty[$, and also $v_x \to e_x$ is a one to one application from $]-\infty, 0]$ onto $]-\infty, -\sqrt{2U(x)/m}]$ so that we have

$$\text{for } |e_x| > \sqrt{2U(x)/m},\ v_x(x, e_x) = sgn(e_x)\sqrt{e_x^2 - \frac{2}{m}U(x)}.$$

The jacobian of the application $e_x \to v_x$ (for $e_x > 0$ for instance) is given by

$$\text{for } v_x > 0,\ dv_x = |e_x|\sigma_x(x, e_x)de_x,$$

where

$$\sigma_x(x, e_x) = (e_x^2 - \frac{2}{m}U(x))^{-1/2},\ \text{ for } |e_x| > \sqrt{2U(x)/m}.$$

and in the same way

$$\text{for } v_x < 0,\ dv_x = |e_x|\sigma_x(x, e_x)de_x.$$

Then denoting

$$\mathcal{E}_x(x) = \{e_x,\ |e_x| > (2U(x)/m)^{1/2}\},$$

we have for every integrable function $\psi(v_x)$,

$$\int_{v_x} \psi(x, v_x)dv_x = \int_{\mathcal{E}_x(x)} \psi(x, v_x(x, e_x))|e_x|\sigma_x(x, e_x)\ de_x.$$

The trajectories of the molecules in the (x, v_x) plane are the level curves of the the total energy $E(x, v_x) = me_x^2/2$ (see fig 3). If the energy of a molecule is less than U_m, then its trajectory is a closed curve (*bound molecule*), the molecule is trapped in a potential well. On the other hand, if its energy is larger than U_m its trajectory is an open curve (*unbound molecule*) and those unbound molecules generate a flow in the x-direction.

Since the tangential potential U is periodic with a small period 2δ, the velocity $v_x(x, e_x) = sgn(e_x)\sqrt{e_x^2 - \frac{2}{m}U(x)}$ is rapidly oscillating. If we look at the surface molecules on a space scale $x^* >> \delta$, the average velocity of the bound molecules is

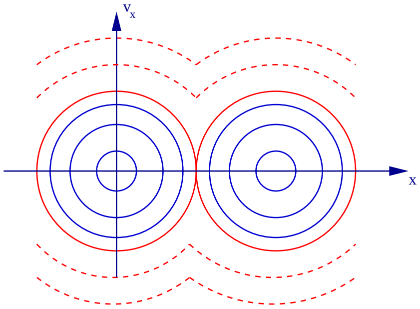

FIGURE 3. trajectories in the phase space (x, v_x) for $\hat{U}(y) = ky^2/2$.

equal to zero. On the other hand the average velocity of an unbound molecule can be obtained as follows. We introduce $-1 \le y_-(e_x) \le y_+(e_x) \le +1$, defined by

$$\hat{U}(y_\pm(e_x)) = \frac{m}{2}e_x^2, \text{ for } e_x^2 \le \frac{2}{m}U_m, \tag{31}$$

$$y_\pm(e_x) = \pm 1, \text{ for } e_x^2 > \frac{2}{m}U_m, \tag{32}$$

and we define for $y \in [-1, +1]$,

$$\begin{aligned} v_x^\#(y, e_x) &= sgn(e_x)\sqrt{e_x^2 - \frac{2}{m}\hat{U}(y)}, \quad \text{if } e_x^2 > \frac{2U_m}{m}, \\ v_x^\#(y, e_x) &= sgn(e_x)\sqrt{e_x^2 - \frac{2}{m}\hat{U}(y)}, \quad \text{if } e_x^2 \le \frac{2U_m}{m} \text{ and } y \in [y_-(e_x), y_+(e_x)], \\ v_x^\#(y, e_x) &= 0, \quad \text{if } e_x^2 \le \frac{2U_m}{m} \text{ and } y \notin [y_-(e_x), y_+(e_x)], \end{aligned}$$

and

$$\sigma_x^\#(y, e_x) = \frac{sgn(e_x)}{v_x^\#(y, e_x)},$$

so that $\sigma_x^\#(y, e_x) = +\infty$, for $y \notin [y_-(e_x), y_+(e_x)]$. Finally, we introduce $\overline{\sigma}_x(e_x)$ defined by

$$\overline{\sigma}_x(e_x) = \frac{1}{2}\int_{y_-(e_x)}^{y_+(e_x)} \sigma_x^\#(y, e_x)dy = \frac{1}{2}\int_{y_-(e_x)}^{y_+(e_x)} (e_x^2 - \frac{2}{m}\hat{U}(y))^{-1/2}dy.$$

Let us consider now an unbound molecule moving in the one dimensional periodic field $U(x) = \hat{U}(\frac{x}{\delta})$ with an "equivalent velocity" e_x. The position x of the molecule is a monotonic function of t, so that we can consider also $t = t(x)$ as a monotonic function of x. Since

$$dx = (e_x^2 - \frac{2}{m}\hat{U}(\frac{x}{\delta}))^{1/2}dt,$$

we have

$$dt = (e_x^2 - \frac{2}{m}\hat{U}(\frac{x}{\delta}))^{-1/2}dx,$$

and the "time of flight", necessary for the considered molecule to cross a potential well (i.e. for going from $x = (i-1)\delta$ to $x = (i+1)\delta$) is

$$\begin{aligned}\tau_{fl}(e_x) &= \int_{(i-1)\delta}^{(i+1)\delta} (e_x^2 - \frac{2}{m}\hat{U}(\frac{x}{\delta}))^{-1/2} dx = \delta \int_{-1}^{+1} (e_x^2 - \frac{2}{m}\hat{U}(y))^{-1/2} dy, \\ &= \delta \int_{-1}^{+1} \sigma_x^{\#}(y, e_x) dy = \frac{2\delta}{|w_x(e_x)|},\end{aligned}$$

where the mean velocity $w_x(e_x)$ of the molecule is given by

$$w_x(e_x) \overset{def}{=} \frac{2\ sgn(e_x)\ \delta}{\tau_{fl}(e_x)}.$$

Let us notice that bound molecules, with an "equivalent velocity" e_x with $me_x^2 \leq 2U_m$, are trapped in a potential well, between $(i + y_-(e_x)\delta)$ and $(i + y_+(e_x)\delta)$. Thus for such a molecule, the time necessary to cross a potential well can be considered as infinite and by consequence the average velocity on a large scale $x^* >> \delta$ can be considered as null, which is consistent with the above definitions of $\sigma_x^{\#}(y, e_x)$ and of w_x.

3.2. **Homogenization of the surface kinetic model.** To describe the flow in the x-direction induced by unbound molecules we start from the kinetic equation (24) for trapped surface molecules, in which we express the distribution functions in term of the variable $e_x,\ e_z$, i.e. we introduce h^t given by

$$h^t(t, x, e_x, e_z) \overset{\text{def}}{=} g^t(t, x, v_x(x, e_x), e_z).$$

Moreover we denote $h_c^t(t, x, e_x, e_z) = h^t(t, x, e_x, e_z)\chi_c(e_x),\ c = b, u$, where $\chi_b(e_x)$ is the characteristic function of the set $\{e_x,\ |e_x| \leq \sqrt{2U_m/m}\}$ and $\chi_u(e_x)$ is the characteristic function of the set $\{e_x,\ |e_x| > \sqrt{2U_m/m}\}$. From the definition of $y_\pm(e_x)$ (31-32), it comes for bound molecules

$$h_b^t(t, \delta y_\pm(e_x), e_x, e_z) = h_b^t(t, \delta y_\pm(-e_x), -e_x, e_z) = g^t(t, \delta y_\pm(e_x), 0, e_z). \qquad (33)$$

Let us recall that the evolution of the surface molecules is described by equations (24) which can be written

$$\partial_t g^t + v_x \partial_x g^t - \frac{1}{m} U'(x) \partial_{v_x} g^t \quad = \quad {Q_{ph}}^t,$$

From the definition of h^t, we get $\partial_t h^t = \partial_t g^t$, and $\partial_x h^t = \partial_x g^t + \partial_{v_x} g^t \partial_x v_x$, or $\partial_x h^t = \partial_x g^t - \frac{U'(x)}{m v_x(x, e_x)} \partial_{v_x} g^t$, so that

$$v_x(x, e_x)\partial_x h^t = v_x(x, e_x)\partial_x g^t - \frac{1}{m} U'(x) \partial_{v_x} g^t,$$

and finally the distribution function $h^t(t, x, e_x, e_z)$ satisfies the following kinetic equation

$$\partial_t h^t + v_x(x, e_x)\partial_x h^t \quad = \quad \frac{1}{\tau_{ms}} \left(\Theta[h^t] l(e_z) M - h^t \right), \qquad (34)$$

where

$$\begin{aligned}
\Theta[h] &= \frac{1}{\tau_z(e_z)} \int_{z_-(e_z)}^{z_+(e_z)} (n[h/l]\sigma_z(z,e_z)/\gamma_1(x,z))dz, \\
n[\varphi] &= \int_{\mathcal{E}_z(z)} \int_{\mathcal{E}_x(x)} \varphi(t,x,e_x,e_z)|e_x|\sigma_x(x,e_x)|e_z|\sigma_z(z,e_z)\ de_x\ de_z, \\
M(e_x,e_z) &= e^{-m(e_x^2+e_z^2)/(2kT)}, \\
\gamma_1(x,z) &= \frac{2\pi kT}{m} \exp\left(-\frac{U(x)+W(z)}{kT}\right).
\end{aligned}$$

