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Sound propagation at small scales under continuum and non-continuum transport

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Using an observation by Lamb, namely that continuum sound wave propagation in sufficiently narrow channels is quasi-steady and isothermal, we obtain analytical predictions for the propagation of sound waves at small scales under non-continuum transport. We also extend Lamb's approach to include the effects of inertia and heat conduction for wave propagation at larger characterisitc scales descibed by continuum transport (no-slip and slip-flow regimes). Our theoretical predictions are compared to molecular-based direct Monte Carlo solutions of the Boltzmann equation. Very good agreement is found between theory and numerical solutions.

1. Introduction

In this paper we investigate wave propagation in channels with transverse dimensions at the micrometre and submicrometre scale. Our study is motivated by the recent interest in micro- and nano-scale fluid mechanics as well as the scientific challenges presented by the breakdown of continuum theory at these small scales (Ho & Tai 1998). In gas flows, the deviation from continuum behaviour is quantified by the Knudsen number, $Kn = \lambda/H$, where λ is the molecular mean free path, and H is a characteristic hydrodynamic lengthscale. Although non-continuum effects are always present near the walls, when these non-continuum regions are small ($Kn \lesssim 0.1$), accurate macroscopic fields can still be obtained in the bulk of the flow using the continuum description subject to slip boundary conditions (Cercignani 1988); as a result, this regime is referred to as slip flow. For $Kn \gtrsim 0.1$, the continuum description is known to fail (Cercignani 1988); the regime $0.1 < Kn < 10$ is known as the transition regime because it represents a transition between diffusive (continuum) transport for $Kn \lesssim 0.1$, and ballistic transport (free molecular flow) for $Kn \gtrsim 10$. In this paper, we focus on two-dimensional channels, which are the predominant building blocks in today's microfabrication techniques, although this work can easily be extended to ducts of arbitrary cross-sectional shape. The characteristic lengthscale H in this context is the channel height.

In Hadjiconstantinou (2002) we have shown that Lamb's continuum treatment of narrow channels (Crandall 1926) can be extended to describe wave propagation in the transition regime. Lamb's approach can be applied to narrow systems, that is systems for which the diffusion length based on the oscillation frequency is much larger than the transverse dimension ($\delta = \sqrt{2\nu/\omega}/H \gg 1$ where ν is the kinematic viscosity and ω is the wave angular frequency), and is based on the realization that times long compared

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to this system's diffusive timescale are still very short compared to the characteristic time of oscillation. This allows the coarse graining of the time description to the diffusive timescale of the system; in the resulting description, the effects of inertia and thermal conduction are negligible and the system response is quasi-static and isothermal, that is the wave propagation characteristics of the channel are governed by its steady-state bulk-flow response. Under these simplifications, analytical solutions for wave propagation can be obtained without explicit knowledge of the flow field inside the channel, which requires solution of the Boltzmann equation.

In this paper we use a kinetic formulation to derive more general expressions for the propagation constant in all Knudsen regimes as well as kinetic criteria for the range of applicability of each theoretical prediction. Using this formulation we show that the long-wavelength approximation is always valid in the narrow channel regime provided the wave frequency is small compared to the molecular collision frequency. This generalized narrow channel theory reduces to the slip-flow description and finally the no-slip result of Lamb as H increases. However, as H increases, the narrow channel requirement is not satisfied at high frequencies, that is heat conduction and fluid inertia become important. We have thus extended Lamb's method to include the effects of fluid inertia and heat conduction in the continuum (slip-flow and no-slip) regime. Similarly to Lamb's method, our approach considers steady-state responses, and the terms 'wave propagation' and 'complex propagation constant' used in this paper refer to the steady-state response of the system under oscillatory forcing. All our theoretical results compare very well with direct Monte Carlo solutions of the Boltzmann equation (Bird 1994).

