The Response of a Gas in a Micro-channel to Periodic Boundary Heating

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Abstract.
We study the flow-field generated in a one-dimensional wall-bounded gas layer due to periodic small-amplitude time variation in the temperature of its boundaries. We focus on the Navier-Stokes limit, where the layer width is large compared to the mean free path and the characteristic time-scale of temperature variations is long compared with the mean free time between collisions. The viscous-compressible Navier-Stokes equations with slip-flow boundary conditions are solved analytically for the case of sinusoidal heating. The analysis is then extended to study the system response to arbitrary periodic heating. Results are presented for both triangle- and square-wave heating profiles. These solutions are found to be in good agreement with low-variance Monte-Carlo simulations of the Boltzmann equation, validating the present analysis as an accurate and simple alternative to expensive molecular computations. In addition, the analysis is applied for quantitative examination of the conditions for breakdown of the slip-flow description in non-isothermal flows.

Keywords: micro-channel, slip-flow model, unsteady heating, low-variance Monte Carlo simulations.
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INTRODUCTION

The time response of a fluid confined in a channel and subject to a change in the thermal properties of its boundaries has been studied extensively in the context of both classical fluid mechanics [1] and rarefied gas dynamics [2]. The fluid motion induced in this problem is essentially driven by the mechanism of thermal expansion, coupling temperature variations in the fluid with density gradients. The problem of gradual change in wall thermal properties was studied in the context of continuum gas dynamics in a series of papers (see [3] and papers cited therein) in which a time-scale longer than some modest multiple of the molecular collision time has been assumed. To consider shorter time-scales, several researchers have investigated the problem in the limit of sudden temperature variations by examining the kinetic response of a dilute gas to a step function change in wall temperatures [4-7].

Current interest in the unsteady boundary heating problem is motivated by the common occurrence of time-varying boundary temperatures in a wide scope of micro- and nano-electro-mechanical-system applications, ranging from micro-processor chip heating to ultrafast thermal excitation encountered in the laser industry [8, 9]. Previous works have focused on the gas response to instantaneous [7] and rapidly-varying continuous [10] changes in the wall temperatures with characteristic time-scales on the order of, or smaller than, the mean collision time. Under these conditions, the effect of molecular collisions is small, and a collisionless description is appropriate. Utilizing such a description, closed-form solutions were obtained for the step-jump and high-frequency oscillatory heating problems. In the latter case, the hydrodynamic response was found to be confined to thin bounded layers in the vicinity of the walls at all times.

In this work we complement the above studies by focusing on the problem in the collision-dominated limit; namely, we consider the case where the distance between the walls is large compared with the mean free path and the time-scale of temperature variations is large compared with the mean time between molecular collisions. We study the late-time response of the system to periodic changes in the temperature of its boundaries. The gas behavior in these cases is modeled by the compressible Navier-Stokes equations subject to slip-flow boundary conditions. To first-order in the Knudsen number, the latter reduce to impermeability conditions for the normal component of the flow velocity and temperature jump conditions at the boundaries. This is a commonly-used model which has been applied to the study of various problems [11-13]. The inclusion of slip-flow boundary conditions makes the results presented here applicable to devices with characteristic scales as small as $\approx 1\mu m$ at standard atmospheric conditions. We make use

of the present analysis to examine the breakdown of the slip-flow description with decreasing time- and length-scales through comparison with low-variance Monte Carlo simulations of the Boltzmann equation [14, 15] and existing analyses of the counterpart high-frequency collisionless problem [10].

The paper is organized as follows: first, the linearized problem is formulated. Then an analytical solution is derived and the numerical method used for validation is outlined. Our results for sinusoidal and general periodic heating profiles are presented and discussed. Finally, some concluding remarks are given.