To derive a kinetic model at a ”mesoscopic scale” (i.e. on a characteristic length $x^* >> \delta$), we introduce the following dimensionless quantities

$$\tilde{x} = \frac{x}{x^*},\ \tilde{l} = \frac{l}{z^*},\ \tilde{v}_x = \frac{v_x}{v^*},\ \tilde{e}_{x/z} = \frac{e_{x/z}}{v^*},\ \tilde{t} = \frac{t}{t^*},\ \tilde{\tau} = \frac{\tau_{ms}}{t^*},\ \tilde{n} = \frac{n}{n^*}, \tag{35}$$

and

$$\tilde{\Theta} = \frac{\Theta\ v^{*2}}{n^*},\ \tilde{h}^t = \frac{h^t}{h^*},\ \tilde{\sigma}_x = \frac{\sigma_x}{\sigma^*},\ \tilde{\sigma}_x^{\#} = \frac{\sigma_x^{\#}}{\sigma^*},\ \tilde{U} = \frac{\hat{U}}{U^*},\ \tilde{W} = \frac{\hat{W}}{U^*}, \tag{36}$$

where x^* is a reference length, $v^* = \sqrt{2kT/m}$, $t^* = x^*/v^*$ is a reference time, $U^* = (m/2)v^{*2}$, n^* is a reference number density, $h^* = (n^* z^*)/v^{*2}$, $\sigma^* = 1/v^*$, so that

$$\tilde{v}_x(\tilde{x},\tilde{e}_x) = sgn(\tilde{e}_x)\sqrt{\tilde{e}_x^2 - \tilde{U}(\tilde{x}x^*/\delta)}.$$

Moreover we assume that the reference length $x^* >> \delta$, so that the ratio

$$\varepsilon = \frac{\delta}{x^*} << 1$$

is a small parameter. We now derive an asymptotic model in the limit $\varepsilon \to 0$, and we describe the asymptotic expansion for the trapped molecules.

Inserting (35-36) in the kinetic equation (34) we obtain

$$\partial_{\tilde{t}}(\tilde{h}^t) + sgn(\tilde{e}_x)\sqrt{\tilde{e}_x^2 - \tilde{U}(\tilde{x}/\varepsilon)}\partial_{\tilde{x}}(\tilde{h}^t) = \frac{1}{\tilde{\tau}}\left(\tilde{\Theta}[\tilde{h}^t]\tilde{l}\tilde{M} - \tilde{h}^t\right),$$

and we look for a solution in the following form

$$\tilde{h}^t(\tilde{t},\tilde{x},\frac{\tilde{x}}{\varepsilon},\tilde{e}_x,\tilde{e}_z) = \tilde{h}^{t,0}(\tilde{t},\tilde{x},\frac{\tilde{x}}{\varepsilon},\tilde{e}_x,\tilde{e}_z) + \varepsilon\tilde{h}^{t,1}(\tilde{t},\tilde{x},\frac{\tilde{x}}{\varepsilon},\tilde{e}_x,\tilde{e}_z) + ... \tag{37}$$

where $\tilde{h}^{t,i}(\tilde{t},\tilde{x},y,\tilde{e}_x,\tilde{e}_z)$, $i = 0,1,...$ are periodic functions in y with period 2 and where, for bound molecules (to be consistent with (33) and the definition of $y_-(e_x)$ and $y_+(e_x)$)

$$\tilde{h}_b^{t,i}(\tilde{t},\tilde{x},y_\pm(\tilde{e}_x),\tilde{e}_x,\tilde{e}_z) = \tilde{h}_b^{t,i}(\tilde{t},\tilde{x},y_\pm(-\tilde{e}_x),-\tilde{e}_x,\tilde{e}_z). \tag{38}$$

Then $\tilde{h}^t$ satisfies

$$\partial_{\tilde{t}}(\tilde{h}^t) + sgn(\tilde{e}_x)\sqrt{\tilde{e}_x^2 - \tilde{U}(\tilde{x}/\varepsilon)}\ [\partial_{\tilde{x}} + \frac{1}{\varepsilon}\partial_y](\tilde{h}^t) = \frac{1}{\tilde{\tau}}\left(\tilde{\Theta}[\tilde{h}^t]\tilde{l}\tilde{M} - \tilde{h}^t\right), \tag{39}$$

where

$$\begin{aligned}
\tilde\Theta[\tilde h^t] &= \frac{1}{\tilde{\tau}_z}\int_{\tilde z_-(\tilde e_z)}^{\tilde z_+(\tilde e_z)} (\tilde n[\tilde h^t/\tilde l]\ \tilde\sigma_z(\tilde z,\tilde e_z)/\tilde\gamma_1(\tilde x/\varepsilon,\tilde z))d\tilde z,\\
\tilde n[\tilde\varphi^*] &= \int_{\tilde{\mathcal{E}}_z(\tilde z)}\int_{\tilde{\mathcal{E}}_x^{\#}(y)} \tilde\varphi^*(\tilde t,\tilde x,y,\tilde e_x,\tilde e_z)|\tilde e_x|\tilde\sigma_x^{\#}(y,\tilde e_x)|\tilde e_z|\tilde\sigma_z(\tilde z,\tilde e_z)\ d\tilde e_x\ d\tilde e_z.\\
\tilde{\mathcal{E}}_z(\tilde z) &= \{\tilde e_z, |\tilde e_z| > \sqrt{\tilde W(\tilde z)}\},\\
\tilde{\mathcal{E}}_x^{\#}(y) &= \{\tilde e_x, |\tilde e_x| > \sqrt{\tilde U(y)}\}\\
\tilde\gamma_1(y,\tilde z) &= \pi \exp\left(-\tilde U(y) - \tilde W(\tilde z)\right).
\end{aligned}$$

Moreover since

$$\tilde v_x(\tilde x,\tilde e_x) \quad = \quad sgn(\tilde e_x)\sqrt{\tilde e_x^2 - \tilde U(\tilde x/\varepsilon)} = \tilde v_x^{\#}(\frac{\tilde x}{\varepsilon},\tilde e_x), \tag{40}$$

inserting (37, 40) in (39) and balancing order by order in ε we get at the principal order,

$$\tilde v_x^{\#}\partial_y \tilde h^{t,0} = 0,$$

and thus for molecules with $\tilde v_x^{\#} \neq 0$ we conclude that

$$\tilde h^{t,0}(\tilde t,\tilde x,y,\tilde e_x,\tilde e_z) = \tilde h^{t,0}(\tilde t,\tilde x,\tilde e_x,\tilde e_z). \tag{41}$$

Then from this property and from (38) we deduce that $\tilde h_b^{t,0}(\tilde t,\tilde x,\tilde e_x,\tilde e_z)$ is an even function of $\tilde e_x$.

At the next order we get

$$\partial_{\tilde t}\tilde h^{t,0} + \tilde v_x^{\#}\partial_{\tilde x}\tilde h^{t,0} + \tilde v_x^{\#}\partial_y \tilde h^{t,1} = \frac{1}{\tilde\tau}\left(\tilde\Theta[\tilde h^0]\tilde l\tilde M - \tilde h^{t,0}\right). \tag{42}$$

We consider now separately bound and unbound molecules.

Let us first consider unbound molecules. Taking into account (41) and multiplying (42) by $\tilde v_x^{\#}(\tilde x/\varepsilon,\tilde e_x)^{-1}$, we get, for unbound molecules

$$\frac{1}{\tilde v_x^{\#}(\tilde x/\varepsilon,\tilde e_x)}\partial_{\tilde t}\tilde h_u^{t,0} + \partial_{\tilde x}\tilde h_u^{t,0} + \partial_y\tilde h_u^{t,1} = \frac{1}{\tilde v_x^{\#}(\tilde x/\varepsilon,\tilde e_x)\ \tilde\tau}\left(\tilde\Theta[\tilde h^{t,0}]\tilde l\tilde M - \tilde h_u^{t,0}\right).$$

Then averaging with respect to the fast variable over one period and taking into account that $\tilde h_u^{t,1}$ is periodic in y, we get

$$\frac{1}{\tilde w_x(\tilde e_x)}\partial_{\tilde t}\tilde h_u^{t,0} + \partial_{\tilde x}\tilde h_u^{t,0} = \frac{1}{\tilde w_x(\tilde e_x)\ \tilde\tau}\left(\tilde{\bar{\tilde\Theta}}[\tilde h^{t,0}]\tilde l\tilde M - \tilde h_u^{t,0}\right),$$

where

$$\begin{aligned}
\tilde w_x(\tilde e_x) &= sgn(\tilde e_x)\left(\frac{1}{2}\int_{-1}^{+1}\tilde v_x^{\#}(y,\tilde e_x)^{-1}dy\right)^{-1},\\
\tilde{\bar{\tilde\Theta}}[\tilde h^{t,0}] &= \frac{1}{2\tilde{\bar{\tilde\sigma}}_x(\tilde e_x)}\int_{-1}^{+1}\tilde\sigma_x^{\#}(y,\tilde e_x)\tilde\Theta[\tilde h^{t,0}](\tilde t,\tilde x,y,\tilde e_z)\ dy.
\end{aligned}$$

Finally, multiplying by $\tilde w_x(\tilde e_x)$ we obtain

$$\partial_{\tilde t}\tilde h_u^{t,0} + \tilde w_x(\tilde e_x)\partial_{\tilde x}\tilde h_u^{t,0} = \frac{1}{\tilde{\tau}}\left(\tilde{\bar{\tilde\Theta}}[\tilde h^{t,0}]\tilde l\tilde M - \tilde h_u^{t,0}\right), \tag{43}$$

Let us consider now bound molecules. Since $\tilde{h}_b^{t,0}(\tilde{t},\tilde{x},\tilde{e}_x,\tilde{e}_z)$ is an even function of $\tilde{e}_x$ it is equal to its even part and thus the left-hand-side of (42) writes also for bound molecules

$$\partial_{\tilde{t}}\tilde{h}_b^{t,0}+\frac{1}{2}(\tilde{v}_x^{\#}(e_x)+\tilde{v}_x^{\#}(-e_x))\partial_{\tilde{x}}\tilde{h}_b^{t,0}+\frac{1}{2}\left(\tilde{v}_x^{\#}(e_x)\partial_y\tilde{h}^{t,1}(e_x)+\tilde{v}_x^{\#}(-e_x)\partial_y\tilde{h}^{t,1}(-e_x)\right).$$

