Transient motion of a confined rarefied gas due to wall heating or cooling

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The transient motion that arises in a confined rarefied gas as a container wall is rapidly heated or cooled is simulated numerically. The Knudsen number based on nominal gas density and characteristic container dimension is varied from nearcontinuum to highly rarefied conditions. Solutions are generated with the direct simulation Monte Carlo method. Comparisons are made with finite-difference solutions of the Navier–Stokes equations, the limiting free-molecular values, and (continuum) results based on a small perturbation analysis. The wall heating and cooling scenarios considered induce relatively large acoustic disturbances in the gas, with characteristic flow speeds on the order of 20% of the local sound speed. Steadystate conditions are reached after on the order of 5 to 10 acoustic time units, here based on the initial speed of sound in the gas and the container dimension. As rarefaction increases, the initial gas response time is decreased. For the case of a rapid increase in wall temperature, transient rarefaction effects near the wall greatly alter gas response compared to the continuum predictions, even at relatively small nominal Knudsen number. For wall cooling, the continuum solution agrees well with direct simulation at that same Knudsen number. A local Knudsen number, based on the mean free path and the scale length of the temperature gradient, is found to be a more suitable indicator of transient rarefaction effects.

1. Introduction

The determination of local properties in a gas confined between two plates maintained at different temperatures is a fundamental problem in both continuum gas dynamics (Schlichting 1960) and gas kinetic theory (Patterson 1971). The transient development of this flow as induced by rapid heating or cooling of one or both of the walls is less well understood, though it has features of interest to problems in combustion, acoustics, and shock wave and boundary-layer theory.

Recently a class of micromechanical devices has been proposed (Muntz *et al.* 1992) which would utilize rapid heating and cooling of a small volume of gas in a thermal cycle to generate mechanical work. Rapid heating of a container wall is one of several means available to deposit energy in the gas. These devices will typically operate at standard atmospheric densities but will have a characteristic dimension h on the order of 10^{-4} m. The nominal Knudsen number, based on the lengthscale h and the hard-sphere mean free path λ_0 , is of the order of 0.002 for such conditions. Generalization (Bird 1983) of the hard-sphere mean free path to account for the variation of collision cross-section with temperature leads to larger nominal Knudsen numbers at the elevated operating temperatures of interest. Under these transitional

rarefied conditions a purely continuum analysis could be subject to large error. An additional issue for the transient problem are the large gradients that initially arise in the flow field. In the case of a rapidly heated container wall, for example, these disturbances can develop into shock waves which propagate across the gas (Clarke, Kassoy & Riley 1984*a,b*). A Knudsen number based on the local mean free path and the scale length of the gradient of temperature (Present 1958; Bird 1976) across these disturbances is much larger than the nominal Knudsen number. Hence, the Navier–Stokes equations may be inaccurate over a sizable portion of the flow field during the initial transient period. In either case, the effect of rarefaction on the transient solution, and the deviation of this solution from that predicted from a purely continuum standpoint are of interest.

To address these issues, we consider the model problem of a gas confined between infinite parallel plates and analyse the transient gasdynamic phenomena that develop as one wall is instantaneously cooled or heated to a new temperature. A nominal Knudsen number range of O(0.03)-O(0.4) and a wall temperature ratio of O(4) are considered for the case of a monatomic gas. The details of the gas-surface interaction process are expected to have a definite impact on the flow field as rarefaction increases. Owing to the uncertainties in general analytical models for this process, consideration is restricted to the case of a perfectly diffuse wall. A related paper (Wadsworth 1992) addresses in more detail the effect of the interaction model on the steady-state profiles.

The present authors are aware of no experimental data for this problem. There exist, however, steady-state data (Alofs, Flagan & Springer 1971) corresponding to the conditions considered herein. These data have been used in Wadsworth (1992) to validate the present numerical schemes. In the present paper, we compare results from the direct simulation Monte Carlo (DSMC) method (Bird 1976) wherein molecular motion is directly modelled, with results of finite-difference solutions of the (no-slip) Navier–Stokes (NS) equations, the free-molecular values, and with the approximate (continuum) perturbation results of Clarke *et al.* (1984a,b), Radhwan & Kassoy (1984) and Kassoy (1979) valid for small times after the initiation of wall heating.