The basic assumption behind our approach is that the pressure is constant across the channel. Thus, the velocity and temperature perturbation fields are decoupled, the former responding to the axial pressure gradient and the latter to temporal variations of pressure. This decoupling of the effects of flow and temperature was utilized in the past to describe wave propagation in porous media (for a critical review see Stinson 1991); despite the relatively small pore sizes ($r > 10\,\mu\mathrm{m}$), none of the previous work, including Stinson's, has incorporated non-continuum phenomena. A generalization of these top-down approaches to a method that is essentially equivalent to the extension of Lamb's method used here can be found in Stinson (1991). Stinson also numerically investigates the limits at which Kirchhoff's solution separates into a thermal conductivity contribution and a flow resistance contribution without, however, making a connection to Lamb's original ideas. It is this reformulation that holds the key to extending the theory to the transition and ballistic regimes.

2. Slip-flow theory

Solutions of the Boltzmann equation (Cercignani 1988) show that for $Kn \lesssim 0.1$ accurate hydrodynamic fields can be obtained in the bulk of the flow (outside the Knudsen layer) by using the continuum description subject to slip boundary conditions. For a stationary wall, the velocity-slip boundary condition is given by

$$u_{gas}|_{wall} = \alpha \frac{2-\sigma_v}{\sigma_v} \lambda \left. \frac{\mathrm{d}u}{\mathrm{d}\tilde{\eta}} \right|_{wall}, \tag{2.1}$$

where σ_v is the momentum accommodation coefficient (Beskok & Karniadakis 1999), and $\tilde{\eta}$ is the coordinate normal to the wall. The temperature slip at the wall is given

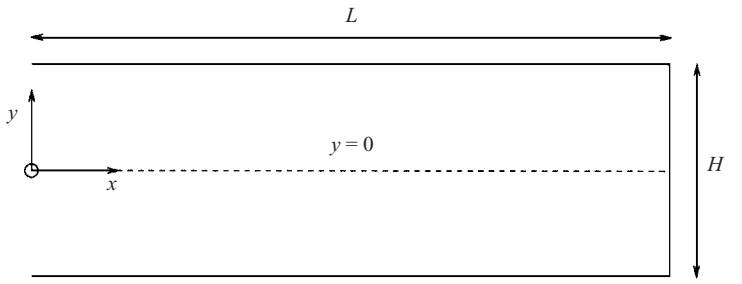

FIGURE 1. Channel geometry.

by a similar expression

$$T_{gas}|_{wall} - T_w = \varepsilon \frac{2\gamma}{\gamma+1} \frac{2-\sigma_T}{\sigma_T} \frac{\lambda}{Pr} \frac{\mathrm{d}T}{\mathrm{d}\tilde{\eta}}\bigg|_{wall} = \zeta \frac{2-\sigma_T}{\sigma_T} \lambda \frac{\mathrm{d}T}{\mathrm{d}\tilde{\eta}}\bigg|_{wall}, \tag{2.2}$$

where T_w is the wall temperature, σ_T is the energy accommodation coefficient, Pr is the gas Prandtl number and γ is the ratio of specific heats.

The coefficients α and ε introduce corrections to the original results of Maxwell ($\alpha = \varepsilon = 1$) obtained through an approximate method (Cercignani 1988). Solutions of the linearized Boltzmann equation by Ohwada, Sone & Aoki (1989*a*) and Sone, Ohwada & Aoki (1989) show that in a hard-sphere gas $\alpha \approx \varepsilon \approx 1.1$. In what follows we will absorb the contribution of the accommodation coefficients into α and ζ.

3. Theory for wave propagation in narrow channels

We now give an outline of Lamb's approach to plane wave propagation in narrow channels and ducts in the no-slip limit (Crandall 1926). The theory is based on the long-wavelength approximation which justifies the neglect of axial derivatives in the viscous terms and the assumption that the pressure is uniform across any section normal to the channel axis. Quantitative criteria for the justification of the above and further assumptions will be developed in the next sections.