But $\tilde{v}_x^{\#}(y,e_x)$ is an odd function of e_x, so that $(\tilde{v}_x^{\#}(e_x)+\tilde{v}_x^{\#}(-e_x))\partial_{\tilde{x}}\tilde{h}_b^{t,0}$ cancels. Then multiplying by $\tilde{\sigma}_x^{\#}(\tilde{x}/\varepsilon,\tilde{e}_x)$ and averaging in the fast variable over one period (between $y_-(\tilde{e}_x)$ and $y_+(\tilde{e}_x)$), we get finally for the bound molecules

$$\partial_{\tilde{t}}\tilde{h}_b^{t,0}=\frac{1}{\tilde{\tau}}\left(\tilde{\overline{\Theta}}[\tilde{h}^{t,0}]\tilde{l}\tilde{M}-\tilde{h}_b^{t,0}\right), \tag{44}$$

where

$$\tilde{\overline{\Theta}}[\tilde{h}^{t,0}]=\frac{1}{(y_+(\tilde{e}_x)-y_-(\tilde{e}_x))\tilde{\overline{\sigma}}_x(\tilde{e}_x)}\int_{y_-(\tilde{e}_x)}^{y_+(\tilde{e}_x)}\tilde{\sigma}_x^{\#}(y,\tilde{e}_x)\tilde{\Theta}[\tilde{h}^{t,0}](\tilde{t},\tilde{x},y,\tilde{e}_z)\,dy.$$

Rewriting equation (43-44) in dimension form and omitting the superscript 0, we get

$$\begin{aligned}\partial_t h_u^t(t,x,e_x,e_z)+w_x(e_x)\partial_x h_u^t(t,x,e_x,e_z) &= \frac{1}{\tau_{ms}}\left(\overline{\Theta}[h^t]lM-h_u^t\right), &(45)\\ \partial_t h_b^t(t,x,e_x,e_z) &= \frac{1}{\tau_{ms}}\left(\overline{\Theta}[h^t]lM-h_b^t\right). &(46)\end{aligned}$$

Proposition 2. *Under the assumptions (4-5-6-27-28-29-30), the solutions of (34) formally converge as $\varepsilon=\delta/x^*\to 0$ to a distibution function $h^t(t,x,e_x,e_z)$, satisfying the following "mesoscopic" kinetic model*

$$\partial_t h^t+w_x(e_x)\partial_x h^t = \frac{1}{\tau_{ms}}\left(\overline{\Theta}[h^t]l(e_z)M-h^t\right),$$

where

$$\begin{aligned}
w_x(e_x) &= \chi_u(e_x)\ sgn(e_x)\left(\frac{1}{2}\int_{-1}^{+1}(e_x^2-2\hat{U}(y)/m)^{-1/2}dy\right)^{-1},\\
\overline{\Theta}[h^t](e_x,e_z) &= \frac{1}{(y_+(e_x)-y_-(e_x))\overline{\sigma}_x(e_x)}\int_{y_-(e_x)}^{y_+(e_x)}\sigma_x^{\#}(y,e_x)\Theta[h^t](y,e_z)\,dy,\\
\Theta[h^t](y,e_z) &= \frac{1}{\tau_z(e_z)}\int_{z_-(e_z)}^{z_+(e_z)}(n[h/l](y,z)\sigma_z(z,e_z)/\gamma_1(y,z))dz,\\
\gamma_1(y,z) &= \frac{2\pi kT}{m}\exp\left(-\frac{\hat{U}(y)+W(z)}{kT}\right),\\
n[g](y,z) &= \int_{\mathcal{E}_z(z)}\int_{\mathcal{E}_x^{\#}(y)}g(e_x,e_z)|e_x|\sigma_x^{\#}(y,e_x)|e_z|\sigma_z(z,e_z)\,de_x\,de_z,\\
\overline{\sigma}_x(e_x) &= \frac{1}{2}\int_{y_-(e_x)}^{y_+(e_x)}\left(\sqrt{e_x^2-\frac{2}{m}\hat{U}(y)}\right)^{-1}dy,\\
\mathcal{E}_x^{\#}(y) &= \{e_x,\ e_x^2>2\hat{U}(y)/m\}.
\end{aligned}$$

Remark 3. 1. The distribution functions h_c^t, for $c=b,u$ describe the number density of gas molecules with velocity (e_x,e_z) per x-unit, obtained by averaging the distribution functions g^t over the periods of the tangential potential

U. Then

$$N(t,x) = \int_{y_-(e_x)}^{y_-(e_x)} \int_0^L n[h/l](t,x,y,z)\;dz\;dy = 2\int_{e_z}\int_{e_x} h|e_x|\overline{\sigma}_x(e_x) de_x\; de_z$$

is the number density of molecules per unit-length, averaged over the periods of the tangential potential U.

2. We can check that $\int_{e_z}\int_{e_x}(\overline{\Theta}[h]lM - h)|e_x|\overline{\sigma}_x(e_x)de_x\; de_z = 0$, which ensures the local conservation of mass.
3. In this model the unbound surface molecules move in the x-direction at an average velocity depending on their total tangential energy, or equivalently, on e_x. On the other hand the bound surface molecules are trapped in a well of the tangential potential U. Their average velocity is null and they relax inside a potential well toward the equilibrium (see equation (46)). Let us notice that, contrary to ([15]), we do not need to assume that the bound molecules are at equilibrium.
4. We have assumed above that $L << \delta << x^*$ (27). It could be interesting to drop this hypothesis and to consider the case where L and δ are comparable. But, in such a case, we cannot uncouple the asymptotic analysis of propositions 1 and 2 and we have to treat both of them together.

4. **Diffusion models for surface molecules.**

In section 2 we derived a multiphase model describing the coupling of the bulk flow with the motion of molecules on the surface. This motion is given by a set of two coupled kinetic equations on variable x, including a Vlasov term due to the interaction potential parallel to the surface. In this section we will consider integration time much greater than the molecule-substrate relaxation time and thus we derive diffusion models. We consider the case of a smooth interaction potential parallel to the surface. We proceed in several steps and we begin with simplifying assumptions.

In a first subsection we consider the same simple configuration as in section 3 where we assumed that the free molecules in the surface layer can be neglected so that all surface molecules are trapped. As before it is reasonable to assume that

$$W_m = +\infty, \tag{47}$$

so that when a molecule enters the surface layer, it cannot escape and moreover we neglect the flux of incoming molecules. Thus there are no free molecules inside the surface layer and it is possible to describe the trapped surface molecules by the following closed model describing the evolution of the distribution function $g = g(v_x, e_z)$

$$\partial_t g + v_x\partial_x g - \frac{U'(x)}{m}\partial_{v_x} g = \frac{1}{\tau_{ms}}\left(\Theta[g]lM - g\right), \tag{48}$$

where

$$M(v_x, e_z) \quad = \quad \exp\left(-m(v_x^2 + e_z^2)/2kT\right),$$

and we denote

$$M_x(v_x) = \exp\left(-\frac{mv_x^2}{2kT}\right),\; M_z(e_z) = \exp\left(-\frac{me_z^2}{2kT}\right),$$

$$\gamma_x = \sqrt{\frac{2k\pi T}{m}},\; \gamma_z(z) = \int_{\mathcal{E}_z(z)} M_z(e_z)|e_z|\sigma_z(z,e_z)de_z = \sqrt{\frac{2k\pi T}{m}}\exp\left(-\frac{W(z)}{kT}\right).$$

The diffusion limit is derived, first in the isothermal case and then extended to the non-isothermal case.
Afterwards, in the second subsection we drop the assumption $W_m = +\infty$ and we extend the analysis of the diffusion limit to the configuration of a flow in a narrow channel where the free molecules are not neglected but where there is no bulk flow.

Before deriving the diffusion models we need a technical lemma related to the collision operator $\Theta[g]lM - g$. Let us denote in the following,

$$((.)) \quad = \quad \int_{e_z}\int_{v_x} dv_x\ de_z.$$

Then we have

Lemma 4.1. *Let us consider the following equation for g:*

$$\Theta[g](x,e_z)l(e_z)M(v_x,e_z) - g(x,v_x,e_z) + \psi(x,v_x)l(e_z)M_z(e_z) = 0, \tag{49}$$

where ψ is a given function.
A necessary and sufficient solvability condition for this equation is

$$\int_{v_x} \psi(x,v_x)\ dv_x = 0. \tag{50}$$

Moreover if (50) is satisfied every solution of (49) writes

$$g = \beta(x)l(e_z)M(v_x,e_z) + \psi(x,v_x)l(e_z)M_z(e_z),$$

where β does not depend on v_x and e_z

Proof. (i) As we have noticed in remarks 1, $((\Theta[g]lM - g)) = 0$ which gives the solvabiliy condition (50).
(ii) It can be easily checked that if $\beta = \beta(x)$ does not depend on v_x and e_z, then $\Theta[\beta lM] = \beta$. Thus $g(x,v_x,e_z) = \beta(x)l(e_z)M(v_x,e_z)$ are solutions of equation (49) with $\psi = 0$. We can prove that they are the only solutions. Indeed if we look for a solution in the form $\beta(x,v_x,e_z)l(e_z)M(v_x,e_z)$, then $\beta(x,v_x,e_z)$ is solution of an integral equation

$$\beta(x,v_x,e_z) = \int_{e'_z}\int_{v'_x} k(v_x,e_z,{v'}_x,e'_z)\ \beta(x,{v'}_x,e'_z)\ d{v'}_x de'_z, \tag{51}$$

where the kernel $k(v_x,e_z,{v'}_x,e'_z) = k(e_z,{v'}_x,{e'}_z)$ is defined by

$$k(e_z,{v'}_x,{e'}_z) = \int_{z_-(e_z,e'_z)}^{z_+(e_z,e'_z)} \frac{\sigma_z(z,e_z)|{e'}_z|\sigma_z(z,e'_z)M_x({v'}_x)M_z(e'_z)}{\gamma_x\ \gamma_z(z)\ \tau_z(e_z)}\ dz,$$

where

$$z_-(e_z,e'_z) = \max(z_-(e_z), z_-(e'_z)),\ \ z_+(e_z,e'_z) = \min(z_+(e_z), z_+(e'_z)),$$

and this kernel k satisfies

$$\forall\ e_z, \quad \int_{e'_z}\int_{v'_x} k(e_z,{v'}_x,{e'}_z)\ d{v'}_x\ d{e'}_z = 1.$$