PROBLEM FORMULATION

Consider a perfect monatomic gas layer of mean density ρ_0 confined between two infinitely long, accommodating walls in the (y^*,z^*) plane at $x^* = \pm L/2$, where * denotes a dimensional variable. The walls are heated uniformly with prescribed periodic time dependence and their common temperature is $T_w^*(t^*) = T_0[1+\varepsilon F(t^*)]$. Here $F(t^*) = F(t^*+\tau_p^*)$, where $\tau_p^* = 2\pi/\omega_p^*$ is the time period and ω_p^* is the angular frequency of the temperature variation. It is assumed that the amplitude ε of the oscillatory term is small ($\varepsilon \ll 1$) so that the system description may be linearized about its equilibrium state of uniform density ρ_0 and temperature T_0. In contrast with previous studies [7, 10], we focus here on the case where the distance L between the walls is large compared with the molecular mean free path l (i.e., the Knudsen number $Kn = l/L \ll 1$) and the characteristic time-scale of the temperature variations at the boundaries is large compared with the mean time between collisions.

We model the system evolution using the viscous-compressible Navier-Stokes equations subject to slip-flow boundary conditions at the boundaries [12]. We assume a one-dimensional setup where all variables are x^*-dependent and the velocity vector $\mathbf{u}^*$ has a non-zero component only in the x^*-direction. To render the problem dimensionless, we scale the position by the layer width L and the time by a time-scale $\tau^* = \omega_p^{*-1}$. The velocity is scaled by $\omega_p^* L$ and the density and temperature are normalized by ρ_0 and T_0, respectively. Linearizing about the initial equilibrium state, we obtain the following balances of mass, momentum and energy for the $O(\varepsilon)$ density ρ, normal velocity u and temperature T perturbations

$$\frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial x} = 0 \quad , \quad \frac{\partial u}{\partial t} = -\frac{1}{St^2}\left(\frac{\partial \rho}{\partial x} + \frac{\partial T}{\partial x}\right) + \frac{4\widetilde{Kn}}{3St}\frac{\partial^2 u}{\partial x^2} \quad \text{and} \quad \frac{\partial T}{\partial t} = \frac{\gamma \widetilde{Kn}}{PrSt}\frac{\partial^2 T}{\partial x^2} - (\gamma-1)\frac{\partial u}{\partial x} \ , \tag{1}$$

together with the boundary conditions

$$u = 0 \text{ and } T = F(t) \pm \xi \frac{\partial T}{\partial x} \text{ at } x = \mp 1/2 \, . \tag{2}$$

In Eq. (1), $St = \omega_p^* L/\sqrt{RT_0}$ is the Strouhal number (with gas constant R); $\widetilde{Kn} = \mu_0/(\rho_0\sqrt{RT_0}L)$ is the modified (viscosity-based) Knudsen number (with μ_0 the gas dynamic viscosity at reference-equilibrium conditions); γ is the ratio of specific heats; and Pr is the Prandtl number. For a perfect monatomic gas $\gamma = 5/3$. We consider here a BGK (Bhatnagar, Gross and Krook [16]) model of molecular interaction for which $Pr = 1$ and efficient low-variance Monte Carlo solution methods exist [15]. In the present notation, our assumption that the characteristic time ω_p^{*-1} is much longer than the mean time between collisions $\tau_{coll}^* = l/\sqrt{8RT_0/\pi}$, can be expressed as $StKn \ll \sqrt{8/\pi} \approx 1.6$. We comment further on the validity of this condition in the Analysis and Results sections.

The boundary conditions (2) impose impermeability and specify the magnitude of temperature jump at the walls. The latter is determined by the value of the temperature gradient at the walls and a temperature-jump coefficient, $\xi = \zeta Kn$, with ζ taking the value $\zeta = 1.3\sqrt{\pi}/2$ for the BGK model [17]. The modified Knudsen number $\widetilde{Kn}$ appearing in (1) is related to Kn through

$$\widetilde{Kn} = \frac{\mu_0}{\rho_0\sqrt{RT_0}l}Kn \, , \tag{3}$$

where $\mu_0/(\rho_0\sqrt{RT_0}l) = \sqrt{\pi/8}$ for a BGK gas [17].