We consider two-dimensional smooth long channels of length L with walls that are a distance $H \ll L$ apart (see figure 1). The gas velocity field is denoted $\boldsymbol{u} = \boldsymbol{u}(x, y, t) = (u(x, y, t), v(x, y, t), w(x, y, t))$. Under an excitation of the form $\exp(\mathrm{i}\omega t)$, a response of the form $u(x, y, t) = \tilde{u}(x, y)\exp(\mathrm{i}\omega t)$, $P(x, t) = \tilde{P}(x)\exp(\mathrm{i}\omega t) + P_0$ is expected. The gas density and temperature will also vary according to $\rho(x, y, t) = \tilde{\rho}(x, y)\exp(\mathrm{i}\omega t) + \rho_0$ and $T(x, y, t) = \tilde{T}(x, y)\exp(\mathrm{i}\omega t) + T_0$. Here P_0, ρ_0 and $T_0 = T_w$ are the average values of pressure, density and temperature, respectively.

Lamb's approach is based on the premise that when a channel is narrow, the system response is quasi-static and isothermal. As a result, the wave propagation characteristics are dictated by the isothermal steady-state response of the channel to a pressure gradient, typically expressed in the following form:

$$\tilde{u}_b = -\frac{1}{\mathscr{R}} \frac{\mathrm{d}\tilde{P}}{\mathrm{d}x}, \tag{3.1}$$

where $\mathscr{R}$ is usually referred to as the flow resistance and u_b is the bulk velocity.

The next step to determining the wave propagation characteristics is the substitution of the pressure gradient in terms of the fluid particle displacement ξ, where

$$u(x, y, t) = \frac{\partial \xi(x, y, t)}{\partial t}, \quad u_b(x, t) = \tilde{u}_b(x) \exp(\mathrm{i}\omega t) = \frac{1}{H} \int_{-H/2}^{H/2} \frac{\partial \xi(x, y, t)}{\partial t} \, \mathrm{d}y = \frac{\partial \bar{\xi}(x, t)}{\partial t}, \tag{3.2}$$

This is accomplished through the continuity equation, expressed here as a kinematic relation integrated across the channel width (Crandall 1926)

$$\frac{\mathrm{d}P}{\mathrm{d}x} = -\left(\frac{\partial P}{\partial \rho}\right)_{av} \rho_0 \frac{\partial^2 \bar{\xi}}{\partial x^2}, \tag{3.3}$$

where $(\partial P/\partial \rho)_{av}$ indicates that this derivative is based on average values across the channel. We may expect, as Lamb has argued, the flow to be isothermal; this will be formally shown in the next section where the narrow channel assumption is lifted.

The equation for the steady state response can thus be written as

$$\mathrm{i}\omega \bar{\xi} = \frac{\rho_0 (\partial P/\partial \rho)_T}{\mathscr{R}} \frac{\partial^2 \bar{\xi}}{\partial x^2}, \tag{3.4}$$

where we have assumed isothermal conditions appropriate to Lamb's formulation. The complex propagation constant β ($u_b \propto \exp(-\beta x)$) is thus given by

$$\beta^2 \equiv (m + \mathrm{i}k)^2 = \frac{\mathrm{i}\omega \mathscr{R}}{P_0}, \tag{3.5}$$

where $k = 2\pi/\ell$ is the wavenumber, ℓ is the wavelenth and m is the attenuation coefficient. If we substitute the Poiseuille expression $\mathscr{R} = 12\mu/H^2$, where μ is the gas viscosity, we obtain the well-known result

$$\beta^2 = \frac{12\mathrm{i}\omega\mu}{P_0 H^2} \tag{3.6}$$

for wave propagation in narrow channels that was originally obtained by taking the narrow-channel limit in Kirchhoff's theory (Kirchhoff 1868).

4. Wave propagation in the presense of inertia and heat conduction

In this section we generalize Lamb's theory to channels that do not satisfy the narrow channel criterion, that is channels where fluid inertia and heat conduction will play a role. This is achieved by solving the linearized momentum and energy equations subject to the long-wavelength approximation.