Moreover, since the kernel k is independent of v_x, so is β and the integral equation (51) writes

$$\beta(x,e_z) = \int_{{e'}_z} \hat{k}(e_z,{e'}_z)\ \beta(x,{e'}_z)\ d{e'}_z, \tag{52}$$

where the kernel $\hat{k}(e_z, e'_z) = \int_{v'_x} k(e_z, v'_x, e'_z) dv'_x$ satisfies

$$\forall\ e_z,\ \ \hat{k}(e_z, .) \in L^1_{e'_z} \quad \text{and} \int_{e'_z} \hat{k}(e_z, e'_z)\ de'_z = 1.$$

It is easy to check that functions $\beta = \beta(x)$ (constant with respect to e_z) are solutions of this equation. Moreover we prove now that they are the only solutions in $L^\infty_{e_z}$. First we prove by contradiction that the only solutions of $\alpha(e_z) = \int_{e'_z} \hat{k}(e_z, e'_z)\alpha(e'_z) de'_z$ are constant functions. If we denote $m = \text{ess sup}_{e'_z} \alpha(e'_z)$, since α is not a constant function of e'_z

$$\exists \eta\ > 0,\ \ \alpha(e'_z) \leq m - \eta,\ \ \text{a.e. in}\ \ e'_z \text{ on a set } \mathcal{F}_{x,\eta} \text{ with positive measure in } e'_z,$$

so that

$$\begin{aligned} \alpha(e_z) \quad &= \quad \int_{e'_z} \hat{k}(e_z, e'_z)\alpha(e'_z) de'_z, \\ &\leq \quad m - \eta \int_{\mathcal{F}_{x,\eta}} \hat{k}(e_z, \epsilon_z) d\epsilon_z \leq m - \eta k_0, \end{aligned}$$

where

$$0 < k_0 = \sqrt{\frac{m}{2k\pi T}} \int_{\mathcal{F}_{x,\eta}} M_z(e'_z) de'_z \leq \int \frac{\sigma_z(z, e_z)}{\tau_z(e_z)\gamma_z(z)} \int_{\mathcal{F}_{x,\eta}} |e'_z| \sigma_z(z, e'_z) M_z(e'_z) de'_z\ dz.$$

This last inequality is in contradiction with the definition of m so that we conclude that necessarily α does not depends on e_z. We easily deduce of this property that the only solutions of (52) are functions $\beta(x, .)$ which, for almost x, are constant functions in e_z. Indeed, for ξ given in C^0_K, let us denote $\alpha_\xi(e_z) = \int_x \xi(x)\beta(x, e_z) dx$. Then α_ξ is solution of the integral equation $\alpha_\xi(e_z) = \int_{e'_z} \hat{k}(e_z, e'_z)\alpha_\xi(e'_z) de'_z$, so that α_ξ is a constant. But $\xi \to \alpha_\xi$ is a linear form that can be written $\int_x \zeta(x)\xi(x) dx$, so that almost everywhere in x we have $\beta(x, e_z) = \zeta(x)$. Thus every solution of the homogeneous equation (49) writes $\beta(x) l(e_z) M(v_x, e_z)$.

(iii) Let us now consider the nonhomogeneous equation. First, we remark that (50) implies that

$$n[\psi M_z] = \left(\int_{v_x} \psi(x, v_x) dv_x \right) \left(\int_{e_z} |e_z| \sigma_z(z, e_z) M_z(e_z) de_z \right) = 0,$$

so that $\psi l M$ is a particular solution of (49), and then, from (ii), every solution writes

$$g(x, v_x, e_z) = \beta(x) l(e_z) M(v_x, e_z) + \psi(x, v_x) l(e_z) M_z(e_z).$$

□

4.1. **Diffusion model for the trapped surface-molecules.** For the sake of simplicity, we assume in a first step that the temperature T is a fixed given constant.

4.1.1. *The isothermal case.* Under the above assumptions the kinetic model obtained in the previous sections writes

$$\partial_t g + v_x \partial_x g - \frac{U'(x)}{m} \partial_{v_x} g = \frac{1}{\tau_{ms}} \left(\Theta[g] l M - g \right). \tag{53}$$

To obtain a dimensionless form of this equation we introduce the following reference quantities. $z^* = L$ is a reference length in the z-direction, $v^* = \sqrt{2kT/m}$ is a reference velocity, t^*_d is a reference *diffusion time*, τ^*_{ms} is a reference *molecule-phonon* *relaxation time*, $\tau_z^* = z^*/v^*$ is a reference time for crossing the surface layer, n^* is a reference number density and $g^* = (n^* z^*)/v^{*2}$, $U^* = mv^*$ and $\tilde{M}(\tilde{v}_x, \tilde{e}_z) = \exp\left(-(\tilde{v}_x^2 + \tilde{e}_z^2)\right)$. Moreover we introduce another reference time t_c^* such that

$$\tau_z^* << \tau_{ms}^* << t_c^* << t_d^*,$$

and the small parameter ε, and we set

$$\varepsilon = \frac{\tau_{ms}^*}{t_c^*} = \frac{t_c^*}{t_d^*}.$$

Finally we introduce x^{**}, a reference length in the x-direction defined by

$$x^{**} = v^* t_c^*.$$

We rescale the problem according to

$$\tilde{x} = \frac{x}{x^{**}}, \tilde{z} = \frac{z}{z^*}, \tilde{l} = \frac{l}{z^*}, \tilde{t} = \frac{t}{t_d^*}, \tilde{\tau}_{ms} = \frac{\tau_{ms}}{\tau_{ms}^*}, \tilde{v}_x = \frac{v_x}{v^*}, \tilde{e}_{x/z} = \frac{e_{x/z}}{v^*}, \tag{54}$$

and

$$\tilde{g} = \frac{g v^{*2}}{n^* z^*}, \quad \tilde{U} = \frac{U}{U^*}, \quad \tilde{\Theta} = \frac{\Theta v^{*2}}{n^*}. \tag{55}$$

With the previous notations and the above assumption, the dimensionless form of equation (53) writes

$$\varepsilon \partial_{\tilde{t}} \tilde{g} + \tilde{v}_x \partial_{\tilde{x}} \tilde{g} - \tilde{U}'(\tilde{x}) \partial_{\tilde{v}_x} \tilde{g} \quad = \quad \frac{1}{\varepsilon \tilde{\tau}_{ms}} \left(\tilde{\Theta}[\tilde{g}] \tilde{l} \tilde{M} - \tilde{g} \right), \tag{56}$$

We consider the asymptotic analysis of this problem when ε tends to 0. We look for

$$\tilde{g} \quad = \quad \tilde{g}^{(0)} + \varepsilon \tilde{g}^{(1)} + \varepsilon^2 \tilde{g}^{(2)} + ... \tag{57}$$

Inserting (57) in (56) and balancing order by order in ε we get
At leading order

$$\tilde{g}^{(0)} = \tilde{\Theta}[\tilde{g}^{(0)}] \tilde{l} \tilde{M}. \tag{58}$$

From the dimensionless form of Lemma 1 the solutions of (58) write

$$\tilde{g}^{(0)} = \alpha(\tilde{t}, \tilde{x}) \tilde{l} \tilde{M} = \frac{\tilde{N}^0(\tilde{t}, \tilde{x})}{\tilde{\gamma}} \tilde{l} \tilde{M}, \tag{59}$$

where $\tilde{N}^0(\tilde{t}, \tilde{x})$ is defined by

$$\tilde{N}^0(\tilde{t}, \tilde{x}) = \alpha(\tilde{t}, \tilde{x}) \; \tilde{\gamma},$$

and where the constant $\tilde{\gamma}$ (depending only on W and T) is defined by

$$\tilde{\gamma} = \int_{\tilde{e}_z} \int_{\tilde{v}_x} \tilde{M}(\tilde{v}_x, \tilde{e}_z) \tilde{l}(\tilde{e}_z) \; d\tilde{v}_x d\tilde{e}_z.$$

Then we get
at order +1

$$\tilde{v_x} \; \partial_{\tilde{x}} \tilde{g}^{(0)} - \tilde{U}'(\tilde{x}) \partial \tilde{v}_x \tilde{g}^{(0)} \quad = \quad \frac{1}{\tilde{\tau}_{ms}} \left(\tilde{\Theta}[\tilde{g}^{(1)}] \tilde{l} \tilde{M} - \tilde{g}^{(1)} \right).$$