ANALYSIS

Sinusoidal heating

The problem specified by Eqs. (1)-(2) is amenable to analytical solution for the case of sinusoidal heating, $F(t) = \sin(t)$. Towards this end, we seek for the long-time periodic (rather than the initial transient) behaviour of the system. We assume harmonic time-dependence of the hydrodynamic perturbations

$$G(x,t) = \bar{G}(x)\mathrm{e}^{\mathrm{i}t} \ , \ G \in \{\rho, u, T\} \tag{4}$$

and substitute (4) into (1). The density and velocity perturbations can be eliminated using

$$\bar{\rho} = \mathrm{i}\bar{u}' \ , \ \bar{u} = -\frac{5\widetilde{Kn}}{2PrSt^2}\left(\frac{1}{St} + \frac{4\mathrm{i}\widetilde{Kn}}{3}\right)\bar{T}''' - \frac{1}{St}\left(2\widetilde{Kn} - \frac{5\mathrm{i}}{2St}\right)\bar{T}' \tag{5}$$

to yield a single equation for the temperature

$$\frac{5\widetilde{Kn}}{3PrSt^2}\left(\frac{1}{St} + \frac{4\mathrm{i}\widetilde{Kn}}{3}\right)\bar{T}'''' + \frac{1}{3St}\left(4\widetilde{Kn} + \frac{5\widetilde{Kn}}{Pr} - \frac{5\mathrm{i}}{St}\right)\bar{T}'' - \mathrm{i}\bar{T} = 0\,. \tag{6}$$

The solution of (6) satisfying the boundary conditions (2) is given by

$$\bar{T}(x) = A\cosh(r_1 x) + B\cosh(r_2 x)\,, \tag{7}$$

where the constants A, B, r_1 and r_2 are tabulated in Ref. [18]. The expressions for the density and velocity perturbations follow subsequently from (5). In addition, the normal heat-flux is given by Fourier's law, which in non-dimensional representation (after scaling by $\rho_0(RT_0)^{3/2}$) takes the form $\bar{q}(x) = -(5\widetilde{Kn}/2Pr)\bar{T}'$. The physical fields are obtained by taking the imaginary parts of the pertinent expressions.

General periodic heating

The above solution can be extended to obtain the gas response to arbitrary small-amplitude periodic heating. This can be achieved by representing the system behavior as a linear superposition of single-harmonic responses, with varying amplitudes determined from the Fourier expansion of $F(t)$.

We demonstrate this procedure by studying the gas response to the "triangle wave" (tw) and "square-wave" (sw) heating signals. These profiles can be represented by their Fourier series expansions

$$F_{tw}(t+2\pi k) = \begin{cases} 2t/\pi & , \quad 0 \le t < \pi/2 \\ -2t/\pi + 2 & , \quad \pi/2 \le t < 3\pi/2 \\ 2t/\pi - 4 & , \quad 3\pi/2 \le t < 2\pi \end{cases} = \frac{8}{\pi^2}\sum_{n=1,3,5,\ldots}^{\infty} \frac{(-1)^{(n-1)/2}}{n^2}\sin(nt) \tag{8}$$

and

$$F_{sw}(t+2\pi k) = \begin{cases} 1 & , \quad 0 \le t < \pi \\ -1 & , \quad \pi \le t < 2\pi \end{cases} = \frac{4}{\pi}\sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n}\sin(nt)\,, \tag{9}$$

where $k = 0, \pm 1, \pm 2, \ldots$. Using linear superposition, the system response is now obtained as an infinite sum over the corresponding responses to each of the sum components in (8) and (9). The solution for each component depends on the Strouhal number based on the corresponding frequency component, $St(n) = n\omega_p^* L/\sqrt{RT_0}$. Since n can become arbitrarily large, it is inevitable that the slip-flow regime requirement, $St(n)Kn \ll \sqrt{\pi/8}$, will not be satisfied for sufficiently large n. In practice, however, only a finite number of terms is needed for a converged result, owing to the decaying contribution of the high-frequency terms ($\sim 1/n^2$ in the triangle-wave and $\sim 1/n$ in the square-wave distributions). More specifically, our numerical calculations indicate that only $N \approx 10$ and $N \approx 100$ terms are required for obtaining a converged result in the triangle- and square-wave cases, respectively. These considerations lead to a bound on the dimensional frequency ω_p^* which, for a given Kn, satisfies the condition $St(N)Kn \ll \sqrt{\pi/8}$. This limitation becomes particularly important, as shown in Fig. 3, at short times after wall-temperature discontinuities, where high-frequency components are non-negligible.