4.1. *The momentum equation*

Starting from the linearized equation of motion

$$\rho_0 \frac{\partial u}{\partial t} = \mu \frac{\partial^2 u}{\partial y^2} - \frac{\partial P}{\partial x} \tag{4.1}$$

we arrive at an equation for the amplitudes $\tilde{u}$ and $\tilde{P}$

$$\frac{\partial^2 \tilde{u}}{\partial y^2} + \phi^2 \tilde{u} = \frac{1}{\mu} \frac{\mathrm{d}\tilde{P}}{\mathrm{d}x}, \tag{4.2}$$

where $\phi^2 = -\mathrm{i}\rho_0\omega/\mu$. Our neglect of axial derivatives in the viscous terms and assumption of constant pressure across the channel width requires $|\phi^2| \gg |\beta^2|$ and

$|\beta H| \ll 1$ (an extensive discussion can be found in Stinson 1991). Due to the long-wavelength approximation we have neglected thermal creep effects which could result from the axial temperature gradient in the gas close to the wall. A discussion of thermal creep effects can be found in Karniadakis & Beskok (2002) and references therein.

The solution of the momentum equation subject to a symmetry condition at the channel centreline and the slip boundary condition (2.1) at the walls is

$$\tilde{u} = \frac{1}{\mu\phi^2}\frac{\mathrm{d}\tilde{P}}{\mathrm{d}x} + \frac{\cos\phi y}{\mu\phi^2\left(\alpha\lambda\phi\sin\frac{1}{2}\phi H - \cos\frac{1}{2}\phi H\right)}\frac{\mathrm{d}\tilde{P}}{\mathrm{d}x}. \tag{4.3}$$

The bulk velocity is given by

$$\tilde{u}_b(x) = \frac{1}{\mu\phi^2}\frac{\mathrm{d}\tilde{P}}{\mathrm{d}x} + \frac{2}{\mu\phi^3 H}\frac{\mathrm{d}\tilde{P}}{\mathrm{d}x}\left(\frac{1}{\alpha Kn\phi H - \cot\frac{1}{2}\phi H}\right) \equiv -\frac{1}{\mathscr{R}(Kn)}\frac{\mathrm{d}\tilde{P}}{\mathrm{d}x}. \tag{4.4}$$

Lamb's result is recovered when $\phi H/2 \to 0$ ($\delta \to \infty$); in this case the effect of inertia becomes negligible and the bulk flow rate reduces to the slip-flow Poiseuille expression

$$\tilde{u}_b = -\frac{H^2}{12\mu}\frac{\mathrm{d}\tilde{P}}{\mathrm{d}x}(1 + 6\alpha Kn), \tag{4.5}$$

that is the response is quasi-static.

4.2. *The energy equation*

The linearized energy equation reduces for this problem to

$$\rho_0 c_P \frac{\partial T}{\partial t} - \kappa\frac{\partial^2 T}{\partial y^2} = \frac{\partial P}{\partial t}, \tag{4.6}$$

where κ is the gas thermal conductivity and c_P is the gas specific heat at constant pressure. Our assumption of constant pressure across the channel allows us to treat the term on the right-hand side as a constant source term with the axial dependence implied. Using the same nomenclature, we rewrite the above equation as

$$\frac{\partial^2\tilde{T}}{\partial y^2} + \psi^2\tilde{T} = \psi^2\frac{(\gamma-1)}{\gamma}\frac{T_0}{P_0}\tilde{P}, \tag{4.7}$$

where $\psi^2 = -\rho_0 \mathrm{i}\omega c_P/\kappa = \phi^2\, Pr$. Using the temperature jump boundary conditions (2.2), the transverse temperature distribution is given by

$$\tilde{T}(x, y) = \frac{(\gamma-1)}{\gamma}\tilde{P}\frac{T_0}{P_0}\left(1 + \frac{\cos\psi y}{\zeta\psi H Kn\sin\frac{1}{2}\psi H - \cos\frac{1}{2}\psi H}\right). \tag{4.8}$$

The average temperature across the channel is given by

$$\tilde{T}_{av}(x) = \frac{1}{H}\int_{-H/2}^{H/2}\tilde{T}\,\mathrm{d}y = \frac{(\gamma-1)}{\gamma}\tilde{P}\frac{T_0}{P_0}\left(1 + \frac{2}{\psi H}\frac{1}{\zeta\psi H Kn - \cot\frac{1}{2}\psi H}\right). \tag{4.9}$$