We notice that the left-hand-side of this relation writes

$$\left(\tilde{v_x} \; \partial_{\tilde{x}} \tilde{N} \frac{M_x(v_x)}{\tilde{\gamma}_x} + 2\tilde{U}'(\tilde{x}) \tilde{v}_x \tilde{N} \tilde{M}_x(\tilde{v}_x) \right) \tilde{l}(\tilde{e}_z) \tilde{M}_z(\tilde{e}_z),$$

so that we can use the dimensionless form of Lemma 1 and thus solutions of this relation write

$$\tilde{g}^{(1)} = \tilde{\alpha}^1(\tilde{t},\tilde{x})\tilde{l}\tilde{M} - \frac{\tilde{\tau}_{ms}}{\tilde{\gamma}}\left(\partial_{\tilde{x}}\tilde{N}^0(\tilde{t},\tilde{x})\right)\tilde{l}\tilde{v_x}\tilde{M} + \frac{\tilde{\tau}_{ms}}{\tilde{\gamma}}\tilde{U}'(\tilde{x})(\partial_{\tilde{x}}\tilde{N}^0(\tilde{t},\tilde{x}))\tilde{l}\tilde{M}. \quad (60)$$

$$\tilde{g}^{(1)} = \tilde{\alpha}^1(\tilde{t},\tilde{x})\tilde{l}\tilde{M} - \frac{\tilde{\tau}_{ms}}{\tilde{\gamma}}\left(\partial_{\tilde{x}}\tilde{N}^0(\tilde{t},\tilde{x})\right)(\tilde{v_x} - \tilde{U}'(\tilde{x}))\tilde{l}\tilde{M}. \quad (61)$$

at order +2

$$\partial_{\tilde{t}}\tilde{g}^{(0)} + \tilde{v_x}\ \partial_{\tilde{x}}\tilde{g}^{(1)} - \tilde{U}'(\tilde{x})\partial\tilde{v_x}\tilde{g}^{(1)} = \frac{1}{\tilde{\tau}_{ms}}\left(\tilde{\Theta}[\tilde{g}^{(2)}]\tilde{l}\tilde{M} - \tilde{g}^{(2)}\right).$$

As above and taking into account (61), the left hand side of this relation can be written in the form $\tilde{\psi}(\tilde{x},\tilde{v_x})\tilde{l}(\tilde{e}_z)\tilde{M}_z(\tilde{e}_z)$, and thus existence of a solution in $\tilde{g}^{(2)}$ is ensured under the solvability condition

$$\int_{\tilde{v_x}}\int_{\tilde{e}_z}\left(\partial_{\tilde{t}}\tilde{g}^{(0)} + \tilde{v_x}\ \partial_{\tilde{x}}\tilde{g}^{(1)} - \tilde{U}'(\tilde{x})\partial\tilde{v_x}\tilde{g}^{(1)}\right)d\tilde{e}_z d\tilde{v_x} = 0. \quad (62)$$

Inserting (59-61) into (62) and noting that $\int_{\tilde{v_x}}\int_{\tilde{e}_z}\tilde{U}'(\tilde{x})\partial\tilde{v_x}\tilde{g}^{(1)}d\tilde{e}_z d\tilde{v_x} = 0$, we get

$$\partial_{\tilde{t}}\tilde{N}^0 - \tilde{D}_0^{(n)}\partial^2_{\tilde{x}^2}\tilde{N}^0 - \tilde{\tau}_{ms}\partial_{\tilde{x}}\left(\tilde{U}'(\tilde{x})\tilde{N}^0\right) = 0, \quad (63)$$

where the diffusion coefficient $\tilde{D}_0^{(n)}$ is given by

$$\tilde{D}_0^{(n)} = \frac{\tilde{\tau}_{ms}}{\tilde{\gamma}}\int_{\tilde{e}_z}\int_{\tilde{v_x}}\tilde{v_x}^2\ \tilde{M}(\tilde{v_x},\tilde{e}_z)\tilde{l}(\tilde{e}_z)\ d\tilde{v_x}d\tilde{e}_z.$$

Then we come back to dimension quantities and we denote $N(t,x) = n^* z^* \tilde{N}^0(\tilde{t},\tilde{x})$. With this definition $g^0 = (N/\gamma)lM$, where $\gamma = \langle\langle M\rangle\rangle$, and

$$\langle\langle . \rangle\rangle = \int_{e_z}\int_{e_x} \cdot\ dv_x\ de_z,$$

so that the number density of molecules

$$n[g^0/l] = \int_{\mathcal{E}_z(z)}\int_{v_x}\frac{g^0(t,x,v_x,e_z)}{l(e_z)}|e_z|\sigma_z(z,e_z)\ dv_x de_z$$

satisfies

$$\int_0^L n[g/l]\ dz = \frac{N(t,x)}{\gamma}\int_{e_z}\int_{v_x} M(v_x,e_z)dv_x de_z = N(t,x).$$

Thus $N(t,x)$ can be interpreted as the number density of molecules per unit x-length in the surface layer, obtained by integrating (with respect to z) over the width of the layer and from (63) we get

$$\partial_t N - D_0^{(n)}\partial^2_{x^2}N - \tau_{ms}\partial_x\left(\frac{U'(x)}{m}N\right) = 0,$$

Finally we have obtained the following result

Proposition 3. *Under the hypothesis (4-5-6-29-47), the solutions of (48) formally converge as* $\varepsilon (= t_c^*/t_d^* = \tau_{ms}^*/t_c^*) \to 0$ *to* $(N(t,x)/\gamma)\, l(e_z) M(v_x,e_z)$ *where the function* $N(t,x)$ *is solution of the following diffusion equation*

$$\partial_t N - D_0^{(n)}\partial^2_{x^2}N - \tau_{ms}\partial_x\left(\frac{U'(x)}{m}N\right) = 0,$$

where

$$D_0^{(n)} = \frac{\tau_{ms}}{\gamma}\langle\langle {v_x}^2\ lM\rangle\rangle,\ \gamma = \langle\langle M\rangle\rangle,\ M(v_x,e_z) = e^{-m(v_x^2+e_z^2)/2kT}.$$

Remark 4. 1. This diffusion equation describes the gas flow in the limit $\varepsilon \to 0$ only on a long time scale $\approx t_d$, or, which is in some sense equivalent, for an initial distribution of the form $(N/\gamma)M(v_x,e_z)$. It does not give a correct description of the flow for a general initial condition and on a short time scale.

4.1.2. *The non-isothermal case.* In this section we assume that the temperature is a (given) function of x, and we perform the same asymptotic analysis as in the previous section. We only indicate the modification induced by this assumption. We first notice that $M = \exp\big(-(v_x^2+e_z^2)/(2kT(x)\big)$ and that $\gamma = \gamma(T(x))$. Moreover the derivative of γ with respect to the temperature, denoted by γ', is given by

$$\gamma'(T) = \partial_T\gamma = \frac{1}{2kT^2}\langle\langle(v_x^2+e_z^2)M\rangle\rangle.$$

The asymptotic analysis follows the same steps as in the previous section. The first difference occurs at the identification of the expansion at order +1. Taking into account the variation of T with respect to x, the first term in the expansion reads now instead of (61)

$$\begin{aligned}\tilde{g}^{(1)} &= \tilde{N}^1\tilde{l}\tilde{M} - \frac{\tilde{\tau}_{ms}\tilde{v_x}}{\tilde{\gamma}}\left(\partial_{\tilde{x}}\tilde{N}^0 - \tilde{N}^0\partial_{\tilde{x}}T(x)\left(\frac{\tilde{\gamma}'(T(x))}{\tilde{\gamma}} + \frac{\tilde{v}_x^2+\tilde{e}_z^2}{2kT(x)^2}\right)\right)\tilde{M}\\ &\quad +\tilde{\tau}_{ms}\tilde{U'}(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}^0,\end{aligned}$$

where the effect of the temperature gradient is included. Finally the asymptotic analysis leads to the diffusion equation

$$\partial_t N - \partial_x(D_0^{(n)}\partial_x N) - \partial_x(D_0^{(T)}\partial_x T) - \tau_{ms}\partial_x\left(\frac{U'(x)}{m}N\right) = 0, \tag{64}$$

where

$$\begin{aligned}D_0^{(n)} &= D_0^{(n)}(T) = \frac{\tau_{ms}}{\gamma(T(x))}\langle\langle v_x^2 lM\rangle\rangle,\\ D_0^{(T)} &= D_0^{(T)}(N,T) = \frac{\tau_{ms}}{\gamma(T(x))}\langle\langle v_x^2\left(\frac{m(v_x^2+e_z^2)}{2kT(x)^2} - \frac{\gamma'(T(x))}{\gamma^2(T(x))}\right)lM\rangle\rangle\ N.\end{aligned}$$

Of course, this approach can be easily extended to the case where the temperature field is not given but determined by a conduction equation (for instance).

It is sometimes preferred to write the diffusion equation (64) with the mass flux defined with respect to $\partial_x p$ rather than with respect to $\partial_x N$. Assuming that the pressure of the gas is given by the ideal gas law $p = kNT$, the diffusion equation (64) writes

$$\partial_t N - \partial_x(C_0^{(p)}\partial_x p) - \partial_x(C_0^{(T)}\partial_x T) = 0,$$

where

$$\begin{aligned}C_0^{(p)} &= \frac{1}{kT}D_0^{(n)}\\ C_0^{(T)} &= D_0^{(T)} - \frac{N}{T}D_0^{(n)}.\end{aligned}$$

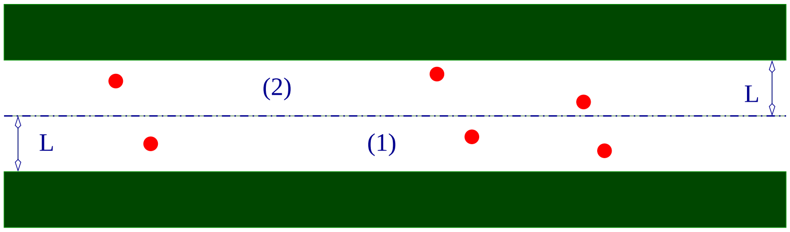

FIGURE 4. narrow channel with two surface layers.