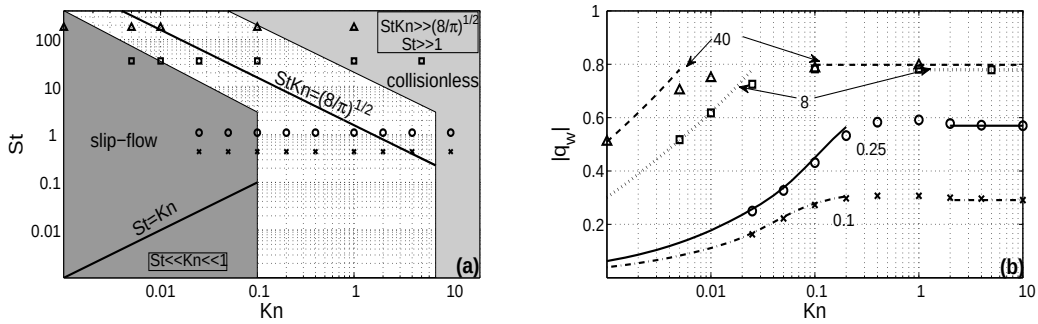

FIGURE 1. (a) Schematic partition of the (Kn, St) plane to the different flow domains in the sinusoidal heating problem. The dark-shaded and bright-shaded zones mark the domains of slip-flow and collisionless-flow regimes, respectively. The line $StKn = \sqrt{8/\pi}$ corresponds to the locus of states where the characteristic time-scale $\tau = 1/\omega_p$ is equal to the mean collision time τ_{coll}. The limit cases $St \ll Kn \ll 1$ (of small dynamical compressibility) and $StKn \gg \sqrt{8/\pi}, St \gg 1$ (of thin bounded layers) are discussed in Refs. [18] and [10]. The crosses, circles and triangles mark the (St, Kn) combinations for which LVDSMC data is presented in Fig. 1b. (b) The Knudsen-number variation of the walls heat-flux amplitude, $|q_w| = \max\{q(x = \pm 0.5)\}$, at the indicated values of $St/(\pi\sqrt{2})$ for a BGK gas subject to sinusoidal heating. The lines mark the analytical slip-flow and collisionless solutions and the symbols denote LVDSMC data.

NUMERICAL SIMULATIONS

Slip-flow theory can be rigorously derived from asymptotic analysis of the Boltzmann equation. In this section we briefly describe the method used for obtaining numerical solutions of the Boltzmann equation for validating the present analysis. Since Boltzmann equation solutions are valid for all Kn and St, they will allow us to find the limits of applicability of our results.

The prevalent numerical scheme for solving the Boltzmann equation is a stochastic particle method known as the direct simulation Monte Carlo (DSMC) method [19]. However, since typical flow-velocities in the present problem are small compared to the speed of sound, use of the DSMC method with existing computational resources becomes extremely time consuming. Our numerical solutions are therefore obtained using a recently developed variance-reduced particle method akin to DSMC known as low-variance deviational simulation Monte Carlo (LVDSMC), which, by simulating only the *deviation* from equilibrium, achieves significant variance reduction, enabling accurate simulation of weak-signal flows with reasonable computational resources.