Using the equation of state of an ideal gas, and the fact that $\tilde{P}_{av} = \tilde{P}$ we can write

$$\frac{\rho_0}{P_0}\left(\frac{\partial P}{\partial\rho}\right)_{av} = \frac{1}{1 - \dfrac{P_0}{T_0}\left(\dfrac{\partial\tilde{T}}{\partial\tilde{P}}\right)_{av}} = \frac{1}{1 - \dfrac{\gamma-1}{\gamma}\left(1 + \dfrac{2}{\psi H}\dfrac{1}{\zeta Kn\psi H - \cot\frac{1}{2}\psi H}\right)}. \tag{4.10}$$

In the absence of slip flow and for $\psi H/2 \sim \phi H/2 \to 0$, $\rho_0/P_0\,(\partial P/\partial\rho)_{av} \to 1$ $(\tilde{T} \to 0)$, that is the flow is isothermal as assumed by Lamb and shown by Kirchhoff's analysis (Rayleigh 1896). As $\psi H/2 \sim \phi H/2 \to \infty$, $\rho_0/P_0\,(\partial P/\partial\rho)_{av} \to \gamma$, that is the propagation is isentropic, as expected, even though this limit is not relevant here.

4.3. *The complete slip-flow solution*

The complete solution can be thus written as

$$\beta^2 \equiv (m+\mathrm{i}k)^2 = \frac{\mathrm{i}\omega\mathscr{R}(Kn)}{\rho_0(\partial P/\partial\rho)_{av}} = -\frac{\mathrm{i}\omega\mu\phi^2\left(1-\dfrac{\gamma-1}{\gamma}\left(1+\dfrac{2}{\psi H}\dfrac{1}{\zeta Kn\psi H-\cot\frac{1}{2}\psi H}\right)\right)}{P_0\left(1+\dfrac{2}{\phi H}\dfrac{1}{\alpha Kn\phi H-\cot\frac{1}{2}\phi H}\right)}, \tag{4.11}$$

which can be also written as

$$\beta^2\lambda^2 = -\frac{5\mathrm{i}\pi}{2}\frac{\tau_c}{\tau}\phi^2H^2Kn^2\frac{1-\dfrac{\gamma-1}{\gamma}\left(1+\dfrac{2}{\psi H}\dfrac{1}{\zeta Kn\psi H-\cot\frac{1}{2}\psi H}\right)}{1+\dfrac{2}{\phi H}\dfrac{1}{\alpha Kn\phi H-\cot\frac{1}{2}\phi H}}, \tag{4.12}$$

where $\tau = 2\pi/\omega$ is the wave period and $\tau_c = \lambda/\bar{c}$ is the molecular collision time. For generality, we have used a viscosity-based mean free path definition $\lambda = 4\bar{c}\mu/(5P_0)$. Here $\bar{c} = \sqrt{8k_bT/(\pi m_m)}$ is the average molecular speed, m_m is the molecular mass, and k_b is Boltzmann's constant. This result is valid for $|\beta H| \ll 1$ and $|\phi^2| \gg |\beta^2|$, and is in agreement with the full Kirchhoff solution subject to slip boundary conditions (numerically solved) to within 0.5% for $|\beta H| \leqslant 0.15$ and $|\phi^2| \gg |\beta^2|$.

For narrow channels, $|\phi H| < 0.1$, the above expression reduces to

$$\beta^2\lambda^2 = \frac{12\mathrm{i}\omega\mu Kn^2}{P_0(1+6\alpha Kn)} = \frac{30\mathrm{i}\pi Kn^2}{1+6\alpha Kn}\frac{\tau_c}{\tau}, \tag{4.13}$$

which is the slip-flow extension of Lamb's result (3.6). By rewriting the narrow channel requirement, $|\phi H| < 0.1$, as $\tau/\tau_c > 1280/Kn^2$ we find that the long-wavelength approximation is always satisfied for narrow channels in the slip-flow regime.