2. Problem definition

Consider the model problem geometry shown in figure 1. Two infinite parallel plates separated by a distance h and initially at temperatures $T_{w_1} = T_{w_2} = T_0$ enclose a gas of nominal number density n_0 and temperature T_0 . The transient gasdynamic phenomena that develop as one wall is instantaneously brought to a new temperature are of interest.

Two distinct initial conditions arise. In case I the temperature of wall 2 is increased to χT_0 , while for case II the temperature of wall 1 is decreased to T_0/χ . Here $\chi = 3.72$ and $T_0 = 79$ K or $T_0 = 294$ K have been chosen to correspond to the (steady-state) data of Alofs *et al.* (1971). Owing to the low temperatures involved we consider only a monatomic gas (helium), thought the previous reference does contain data for diatomic nitrogen.

A characteristic rarefaction parameter, the Knudsen number, $Kn_0 = \lambda_0/h$, can be used to estimate the gasdynamic phenomena expected. We consider variations in the gas density such that near-continuum to highly rarefied gasdynamic phenomena are experienced. At higher Knudsen number indicative of more rarefied conditions, the details of the gas-surface interaction process at the plate surface are expected



FIGURE 1. Schematic of problem geometry.

to become increasingly important in establishing the flow field. Lacking accurate models for this process, consideration is limited to the case where the plates are perfectly diffuse reflectors at the wall temperature. This assumption will allow direct assessment of bulk rarefaction effects. Some estimates of the influence of the wall model are made below, however.

The nominal Knudsen number is not useful in quantifying the transient rarefaction processes which arise. Also, definition of a characteristic time parameter for this unsteady problem is made difficult by the lack of definite periodic phenomena. The acoustic and condition times discussed below are the most useful timescales which can be determined *a priori*.

3. Theory

Clarke *et al.* (1984*a,b*), Radhwan & Kassoy (1984) and Kassoy (1979) have considered the continuum wall heating problem extensively, and have given a sophisticated analytical exposition based on perturbation methods. They have also presented numerical calculations in support of their analytical results. Here we summarize their results and discuss major differences in the present problem. In their analyses, the ratio between the acoustic time t_a and the conduction or diffusion time t_c is used as the small parameter in the perturbation approach. Here, $t_a = h/a_0$ where a_0 is the speed of sound in the gas at the initial temperature and $t_c = h^2/\alpha_0$ where α_0 is the thermal diffusivity of the gas. The ratio between these two timescales can be identified as a nominal Knudsen number with the additional assumption that the Strouhal number St = 1. Based on these timescales, the analysis shows the gas near the wall to be made up of a conduction zone (or boundary layer), and an isentropic core. The expansion of the conduction zone and its effect on the core gas is the fundamental basis of the piston analogy (Moody 1990) typically used in compressible flow analysis.

The distinct transient features which arise in the gas can be categorized based on the amplitude and time over which heat addition at the boundary is applied. For the case of small and slow (based on t_c) wall heating (Kassoy 1979; Radwhan & Kassoy 1984), a linear acoustic field develops where the gas pressure is spatially homogeneous and rises monotonically to its steady-state value. Owing to acoustic effects, the gas response time is shorter than that of an equivalent heat-conducting solid (see also Larkin 1967).

In the case of large and rapid (compared to t_a) heat addition rates (Clarke *et al.* 1984*a,b*), the analysis retains the full Navier–Stokes equations and predicts the development of a shock wave which propagates away from the heated wall. Similar wall heating and cooling rates are considered here. Several key differences exist between this and the previous work, however.