4.2. **Diffusion model for trapped and free molecules in a narrow channel.** In the previous subsection we derived a diffusion limit of the tangential model under the assumption that all molecules in the surface layer are trapped. Now we drop this limitation so that the flow of trapped molecules is coupled with the flow outside the surface layer by the free molecules. We consider the following configuration: the gas molecules move in a narrow channel with diameter $2L$, with a lower boundary (denoted 1), located at $z = 0$ and an upper boundary (denoted 2), located at $z = 2L$ (see figure 4). In this simple configuration there is no bulk flow and the incoming free molecules in the lower surface layer are the free molecules going out of the upper surface layer and conversely. We assume moreover that the two boundaries are similar (same temperature, same interaction potential) so that

$$T_1 = T_2, \qquad U_1(x) = U_2(x), \qquad W_1(z) = W_2(2L - z). \tag{65}$$

Using the same approach as in section 2, the flow of molecules in the channel can be described (in the isothermal case) by the following system of two coupled monodimensional kinetic equations

$$\partial_t g_1 + v_x \partial_x g_1 - \frac{U'(x)}{m} \partial_{v_x} g_1 = Q_{ph}[g_1] + \frac{\chi^f(e_z)}{2\tau_z(e_z)} \left(g_2(-|e_z|) - g_1(|e_z|) \right), \tag{66}$$

$$\partial_t g_2 + v_x \partial_x g_2 - \frac{U'(x)}{m} \partial_{v_x} g_2 = Q_{ph}[g_1] + \frac{\chi^f(e_z)}{2\tau_z(e_z)} \left(g_1(|e_z|) - g_2(-|e_z|) \right), \tag{67}$$

where g_1 is the distribution function describing the (trapped and free) molecules inside the lower surface layer and g_2 is the distribution function describing the (trapped and free) molecules inside the upper surface layer. From hypothesis (65) the times τ_z is the same in the two equations and we have the same property for τ_{ms}, for the length l, for the characteristic function χ^f, for the operator Θ and the distribution M.

We denote $g_* = g_1 + g_2$, the distribution function of molecules in the channel. Then if we add equation (66) and equation (67), the sum of the coupling terms vanishes since the free molecules outgoing from the lower surface layer are the free molecules incoming into the upper surface layer and conversely. Thus (using that the operator Θ is linear in g), we obtain for g_* the following closed kinetic equation

$$\partial_t g_* + v_x \partial_x g_* - \frac{U'(x)}{m} \partial_{v_x} g_* \quad = \quad Q_{ph}[g_*] = \frac{1}{\tau_{ms}} \left(\Theta[g_*] l M - g_* \right),$$

which is very similar to (53), but includes the free molecules ($g_i = \chi^t g_i^t + \chi^f g_i^f$, $i = 1, 2$). If we rescale this equation as in (54-55), we get the following dimensionless equation for g_*

$$\varepsilon\partial_{\tilde{t}}\tilde{g}_* + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_* - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_* \quad = \quad \frac{1}{\varepsilon\ \tilde{\tau}_{ms}}\left(\tilde{\Theta}[\tilde{g}_*]\tilde{l}\tilde{M} - \tilde{g}_*\right),$$

and the same asymptotic analysis as in section 4.1 leads to the following diffusion equation for $N_* = \int_0^L n[(g_1+g_2)/l]dz$

$$\partial_t N_* - D_0^{(n)}\partial^2_{x^2}N_* - \tau_{ms}\partial_x\left(\frac{U'(x)}{m}N^*\right) = 0, \tag{68}$$

where

$$D_0^{(n)} = \frac{\tau_{ms}}{\gamma}\langle\langle {v_x}^2 lM\rangle\rangle,\ \gamma = \langle\langle M\rangle\rangle,\ M(v_x,e_z) = e^{-m(v_x^2+e_z^2)/2kT}.$$

Let us look now for a diffusion limit of equations (66-67). We need some more assumptions. We rescale these equations as in (54-55) with, in addition

$$\tilde{\tau}_z = \frac{\tau_z}{\tau_z^*}, \qquad \tilde{\chi}^f\tilde{g}_i = \frac{\chi^f g_i}{(n_f^*/v^{*2})},$$

where $\tau_z^* = z^*/v^*$. We denote

$$\varepsilon_0 = \frac{\tau_z^*}{t_c^*} = \frac{z^*}{x^*},$$

and as in 4.1.1 we assume that

$$\varepsilon = \frac{\tau_{ms}^*}{t_c^*} = \frac{tc^*}{t_d^*}.$$

With these notations (66) writes in dimensionless form

$$\begin{aligned}\varepsilon\partial_{\tilde{t}}\tilde{g}_1 + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_1 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_1 \quad &= \quad \frac{1}{\varepsilon}\left(\tilde{\Theta}[\tilde{g}_1]\tilde{l}\tilde{M} - \tilde{g}_1\right)\\ &\quad + \frac{n_f^* t_c^*}{n^*\tau_z^*}\frac{\chi^f(\tilde{e}_z)}{2\tilde{\tau}_z(\tilde{e}_z)}\left(\tilde{g}_2(-|\tilde{e}_z|) - \tilde{g}_1(|\tilde{e}_z|)\right),\end{aligned}$$

and we have a similar formula for (67). The right-hand-side of those two equations contains a collision term (of order $\frac{1}{\varepsilon}$) and a coupling term which makes the two equations relax one towards the other. To go further we must precise the relative size of the coupling term with respect to the collision term which is determined by the ratio $\frac{n_f^* t_c^*}{n^*\tau_z^*} = \frac{n_f^*}{n^*\varepsilon_0}$. Different regimes can be encountered according to the size of n_f^*/n^* compared with the small quantities ε and ε_0, and we study several ones in the following.

4.2.1. *Strong coupling of the two surface layers.* We assume there that

$$\varepsilon_0 \leq \varepsilon,\ \ \frac{n_f^*}{n^*} = \frac{\varepsilon_0}{\varepsilon}.$$

The first assumption means that $\tau_z^* \leq \tau_{ms}^*$. The second assumption means that the ratio of free molecules is of order $\frac{\varepsilon_0}{\varepsilon}$, so that the number of free molecules can be (smaller than but) comparable to the total number of molecules (when $\varepsilon_0 = \varepsilon$). This is a reasonable assumption when $W_m \approx kT$. Under those assumptions the ratio $\frac{n_f^* t_c^*}{n^*\tau_z^*} = 1/\varepsilon$ so that the coupling term of the two equations is strong and is comparable to the collision term. Then the dimensionless form of the system is given by

$$\begin{aligned} \varepsilon\partial_{\tilde{t}}\tilde{g}_1 + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_1 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_1 &= \Lambda[\tilde{g}_1, \tilde{g}_2], && (69)\\ \varepsilon\partial_{\tilde{t}}\tilde{g}_2 + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_2 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_2 &= \Lambda[\tilde{g}_2, \tilde{g}_1], && (70) \end{aligned}$$

where $\Lambda[\tilde{g}_a, \tilde{g}_b] = \frac{1}{\varepsilon\ \tilde{\tau}_{ms}}\left(\tilde{\Theta}[\tilde{g}_a]\tilde{l}\tilde{M} - \tilde{g}_a\right) + \frac{\chi^f}{2\varepsilon\ \tilde{\tau}_z}\left(\tilde{g}_b(-|\tilde{e}_z|) - \tilde{g}_a(|\tilde{e}_z|)\right)$.
Since we have derived a diffusion limit for $g_* = g_1 + g_2$, in order to get the diffusion limit of the system of equations modeling the evolution of g_1 and g_2 it is sufficient to study the diffusion limit of the equation giving the evolution of $g_{**} = g_1 - g_2$ obtained by subtracting (70) from (69). Looking for $\tilde{g}_{**} = \tilde{g}^0_{**} + \varepsilon\tilde{g}^1_{**} + ...$, inserting in (70)-(69) and balancing order by order we obtain
At the leading order

$$\left(\tilde{\Theta}[\tilde{g}^0_{**}]\tilde{l}\tilde{M} - \tilde{g}^0_{**}\right) - \frac{\tilde{\tau}_{ms}\chi^f(\tilde{e}_z)}{2\ \tilde{\tau}_z(\tilde{e}_z)}\left(\tilde{g}^0_{**}(|\tilde{e}_z|) + \tilde{g}^0_{**}(-|\tilde{e}_z|)\right) = 0.$$

We first remark that this relation implies that $\tilde{g}^0_{**}$ is an even function of $\tilde{e}_z$, so that it can be written

$$\left(\tilde{\Theta}[\tilde{g}^0_{**}]\tilde{l}\tilde{M} - \tilde{g}^0_{**}\right) - \frac{\tilde{\tau}_{ms}\chi^f(\tilde{e}_z)}{\tilde{\tau}_z(\tilde{e}_z)}\tilde{g}^0_{**} = 0. \tag{71}$$

To solve this equation we proceed as in the proof of Lemma 1 and we look for $\tilde{g}_{**} = \tilde{\beta}(\tilde{x}, \tilde{v}_x, \tilde{e}_z)\tilde{l}\tilde{M}$. Inserting in (71) we find for $\tilde{\beta}$ the following integral equation

$$\left(1 + \frac{\tilde{\tau}_{ms}\chi^f(\tilde{e}_z)}{\tilde{\tau}_z(\tilde{e}_z)}\right)\tilde{\beta}(\tilde{x}, \tilde{v}_x, \tilde{e}_z) = \int_{\tilde{\epsilon}_z}\int_{\tilde{w}_x}\tilde{k}(\tilde{v}_x, \tilde{e}_z, \tilde{w}_x, \tilde{\epsilon}_z)\tilde{\beta}(\tilde{x}, \tilde{w}_x, \tilde{\epsilon}_z)d\tilde{w}_x d\tilde{\epsilon}_z, \tag{72}$$

where the kernel $\tilde{k}$ (the dimensionless form of the kernel k introduced in Lemma 1) is nonnegative and satisfies

$$\int_{\tilde{\epsilon}_z}\int_{\tilde{w}_x}\tilde{k}(\tilde{v}_x, \tilde{e}_z, \tilde{w}_x, \tilde{\epsilon}_z)d\tilde{w}_x d\tilde{\epsilon}_z = 1. \tag{73}$$