In the following, the BGK model is simulated using a particular LVDSMC method developed by Radtke and Hadjiconstantinou [15] for treating the linearized Boltzmann equation in the relaxation-time approximation. In contrast with the DSMC method, the low Knudsen numbers considered here do not pose particular problems for the LVDSMC method, as the latter simulates the deviation from a spatially variable equilibrium and is able to take advantage of the near-local-equilibrium conditions prevalent at low Kn. The simulations use $N_{cell} = 200$ cells for $Kn = 0.025$ and $N_{cell} = 100$ cells for all other values of Kn. The time-step used was a small fraction (typically 0.2) of the cell traversal time based on the most probable speed $L/(N_{cell}\sqrt{2RT_0})$. The results shown were sampled after allowing the simulation to achieve a “steady" oscillatory state by integrating in time for at least 20 acoustic time-scales $L/\sqrt{2RT_0}$.

RESULTS

The slip-flow analysis of the system response to sinusoidal heating has been validated in Ref. [18] through comparison with LVDSMC results. For completeness, we describe here the limits of applicability of our theory. Figure 1 presents schematic mapping of the different flow regimes obtained in the sinusoidal heating problem in the (Kn, St) plane. In Fig. 1a, The dark-shaded and bright-shaded zones mark the domains of slip-flow and free-molecular regimes, respectively, while the unshaded zone corresponds to the transition regime domain of “intermediate" Knudsen numbers. Fig. 1b presents the Kn-variation of the walls heat-flux amplitude at the indicated values of St.

When $St < 1$, the characteristic time-scale of temperature variations at the boundaries is always considerably larger than the mean collision time. As a result, the limit of validity of the slip-flow theory is determined only by the Knudsen number. Our comparison with LVDSMC simulations (cf. Fig. 1b and [18]) confirms the commonly accepted value of

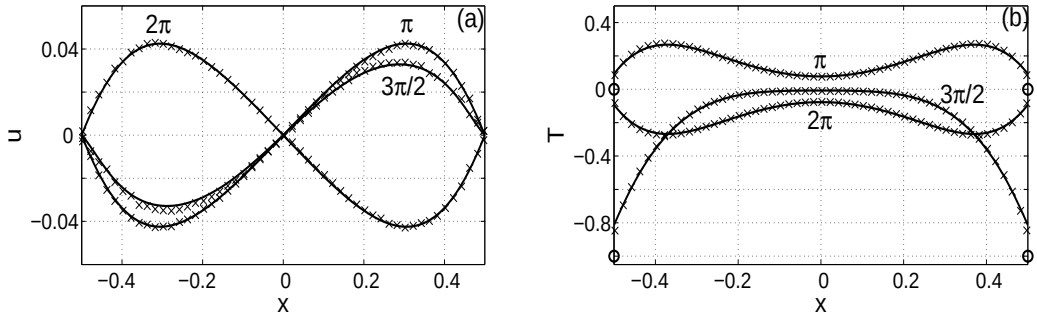

FIGURE 2. The (a) velocity and (b) temperature perturbations for a BGK gas subject to triangle-wave heating profile at $Kn = 0.025$, $St = \pi\sqrt{2}/4 \approx 1.11$ and the indicated values of time. The solid lines correspond to the Fourier-series results and the crosses mark LVDSMC data. The circles denote the wall-temperature perturbations, added to mark the magnitude of temperature-jumps at the walls.

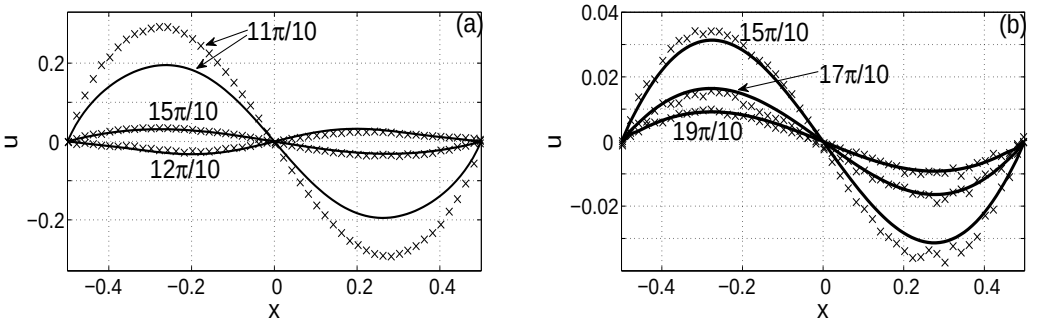

FIGURE 3. The velocity perturbation for a BGK gas subject to square-wave heating profile at $Kn = 0.025$, $St = \pi\sqrt{2}/4 \approx 1.11$ and the indicated values of time. The solid lines correspond to the Fourier-series results and the crosses mark LVDSMC data.