(i) In the continuum limit, analysis of the relatively slow heating rate problem

must be explicitly restricted to the case of a gas in zero gravity. This is required to eliminate buoyancy and free convection effects which would mask the wall-induced phenomena. In the rarefied problem, the gas density arises as a parameter through the Knudsen number. The characteristic free convection parameter, the Grashof number, can then be written as $Gr \sim Kn_0^{-2}$. For all cases considered, Gr is several orders of magnitude below that at which convection effects are expected (Eckert & Carlson 1961; Alofs *et al.* 1971). Under rarefied conditions, the induced motion is thus experimentally accessible over the whole range of heat addition rates. In fact, the magnitude and timescales of the phenomena of interest are such that detailed measurements of both macroscopic and microscopic quantities can be made. The present results are of use in defining such an experiment.

(ii) Under the case of rapid boundary heating, the development of large-amplitude (nonlinear) waves restricts the aforementioned analytical results to very small times, i.e. where an acoustic disturbance has travelled much less than the gap height, $t \ll t_a$. In fact, the confined nature of the gas does not directly arise in the analysis, and the parameter h is carried through only for pedagogical reasons (Clarke *et al.* 1984*a*). Under those limitations, the perturbation results are more suited to the Rayleigh problem. There, the motion induced in a semi-infinite expanse of gas as a bounding wall is instantaneously given a new temperature or heat flux value is of interest. Aoki *et al.* (1991) have recently considered this problem using a model form of the Boltzmann equation. Both of these analyses are useful in characterizing the initiation process. The interaction between the induced gas disturbances and the bounding walls, which make the analytical approach intractable, are the dominant features in the relaxation. These events, and the effect of rarefaction upon them, are quantified here by numerical simulation.

For the temperature ratios considered herein a definite acoustic disturbance arises and crosses the gas several times before steady-state conditions are reached. The maximum induced bulk velocity in the gas is of the order of 20% of the local speed of sound. In an actual gas-driven micromachine much larger temperature ratios, and thus much stronger disturbance fields, will arise.

(iii) The aforementioned analysis allows definition of a general wall heat flux function. In the case of rapid heating, such as would result in the development of shock waves, a constant heat flux and thus a constant energy flow into the gas was typically assumed. This leads to a fundamental description of the piston analogy discussed above. Here, in deference to a realistic mechanical system, we consider a wall medium with a characteristic temperature response time of a few gas collision times. As a result, the wall heat transfer rates are not known *a priori*. Large temporal variations will arise as the disturbances travel across the gas. Larkin (1967) presents calculations using a simplified continuum model which qualitatively show the relative differences between the constant temperature and constant heat flux cases. Finally, note that for the case of wall cooling, expansion rather than compression waves will propagate through the gas and determine the transient relaxation.

4. Approach

A variety of analytical and numerical schemes have been proposed for application to rarefied gasdynamic flows. The second-order approximation to the Boltzmann equation under the Chapman–Enskog expansion, i.e. the Burnett equations, have recently been shown to provide improved results compared to the Navier–Stokes equations for certain applications (Fiscko & Chapman 1988; Pham-Van-Diep, Erwin & Muntz 1991; Zhong, MacCormack & Chapman 1991). As with the Navier–Stokes equations, these appear to be limited by the lack of a physically realistic and accurate boundary condition model. The Burnett equations contain (second-order) correction terms to the Navier–Stokes stress tensor and heat flux vector. The additional terms will be non zero for the unsteady problem of interest here. In the steady-state limit, however, the Burnett heat flux vector reduces to that of the Navier–Stokes equations, though the normal component of the pressure tensor retains additional terms (Wadsworth 1992).

Techniques based on more direct solution of the Boltzmann equation (or a simplified form) can be generally grouped into moment methods (Liu & Lees 1961), finite-difference (Huang 1967; Huang & Hwang 1973) or iterative (Willis 1962) solution of a model equation, or direct simulation (Bird 1976). Here we utilize the direct simulation approach.