5. Extension to non-continuum regimes

The more general form of the linearized momentum and energy conservation equations in the wave propagation context can be written as

$$\mathrm{i}\rho_0\omega\tilde{u} - \frac{\partial\tilde{\tau}_{xy}}{\partial y} = -\frac{\mathrm{d}\tilde{P}}{\mathrm{d}x}, \qquad \mathrm{i}\rho_0c_P\omega\tilde{T} + \frac{\partial\tilde{q}_y}{\partial y} = \mathrm{i}\omega\tilde{P}, \tag{5.1a, b}$$

where $\tilde{\tau}_{xy}$ is the amplitude of the x, y-component of the stress tensor, and $\tilde{q}_y$ is the amplitude of the y-component of the heat-flux vector. However, closures for the heat flux vector and shear stress tensor beyond the slip-flow regime ($Kn \gtrsim 0.1$) do not exist and thus integration of these equations is, in general, not possible. Solution can be achieved by resorting to molecular-kinetic descriptions such as the Boltzmann equation or molecular simulation. Here we show that we can obtain an analytical solution by taking advantage of the physical significance of the narrow channel limit.

The narrow channel requirement is easily met for $Kn \gtrsim 0.1$ if we assume that the neglect of inertial effects is still governed by the (continuum-based) criterion

given above, namely $\delta \gg 1$. Consider gaseous argon at atmospheric pressure as an example: at $Kn = 0.1$, any frequency $\omega < 10^7$ rad s^{-1} leads to $\delta \gg 1$; at $Kn = 10$, δ is much larger than 1 for any frequency $\omega < 10^{11}$ rad s^{-1} (molecular collision-rate effects become important well before this frequency (Hadjiconstantinou & Garcia 2001)).

Thus, if we are able to provide a model for the steady-state flow resistance $\mathscr{R} = \mathscr{R}(Kn)$ defined by

$$\tilde{u}_b = -\frac{1}{\mathscr{R}(Kn)}\frac{\mathrm{d}\tilde{P}}{\mathrm{d}x} \tag{5.2}$$

that describes the flow rate in channels for all Knudsen numbers under isothermal conditions, we will be able to predict the characteristics of wave propagation at arbitrary Knudsen numbers for narrow channels. It has been shown both experimentally (Knudsen 1909) and theoretically (Cercignani 1988) that in the linear steady-flow regime there exists such a description of isothermal pressure-driven flow. It is usually presented (Cercignani 1988) in the form

$$\dot{Q} = u_b H = -\frac{1}{P_0}\frac{\mathrm{d}P}{\mathrm{d}x} H^2 \sqrt{\frac{RT_0}{2}}\,\bar{Q}, \tag{5.3}$$

where $\dot{Q}$ is the flow rate per unit depth, $R = k_b/m_m$ is the gas constant, and $\bar{Q} = \bar{Q}(Kn)$ is a proportionality coefficient that has been accurately determined by solution of the Boltzmann equation, and exists in tabular form (Cercignani 1988). In the transition regime, $\bar{Q}(Kn)$ varies slowly about its minimum value ($1.5 < \bar{Q}(0.1 < Kn < 10) < 3$) occurring at $Kn \approx 1$, which explained Knudsen's experimental discovery (Knudsen 1909) of a minimum in the normalized (as above) flow rate. For the purposes of comparison with our hard-sphere DSMC calculations in § 6, we will use $\bar{Q}(Kn)$ as determined by solution of the linearized Boltzmann equation (Ohwada, Sone & Aoki 1989*b*) for a hard-sphere gas. For real gas applications, appropriate values of $\bar{Q}(Kn)$ that describe real-gas behaviour can be used. However, experiments, linearized solutions of the Boltzmann equation, and molecular simulations have been found to be in very good agreement (Beskok & Karniadakis 1999), even when the latter two employ the hard-sphere model or even simpler models such as that of Maxwellian molecules (Cercignani 1988).