$Kn \approx 0.1$ to be the upper limit of applicability of the slip-flow model. The transition regime then extends up to $Kn \approx 7$, where the effect of molecular collisions vanishes and the free-molecular description, analyzed in Ref. [10], prevails.

The situation changes markedly in the case of high-frequency heating, $St \gg 1$. Here, the short time-scale of temperature variations at the walls becomes the main factor in determining the type of flow to be developed; specifically, the $StKn$ criterion replaces the Knudsen number condition used in the $St < 1$ case. At $StKn = \sqrt{8/\pi}$ (denoted by a line in Fig. 1a) the characteristic time-scale $\tau = 1/\omega_p$ and the mean collision time τ_{coll} are equal; the slip-flow and collisionless flow regimes are expected to take place at $StKn \ll \sqrt{8/\pi}$ and $StKn \gg \sqrt{8/\pi}$, respectively. In practice, our comparison with LVDSMC data indicate that the transition regime is bounded between $0.2 < StKn < 20$.

The analysis of the system response to the triangle-wave (8) and square-wave (9) signals is examined in Figures 2 and 3, respectively, where the velocity and temperature fields are compared with LVDSMC results. The indicated Strouhal number in both cases ($St = \pi\sqrt{2}/4$) corresponds to the "fundamental" $n = 1$ frequency of the wave. In the triangle-wave case (Fig. 2), the agreement between the present theory and LVDSMC data is very good at all times, apart from thin Knudsen layers observed in the temperature profile at $t = 2\pi$.

A less satisfactory agreement is obtained in the square-wave case (Fig. 3), where large discrepancies appear in the velocity profile shortly after the wall-temperature discontinuity occurs (at $t = \pi$ the wall-temperature perturbation "jumps" from 1 to -1). To rationalize these discrepancies, recall that the Strouhal number is inversely proportional to the characteristic time-scale of the temperature variations at the walls. When wall-temperature discontinuities occur, this local time-scale becomes vanishingly small, making the corresponding Strouhal number infinitely large. In terms of the present Fourier analysis, infinitely large frequency components are required to capture the correct system behaviour. The condition $StKn \ll \sqrt{\pi/8}$ is therefore violated and the full kinetic model of the gas must be taken into account. As can be seen in Fig. 3a, this breakdown of the slip-flow description persists for some (short) time after the discontinuity occurs. This indicates that even when approximating the system behavior using a truncated Fourier

series, a number of high-frequency terms (which are still non-negligible) violate the time-scale restriction. Specifically, for the present case characterized by $St \approx 1.11$ and $Kn = 0.025$, we find that $St(N = 100)Kn \approx 5.6 > \sqrt{\pi/8}$, which is manifested in the disagreement between the two velocity profiles at $t = 11\pi/10$ (Fig. 3a). With increasing time (from the discontinuity at $t = \pi$ to the one at $t = 2\pi$), the discrepancies in the velocity vanish (Fig. 3b). Similar trends are also observed in all other hydrodynamic fields (not shown here).

CONCLUSION

We have studied the linearized response of a gas confined in a micro-channel to periodic variation in the temperature of its boundaries. The results obtained, valid for Knudsen numbers $Kn < 0.1$ and Strouhal numbers $St < Kn^{-1}$, complement existing analyses of the collisionless gas response to high-frequency ($St \gg 1$) heating. In addition, the present scheme provides an accurate and simple description of the gas response in the low-St number limit where numerical calculations are particularly demanding, due to long evolution time-scales and small hydrodynamic response amplitudes. Extensions of the present results to non-periodic heating profiles as well as other models of molecular interaction are presented in a separate paper [18].

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