Thus from (72), we deduce that $\tilde{\beta}$ vanishes or cannot be independent of $\tilde{v}_x$ and $\tilde{e}_z$ and moreover

$$\min_{\tilde{w}_x, \tilde{\epsilon}_z}\tilde{\beta}(\tilde{x}, \tilde{w}_x, \tilde{\epsilon}_z) \leq \left(1 + \frac{\tilde{\tau}_{ms}\chi^f(\tilde{e}_z)}{\tilde{\tau}_z(\tilde{e}_z)}\right)\tilde{\beta}(\tilde{x}, \tilde{v}_x, \tilde{e}_z) \leq \max_{\tilde{w}_x, \tilde{\epsilon}_z}\tilde{\beta}(\tilde{x}, \tilde{w}_x, \tilde{\epsilon}_z).$$

Since $\left(1 + \frac{\tilde{\tau}_{ms}\chi^f(\tilde{e}_z)}{\tilde{\tau}_z(\tilde{e}_z)}\right) > 1$ for $|\tilde{e}_z| > \tilde{W}_m$, this relation implies that $\tilde{\beta}$ reaches its maximum for a value $(\tilde{w}^*_x, \tilde{e}^*_z)$ such that $|\tilde{e}^*_z| \leq \tilde{W}_m$. Then we have

$$\tilde{\beta}(\tilde{x}, \tilde{v}^*_x, \tilde{e}^*_z) = \int_{\tilde{\epsilon}_z}\int_{\tilde{w}_x}\tilde{k}(\tilde{v}^*_x, \tilde{e}^*_z, \tilde{w}_x, \tilde{\epsilon}_z)\tilde{\beta}(\tilde{x}, \tilde{w}_x, \tilde{\epsilon}_z)d\tilde{w}_x d\tilde{\epsilon}_z.$$

But this relation and (73) imply that $\tilde{\beta}$ is independent of $\tilde{w}_x$ and $\tilde{e}_z$, and thus, from the remark above, that $\tilde{\beta} = 0$. Consequently we have proved that $\tilde{g}^0_{**} = 0$.
Using this result we check that $\tilde{g}^1_{**}$ satisfies the same equation as $\tilde{g}^0_{**}$ so that we can also conclude that $\tilde{g}^1_{**} = 0$ and so on. Finally, since $\tilde{g}^0_{**} = 0$, we conclude that $N_1 = N_2 = N_*/2$ and that N_1 and N_2 satisfy the same equation as N_* (68). In fact since the coupling is strong, the distribution functions g_1 and g_2 relax very fast to the same limit $N_*/(2\gamma)lM$, in a time shorter than the diffusion time.

4.2.2. *Moderate coupling of the two surface layers.* We assume now that

$$\frac{n_f^*}{n^*} = \varepsilon_0,$$

so that the ratio $\frac{n_f^* t_c^*}{n^* \tau_z^*} = 1$. This assumption means that the number of free molecules is much smaller than the total number of molecules, which is reasonable when $W_m >> kT$. Under this assumptions the coupling term is moderate (of order 1) and smaller the collision term (of order $1/\varepsilon$).
Then the dimensionless form of the system is given by

$$\begin{aligned} \varepsilon\partial_{\tilde{t}}\tilde{g}_1 + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_1 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_1 &= \Lambda[\tilde{g}_1, \tilde{g}_2], \\ \varepsilon\partial_{\tilde{t}}\tilde{g}_2 + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_2 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_2 &= \Lambda[\tilde{g}_2, \tilde{g}_1], \end{aligned}$$

where

$$\Lambda[\tilde{g}_a, \tilde{g}_b] = \frac{1}{\varepsilon\ \tilde{\tau}_{ms}}\left(\tilde{\Theta}[\tilde{g}_a]\tilde{l}\tilde{M} - \tilde{g}_a\right) + \frac{\chi^f}{2\tilde{\tau}_z}\left(\tilde{g}_b(-|\tilde{e}_z|) - \tilde{g}_a(|\tilde{e}_z|)\right).$$

We look for $\tilde{g}_i = \tilde{g}_i^0 + \varepsilon\tilde{g}_i^1 + ...$, with $\tilde{N}[\tilde{g}_i^k] = \int_0^L n[\tilde{g}_i^k/l]dz = 0$, for $i = 1, 2$ and $k \geq 1$. The asymptotic analysis leads to
At the leading order For $i = 1, 2$, $\tilde{\Theta}[\tilde{g}_i^0]\tilde{l}\tilde{M} - \tilde{g}_i^0 = 0$, which implies $\tilde{g}_i^0 = \frac{\tilde{N}_i}{\gamma}\tilde{l}\tilde{M}$.
At order +1

$$\tilde{\Theta}[\tilde{g}_1]\tilde{l}\tilde{M} - \tilde{g}_1 = \frac{\tilde{\tau}_{ms}\chi^f(\tilde{e}_z)}{2\tilde{\tau}_z(\tilde{e}_z)}(\tilde{g}_2^0 - \tilde{g}_1^0) + \tilde{\tau}_{ms}\left(\tilde{v}_x\partial_{\tilde{x}}\tilde{g}_1^0 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_1^0\right).$$

A necessary condition of solvability is that the integral of the right-hand-side with respect to $\tilde{v}_x$ and $\tilde{e}_x$ vanishes, which implies that

$$(\tilde{N}_2 - \tilde{N}_1)\int_{\tilde{e}_z}\int_{\tilde{v}_x}\frac{\tilde{\tau}_{ms}\chi^f}{2\tilde{\tau}_z(\tilde{e}_z)}\tilde{l}(\tilde{e}_z)\tilde{M}d\tilde{v}_x d\tilde{e}_z = 0,$$

and thus $\tilde{N}_1 = \tilde{N}_2$. With this condition the hypothesis of Lemma 1 is satisfied by the right-hand-side and taking into account that $\tilde{N}[\tilde{g}_i^1] = 0$, we obtain $\tilde{g}_1^i = \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_i^0 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_i^0$. Finally, coming back to dimension variables we conclude that $N_1 = N_2 = N_*/2$ are solution of a the same diffusion equation as N_*.

4.2.3. *Weak coupling between the two surface layer.* We assume now that

$$\frac{n_f^*}{n^*} = \varepsilon\varepsilon_0. \tag{74}$$

This assumption means that the ratio of free molecules is very small. Under this hypothesis the ratio $\frac{n_f^* t_c^*}{n^* \tau_z^*} = \varepsilon$, so that the coupling of the two equations is weak (the coupling term is of order ε while the collision term is of order $1/\varepsilon$) and the dimensionless form of the system governing the evolution of g_1 and g_2 is

$$\begin{aligned} \varepsilon\partial_{\tilde{t}}\tilde{g}_1 + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_1 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_1 &= \Lambda[\tilde{g}_1, \tilde{g}_2], && (75) \\ \varepsilon\partial_{\tilde{t}}\tilde{g}_2 + \tilde{v}_x\partial_{\tilde{x}}\tilde{g}_2 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_2 &= \Lambda[\tilde{g}_2, \tilde{g}_1], && (76) \end{aligned}$$

where

$$\Lambda[\tilde{g}_a, \tilde{g}_b] = \frac{1}{\varepsilon\ \tilde{\tau}_{ms}}\left(\tilde{\Theta}[\tilde{g}_a]\tilde{l}\tilde{M} - \tilde{g}_a\right) + \frac{\varepsilon\ \chi^f(\tilde{e}_z)}{2\tilde{\tau}_z(\tilde{e}_z)}\left(\tilde{g}_b(-|\tilde{e}_z|) - \tilde{g}_a(|\tilde{e}_z|)\right).$$

To study the diffusion limit of this system we integrate the two equations with respect to $\tilde{e}_z$. It comes

$$\varepsilon\partial_{\tilde{t}}\tilde{h}_1 + \tilde{v}_x\partial_{\tilde{x}}\tilde{h}_1 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{h}_1 = \frac{1}{\varepsilon\ \tilde{\tau}_{ms}}\left(\frac{\tilde{N}_1}{\tilde{\gamma}_x}\tilde{M}_x - \tilde{h}_1\right) + \frac{\varepsilon}{2}\left(\tilde{F}_2 - \tilde{F}_1\right), \tag{77}$$

$$\varepsilon\partial_{\tilde{t}}\tilde{h}_2 + \tilde{v}_x\partial_{\tilde{x}}\tilde{h}_2 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{h}_2 = \frac{1}{\varepsilon\ \tilde{\tau}_{ms}}\left(\frac{\tilde{N}_2}{\tilde{\gamma}_x}\tilde{M}_x - \tilde{h}_2\right) + \frac{\varepsilon}{2}\left(\tilde{F}_1 - \tilde{F}_2\right), \tag{78}$$

where $\tilde{h}_i = \int_{\tilde{e}_z}\tilde{g}_i d\tilde{e}_z$, $\tilde{N}_i = \tilde{N}[\tilde{g}_i] = \tilde{N}[\tilde{h}_i]$, $\tilde{F}_i = \int_{\tilde{e}_z}\frac{\chi^f(\tilde{e}_z)}{\tilde{\tau}_z}\tilde{g}_i(\tilde{e}_z)d\tilde{e}_z$. Unfortunately, this system is not closed because, in general, we cannot write $\tilde{F}_i$ as a function of $\tilde{h}_i$. Nevertheless

$$\text{if } \tilde{g}_i = \frac{\tilde{h}_i}{\int\tilde{l}\tilde{M}_z d\tilde{e}_z}\tilde{l}(\tilde{e}_z)\tilde{M}_z(\tilde{e}_z),\ \text{then } \tilde{F}_i = \tilde{c}\ \tilde{h}_i,\ \ \text{where } \tilde{c} = \frac{\int_{\tilde{e}_z}\chi^f(\tilde{e}_z)|\tilde{e}_z|\tilde{M}_z(\tilde{e}_z)d\tilde{e}_z}{\int\tilde{l}\tilde{M}_z d\tilde{e}_z}. \tag{79}$$