Perlmutter (1967) has considered the present problem in the free-molecular limit. Here the Boltzmann equation becomes

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial y} = 0, \tag{1}$$

to be solved for the molecular velocity distribution function f = f(y, v; t). The general solution to this equation is $f = f_0(y - vt, v)$, where f_0 is the initial condition on f. In other words, the distribution function propagates unchanged along the characteristics y - vt. Consideration of general boundary conditions leads to a multiple reflection problem (Bird 1976) requiring solution of coupled Fredholm integral equations. Perlmutter has derived integral equations for the flux of a general macroscopic quantity at any point in the gas for the case of a step increase or decrease in the wall temperature. The equations must be solved numerically. An alternative, but less efficient means to generate the free-molecular solution is to apply a DSMC scheme modified to circumvent the collision subroutine.

In this paper, we utilize time-accurate finite-difference solution of the no-slip Navier-Stokes equations (MacCormack & Baldwin 1975) to establish a reference continuum solution at the lowest Knudsen number considered ($Kn_0 = 0.033$), and the probabilistic DSMC method of Bird (1976) for calculations over the complete range of conditions. This finite-difference scheme is formally of higher temporal accuracy than that used by Clarke *et al.* (1984*a,b*). It has been validated on a wide range of both steady and unsteady problems and will not be discussed in detail here.

The implementation of boundary conditions for the finite-difference solution is rather important, however. The instantaneous change in the wall temperature can lead to certain non-physical results for small times after initiation. For example, the finite-difference approximation for the initial heat flux directed into the gas from the heated wall can be written as $q_w = (T_{w_2} - T_0)/\Delta y_w$. The inverse dependence on cell spacing at the wall, along with the increase of the boundary temperature on a timescale of the order of one molecular collision time in the gas leads to unrealistically large initial wall heat flux values. This in turn leads to larger induced disturbances in the gas and thus accelerated transient response. During the initiation event, heat transfer into the gas is a non-continuum process controlled by molecule impact with the wall. One means to account for this in the continuum formulation is to constrain the wall temperature increase such that the wall heat flux is bounded by the initial free-molecular limit,

$$q_{\mathbf{w}_{\rm fmo}} = \frac{1}{2} m n_0 \frac{(2R)^{\frac{3}{2}}}{\pi^{\frac{1}{2}}} \bigg[T_0^{\frac{3}{2}} - \left(\frac{T_0}{T_{\mathbf{w}_2}} \right)^{\frac{1}{2}} T_{\mathbf{w}_2}^{\frac{3}{2}} \bigg].$$
(2)

Here, m is the gas density and R is the gas constant. This procedure essentially ramps the wall temperature to its final value over a period of several collision times. It will be shown to qualitatively improve the transient response. A similar procedure can be used for the case of wall cooling. Note that this is merely an attempt to improve the physical modelling of the initiation event in the NS solution. No numerical difficulties arose from the excessive boundary heat flux.

For a general rarefied flow, the rigorous no-slip boundary conditions are typically relaxed through allowance of slip (Gupta, Scott & Moss 1985). Though the slip conditions can be formally derived from flux balances across the Knudsen layer, several of the assumptions used in their derivation will be violated during the initial heating period. As the purpose of this paper is not to address extensions to the continuum approach for rarefied conditions, but rather to evaluate general rarefaction effects on the transient motion that develops, slip boundary conditions are not considered further here. An evaluation of slip models for the steady-state problem is given in Wadsworth (1992).

In the DSMC method the behaviour of a gas is modelled probabilistically. Though typically applied to steady gasdynamic problems, the method proceeds in an unsteady manner. The simulated molecules are initialized to some reference condition, and are subsequently tracked through translation and collision events. Macroscopic gas properties are generated by sampling appropriate molecular quantities. In an application to a steady problem, this sampling is begun after the initial transients in the flow field have decayed. Here, the transient portion is of most interest. We utilize ensemble averaging of a series of calculations, identical except for the sequence of random numbers used, to reduce statistical scatter inherent in the necessarily small sample sizes. The time period over which one sample is generated, and thus the minimum temporal resolution, is of the order of one molecular collision time. Since macroscopic features develop over several collision times, it is feasible to use a 'boxcar' sampling scheme where several independent samples are accumulated and considered to be representative of the state of the gas at some intermediate time. For example, the macroscopic quantity z(t) at some spatial location is generated from the appropriate averaged sampled molecular quantity $\zeta(t)$ as

$$z(t) = \frac{1}{2\epsilon} \int_{t-\epsilon}^{t+\epsilon} \zeta(\tau) \,\mathrm{d}\tau.$$
(3)