By combining (3.3) and (5.2), we obtain the counterpart of equation (3.4) governing wave propagation in narrow channels in all Kn-regimes, while from (5.3) we can identify

$$\mathscr{R}(Kn) = \frac{P_0}{H\bar{Q}\sqrt{RT_0/2}} \tag{5.4}$$

leading to

$$\beta^2\lambda^2 = \frac{8\mathrm{i}\sqrt{\pi}Kn}{\bar{Q}}\frac{\tau_c}{\tau}. \tag{5.5}$$

Given the (approximate for $Kn > 0.1$) narrow channel requirement $\tau/\tau_c > 1280/Kn^2$, the above equation predicts that the long-wavelength approximation is satisfied provided $\tau/\tau_c \gtrsim 100$ (molecular collision-frequency effects become important for $\tau/\tau_c \lesssim 100$). Expression (5.5) is expected to hold in all Kn-regimes for $\delta \gg 1$ since both ingredients, equations (3.3) and (5.3), are valid in all Kn-regimes. Although direct solution of the Boltzmann equation becomes computationally expensive in the limit $Kn \to 0$, the transition of (5.3) into (4.5) requires

$$\bar{Q} = \frac{8}{5\sqrt{\pi}}\frac{1 + 6\alpha Kn}{6Kn} \quad \text{for} \quad Kn < 0.1. \tag{5.6}$$

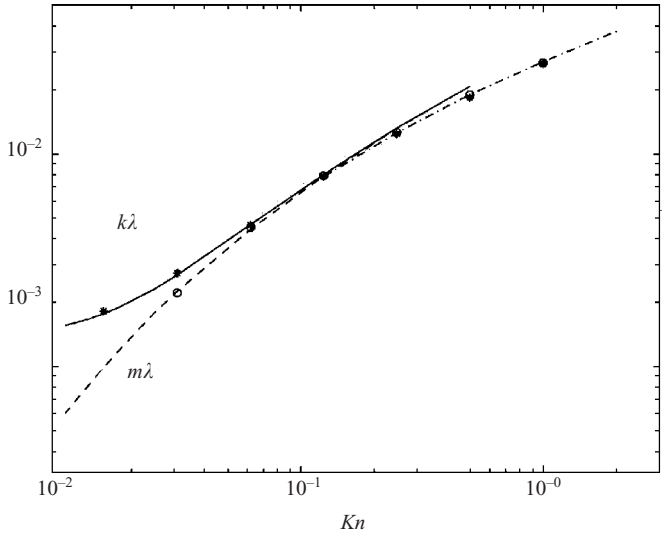

FIGURE 2. Comparison between the theoretical predictions and DSMC simulations for $\omega = 6 \times 10^6$ rad s^{-1}. The dashed and solid lines show the prediction of (4.11) for the attenuation coefficient and the wavenumber, respectively. The dash-dotted line shows the prediction of (5.5). DSMC results for the wavenumber and attenuation coefficient are shown as stars and circles, respectively. Error bars are given by the symbol size.

6. Direct simulation of wave propagation

The direct simulation Monte Carlo (DSMC) is a stochastic molecular simulation technique for solving the Boltzmann equation. Consistency between DSMC solutions and solutions of the Boltzmann equation in the limit of infinitesimal discretization and large number of particles was recently shown by Wagner (1992). Alexander, Garcia & Alder (1998) have shown that the transport coeffcients exhibit quadratic convergence with the cell size, whereas Hadjiconstantinou (2000) and Garcia & Wagner (2000) have shown the same behaviour for the timestep.

For brevity we will not present a description of the DSMC algorithm. Excellent descriptions can be found in the literature (Bird 1994); comparisons of DSMC simulation results with solutions of the linearized Boltzmann equation and experimental results for diverse non-equilibrium phenomena spanning the whole Kn-range can also be found in Bird (1994).

Wave propagation simulations are possible by using standard DSMC techniques (Bird 1994) augmented by a special sampling algorithm that accounts for the transient nature of the phenomenon (Hadjiconstantinou & Garcia 2001). More details on the implementation can be found in Hadjiconstantinou (2002).

The computational cost of DSMC simulations is proportional to the total time simulated and as a result it is inversely proportional to the wave frequency. In order to minimize the computational cost of our molecular simulations, our comparisons were performed at relatively high frequencies, while care was taken to ensure that nonlinear effects, molecular collision frequency effects and homogeneous absorption effects were negligible (Hadjiconstantinou 2002). At high frequencies inertia and heat conduction become important while $|\beta H|$ in some cases exceeds 0.1. Comparison at high frequencies thus has the advantage of providing a more stringent test of the theory presented above.