But an asymptotic analysis from the dimensionless form of (75-76) proves that $\tilde{g}_i^0 = (\tilde{N}_i/\tilde{\gamma})\tilde{l}\tilde{M}$ and $\tilde{g}_i^1 = (\tilde{N}_i/\tilde{\gamma})\tilde{l}\tilde{M} - \frac{\tilde{\tau}_{ms}}{\gamma}\left(\partial_{\tilde{x}}\tilde{N}_i^0\ \tilde{v}_x\tilde{l}\tilde{M} - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{g}_i^0\right)$, so that $\tilde{g}_i^0 + \varepsilon\tilde{g}_i^1$ satisfies the assumption of (79). Thus we can write (77-78) in the following form

$$\begin{aligned}
\varepsilon\partial_{\tilde{t}}\tilde{h}_1 + \tilde{v}_x\partial_{\tilde{x}}\tilde{h}_1 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{h}_1 &= \frac{1}{\varepsilon\ \tilde{\tau}_{ms}}\left(\frac{\tilde{N}_1}{\tilde{\gamma}_x}\tilde{M}_x - \tilde{h}_1\right) + \frac{\varepsilon}{2}\tilde{c}\left(\tilde{h}_2 - \tilde{h}_1\right) + \mathcal{O}(\varepsilon^2),\\
\varepsilon\partial_{\tilde{t}}\tilde{h}_2 + \tilde{v}_x\partial_{\tilde{x}}\tilde{h}_2 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{h}_2 &= \frac{1}{\varepsilon\tilde{\tau}_{ms}}\left(\frac{\tilde{N}_2}{\tilde{\gamma}_x}\tilde{M}_x - \tilde{h}_2\right) + \frac{\varepsilon}{2}\tilde{c}\left(\tilde{h}_1 - \tilde{h}_2\right) + \mathcal{O}(\varepsilon^2),
\end{aligned}$$

where $\tilde{\gamma}_x = \int_{\tilde{v}_x}\tilde{M}_x(\tilde{v}_x)d\tilde{v}_x = \sqrt{2\pi}$. The asymptotic analysis on this system follows the same ideas as in previous subsections and we get
At the leading order

$$\tilde{h}_i^0 = \frac{\tilde{N}_i^0}{\tilde{\gamma}_x}\tilde{M}_x,\ \ i = 1, 2,\ \ \text{with } \tilde{N}_1^0 + \tilde{N}_2^0 = \tilde{N}_*^0. \tag{80}$$

At order +1

$$\tilde{h}_i^1 = \frac{\tilde{N}_i^1}{\tilde{\gamma}_x}\tilde{M}_x - \tilde{\tau}_{ms}\left(\partial_{\tilde{x}}\frac{\tilde{N}_i^0}{\tilde{\gamma}_x}\ \tilde{v}_x\tilde{M}_x - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{h}_i^0\right). \tag{81}$$

At order +2

$$\begin{aligned}
\partial_{\tilde{t}}\tilde{h}_1^0 + \tilde{v}_x\partial_{\tilde{x}}\tilde{h}_1^1 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{h}_1^1 &= \frac{1}{\tilde{\tau}_{ms}}\left(\frac{\tilde{N}[\tilde{h}_1^2]}{\tilde{\gamma}_x}\tilde{M}_x - \tilde{h}_1^2\right) + \frac{\tilde{c}}{2}\left(\tilde{h}_2^0 - \tilde{h}_1^0\right),\\
\partial_{\tilde{t}}\tilde{h}_2^0 + \tilde{v}_x\partial_{\tilde{x}}\tilde{h}_2^1 - \tilde{U}'(\tilde{x})\partial_{\tilde{v}_x}\tilde{h}_2^1 &= \frac{1}{\tilde{\tau}_{ms}}\left(\frac{\tilde{N}[\tilde{h}_2^2]}{\tilde{\gamma}_x}\tilde{M}_x - \tilde{h}_2^2\right) + \frac{\tilde{c}}{2}\left(\tilde{h}_1^0 - \tilde{h}_2^0\right).
\end{aligned}$$

With this form of the equations, we can use Lemma 1 and $\tilde{h}_1^2$ and $\tilde{h}_2^2$, can be defined from those relations if and only if the following solvability conditions holds

$$\begin{aligned} \int_{\tilde{v}_x} \left(\partial_{\tilde{t}} \tilde{h}_1^0 + \tilde{v}_x \partial_{\tilde{x}} \tilde{h}_1^1 - \tilde{U}'(\tilde{x}) \partial_{\tilde{v}_x} \tilde{h}_1^1 - \frac{\tilde{c}}{2} \left(\tilde{h}_2^0 - \tilde{h}_1^0 \right) \right) d\tilde{v}_x &= 0, \\ \int_{\tilde{v}_x} \left(\partial_{\tilde{t}} \tilde{h}_2^0 + \tilde{v}_x \partial_{\tilde{x}} \tilde{h}_2^1 - \tilde{U}'(\tilde{x}) \partial_{\tilde{v}_x} \tilde{h}_2^1 - \frac{\tilde{c}}{2} \left(\tilde{h}_1^0 - \tilde{h}_2^0 \right) \right) d\tilde{v}_x &= 0, \end{aligned}$$

After inserting (80-81) in the above relations and coming back in dimension variables we finally obtain the following result

Proposition 4. *Under the hypothesis (4-5-6-29-65-74), the solutions* g_i, $i = 1, 2$ *of (66-67) formally converge as* $\varepsilon (= t_c^*/t_d^* = \tau_{ms}^*/t_c^*) \to 0$ *to*

$$(N_i(t,x)/\gamma)\, l(e_z)\ M(v_x, e_z), i = 1, 2$$

where the functions $N_i(t,x), i = 1, 2$ *are solutions of the following system of diffusion equations*

$$\begin{aligned} \partial_t N_1 - D_0^{(n)} \partial_{x^2}^2 N_1 - \tau_{ms} \partial_x \left(\frac{U'(x)}{m} N_1 \right) &= c\ (N_2 - N_1), \\ \partial_t N_2 - D_0^{(n)} \partial_{x^2}^2 N_2 - \tau_{ms} \partial_x \left(\frac{U'(x)}{m} N_2 \right) &= c\ (N_1 - N_2), \end{aligned}$$

where

$$\begin{aligned} D_0^{(n)} &= \frac{\tau_{ms}}{\gamma} \langle\langle {v_x}^2 M \rangle\rangle, \\ \gamma = \langle\langle M \rangle\rangle,\ M(v_x, e_z) &= e^{-m(v_x^2 + e_z^2)/2kT},\ c = c(W_m) = \frac{\int_{e_z} \chi^f(e_z) |e_z| M_z(e_z) de_z}{\int_{e_z} l(e_z) M_z(e_z) de_z}. \end{aligned}$$

Remark 5. From this model, thanks to convenient rescalings, we can recover some of the diffusion models obtained above

1. In the limit of a large W_m the number of free molecules tends to 0 and so does the coefficient $c = c(W_m) = (\int_{e_z} \chi^f(e_z)|e_z| M_z(e_z) de_z)/(\int_{e_z} l(e_z) M_z(e_z) de_z)$. Thus we recover in this limit the result of proposition 3, where we found a diffusion equation for the trapped molecules assuming that the free molecules could be neglected. In the present configuration, we obtain, in the limit of a large W_m two independent diffusion equations for N_1 and N_2.

2. In the limit of a small τ_z, then $N_2 = N_1$, and we recover the diffusion model of the moderate coupling regime.

5. **Conclusion.** We have presented the formal derivation of a hierarchy of models describing a gas flow in the vicinity of a wall, using scaling and systematic asymptotic analysis. Following the ideas introduced in [7],[8],[4], [15],[5],[16],[6], the influence of the wall is taken into account through Van der Wall forces acting on the gas molecules and through a relaxation of the gas molecules by the substrate.

In this paper we made some simplifying assumptions: we assumed that the molecules move in a 2D plane, we considered the case where the intermolecular collisions can be neglected and we assumed that the interaction potential has a simplified structure.

With those assumptions we derived a multiphase model involving a classical kinetic equation for the bulk flow coupled with two one-dimensional kinetic equations modeling the trapped and free molecules inside the surface layer. This one-dimensional kinetic model can be interpreted as a non-local boundary condition for the bulk flow.

Then, assuming that the interaction potential is rapidly oscillating in the direction parallel to the solid surface, an averaged mesoscopic kinetic model is obtained by homogeneization.

Finally, in the limit of a small relaxation time, we derived from the multiphase kinetic model diffusion models for the surface molecules. In a first step we assume that the free molecules can be neglected and in a second step we consider a narrow channel constituted by two surface layers. Then we took into account the trapped and free molecules in the channel and we derived several diffusion models according to the (strong, moderate or weak) coupling of the two surface layers.

The extension of those models for more general interaction potentials and for collisional flows will be studied in forthcoming papers.

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