Here ϵ is a small time parameter, chosen to be much less than the characteristic timescale of any macroscopic motion, i.e. $\epsilon \ll t_a$. In practice the integration is replaced by a sum over finite increments of time. This means of generating unsteady data is necessarily diffusive if ϵ becomes comparable to the macroscopic scale. As will be seen, macroscopic phenomena have been well resolved for all conditions of interest by appropriate choice of ϵ .

Several variants of the basic DSMC method used here have been developed. Bird (1991) has recently presented a source listing of a code suitable for the present problem with only minor modifications. The interested reader is referred to that paper for details on the actual implementation of the direct simulation scheme.

For both the NS and DSMC calculations the gas is modelled as an ideal monatomic with a viscosity-temperature dependence given as $\mu \sim T^{\omega}$. The NS calculations utilize no-slip boundary conditions, while the diffuse wall is implemented in DSMC

		Kn_0 0.033 0.075	n_0 (m ⁻³) 3 6.32 × 10 ² 5 2.84 × 10 ² 6 5 20 × 10 ² 7 0 5 20 × 10 ² 7	T_{w_1} (K) 179 179 79 79 79	T _{w2} (K) 294 294	q _{wss} (DSMC) (W m ⁻²) 910 790		$q_{w_{ss}}$ (W_{ss} (W_{ss}) 10	(NS) m ⁻²) 55 	
TABLE 1. Nominal simulation parameters										
(a)						(b)				
Kn_0	Т ₀ (К)	p_0 (N m ⁻²)	t_{a} (s)	$Kn\left(T_{0} ight)$		Kn ₀	Т ₀ (К)	$p_0 \ ({ m Nm^{-2}})$	t_{a} (s)	$Kn(T_0)$
0.033	79	6.90	$4.36 imes 10^{-5}$	0.027		0.033	294	25.66	$2.26 imes10^{-5}$	0.033
0.075	79	3.10	$4.36 imes 10^{-5}$	0.061		0.075	294	11.52	$2.26 imes 10^{-5}$	0.075
0.399	79	0.57	$4.36 imes10^{-5}$	0.325		0.399	294	2.11	2.26×10^{-5}	0.399
		Таві	LE 2. Parame	ters for (a	ı) wall l	neating	; and ((b) wall co	ooling	

by assigning the post-collision velocity components of molecules incident on the wall from an equilibrium distribution at the wall temperature. In the continuum limit, these two boundary conditions are formally identical. It will be shown that, even under conditions of relatively small nominal rarefaction, substantial differences arise between the direct simulation and Navier–Stokes models of the initial gas response near the walls. This in turn leads to large differences in the overall relaxation process.

5. Results

Table 1 summarizes the basic simulation conditions (nominal Knudsen number Kn_0 , number density n_0 , wall temperatures T_{w_1} , T_{w_2} , and the magnitudes of the steady-state wall heat flux values $(q_{w_{ss}})$ as predicted by the DSMC and NS techniques). The Knudsen number is based on the hard-sphere mean free path for helium $\lambda_0 = (\sqrt{2 \pi d^2 n_0})^{-1}$ and the plate separation h = 2.28 cm. Table 2 defines the initial conditions for the cases of wall heating and cooling. These cases differ only in the initial temperature of the gas, and thus result in the same steady-state solution. Also shown in the tables are the reference pressure $p_0 = n_0 kT_0$, acoustic time t_a , and the Knudsen number based on the variable hard sphere (VHS) model of Bird (1983) evaluated at T_0 . In the VHS model, $\lambda = \lambda_r (T/T_r)^{\omega-\frac{1}{2}}$, where λ_r is the reference mean free path measured at temperature T_r , and ω is the exponent in the viscositytemperature relation. Here, for helium, $\lambda_r \equiv \lambda_0$, $T_r = 293$ K, and $\omega = 0.657$ (Bird 1991). For the present results, the VHS model is used to relate a microscopic property (collision cross-section) to a macroscopic phenomenon (the temperature dependence of viscosity used in the NS calculation). It is not expected to give a quantitative measure of the viscosity of helium at low temperatures. For the range of gas temperatures experienced here, the influence of this model is small. Using a test-particle Monte Carlo scheme, Koura & Kondo (1969) have qualitatively shown the effect of the exponent ω on transient and steady-state profiles for a similar problem.