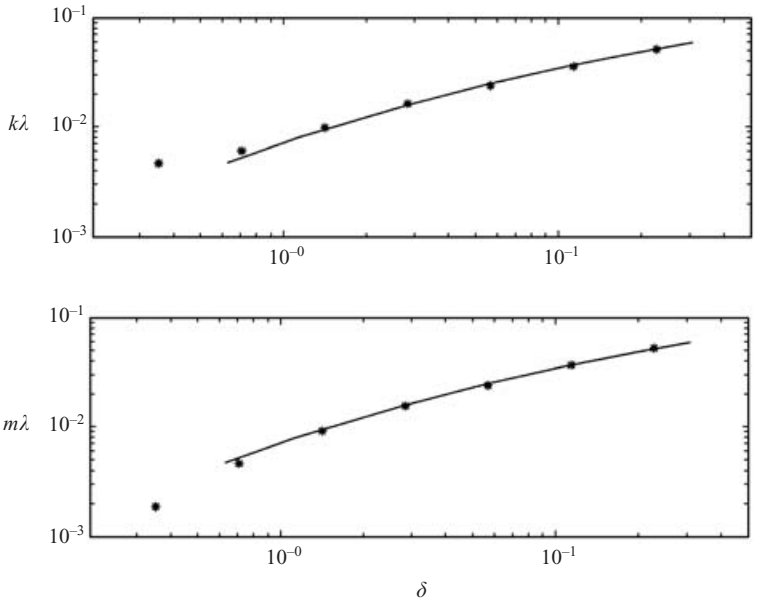

FIGURE 3. Comparison between the theoretical prediction of (5.5) and DSMC simulations for $\omega = 18.5 \times 10^6$ rad s^{-1}. Error bars are given by the symbol size.

Figure 2 shows a comparison between the theoretical results and DSMC simulations for different Knudsen numbers at a fixed frequency $\omega = 6 \times 10^6$ rad s^{-1}. It shows that the theory remains reasonably accurate even when $|\beta H|$ exceeds 0.1; also the slip-flow approximation remains reasonably accurate beyond $Kn \approx 0.1$.

Figure 3 shows the results of simulations at a fixed frequency $\omega = 18.5 \times 10^6$ rad s^{-1} for a variety of channel heights. The solid lines represent the predictions of (5.5). The narrow channel theory appears to be valid for $\delta > 1$ (rather than $\delta \gg 1$) despite the continuum origin of this criterion.

7. Concluding remarks

The agreement between the theoretical results and simulations is very good, suggesting that the theory developed remains robust and reasonably accurate even beyond its expected limits of applicability. The theoretical results remain accurate for $|\beta H| \sim O(0.1)$. The continuum-based criterion $\delta \gg 1$ appears to provide a conservative estimate of the effects of inertia for $Kn > 0.1$. The slip-flow results continue to be relatively accurate beyond $Kn = 0.1$ in agreement with previous studies (Hadjiconstantinou & Simek 2002).

The flow resistance in the early transition regime can be calculated from a Poiseuille model subject to second-order slip-flow boundary conditions such as the ones proposed in Beskok & Karniadakis (1999) and Hadjiconstantinou (2003). However, their use is currently limited to isothermal flows due to the lack of a reliable second-order temperature jump model. When such a model is developed, second-order slip models will enable the use of the continuum theory of § 4 well beyond $Kn = 0.1$ and thus lift the isothermal restriction associated with the narrow channel theory of § 5.

Although in this work we used the dilute hard-sphere gas model to verify our predictions, we expect the results to approximate real gas behaviour well. The slip-flow-based theory incorporates all the physics required to capture polyatomic gas

behaviour, whereas the narrow channel approach only requires the pressure-driven flow characteristics to be known; the latter are captured fairly accurately by the dilute monoatomic gas model (Beskok & Karniadakis 1999). Wave propagation under low-pressure conditions (where slip and non-continuum effects manifest themselves at larger scales) is also captured by the developments presented above; in fact under these conditions, the narrow channel requirement ($\tau/\tau_c > 1280/Kn^2$) is satisfied at even higher frequencies (for the same channel height) because the gas viscosity is not a function of pressure.

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