In the results presented below, figures 2–8 show results for case I, heating of wall 2, while figures 9 and 10 show results for case II, cooling of wall 1.

Figure 2 gives a qualitative view of the overall relaxation process. Shown are



 t/t_a FIGURE 3. Bulk transient pressure response, case I, $Kn_0 = 0.033$: ----, NS; ----, DSMC;, free molecule.

8

1.3

1.0

2

Navier-Stokes pressure profiles across the gas as a function of time. Here and in the following figures time has been normalized by the acoustic time t_a , and pressure by the initial gas pressure p_0 . The propagation of the initial pressure pulse across the gas and its subsequent reflection are clearly evident, as is the slow increase in average pressure toward the steady-state value. Other quantities show similar behaviour.



FIGURE 4. Transient pressure response at wall 1, case I, $Kn_0 = 0.033$.

Yoshizawa (1969) has presented unsteady temperature profiles generated with a testparticle Monte Carlo scheme for a similar problem $(Kn_0 = 0.5, \chi = 4)$.

By evaluating an average instantaneous pressure of the gas, i.e.

$$\overline{p}(t) = \int_0^h p(y, t) \,\mathrm{d}y/h$$

an estimate of the bulk response can be made. Figure 3 compares NS (solid line) and DSMC (dashed line) predictions for wall heating under near-continuum conditions, $Kn_0 = 0.033$. Also shown with a dotted line is the limiting free-molecular value predicted by DSMC calculations in which collisions have been neglected. The difference between the NS and DSMC values at any time is very near the difference in the steady-state values. That difference is a direct measure of the 'slip' effects at the wall, indicating a (temperature) slip on the order of a few percent. A reference steady-state 'linearized' continuum value of the pressure, p_1 , estimated by assuming a centreline temperature $T_{\rm cl} = \frac{1}{2}(T_{\rm w_2} + T_{\rm w_1})$ and density $n_{\rm cl} = n_0$ is indicated on the figure, along with the free-molecular value (Bird 1976).

Figure 3 is qualitatively similar to figure 4 in Radhwan & Kassoy (1984) which considered the case of relatively weak, slow heating. That analysis predicted a spatially homogeneous pressure which monotonically increased to the steady-state value on a conduction timescale $t_c \ge t_a$. For the present conditions, the pressure field is far from spatially homogeneous over essentially all of the rise period owing to the large heating involved. This feature is quantified in figure 4 where the pressure on (unheated) wall 1 is shown as a function of time for the same calculations shown in the previous figure. The difference between the NS and DSMC peak pressures greatly exceeds that between the steady-state values, indicating large local transient rarefaction effects. The propagation of the disturbance across the gas is an acoustic phenomenon, and its transit speed is modelled accurately by both the NS and DSMC



FIGURE 5. Comparison of NS and DSMC heat flux at wall 1, case I, $Kn_0 = 0.033$.



FIGURE 6. Effect of limiting wall heat flux on NS solution, case I, $Kn_0 = 0.033$: ______, limited; _____, unlimited.

techniques. Under continuum conditions, the leading characteristic travels at $c = \frac{1}{2}(\gamma+1)v + a_0$, where a_0 is the initial acoustic speed of the gas and $\gamma = \frac{5}{3}$. From figure 4 we evaluate an average c, $\bar{c} \sim 1.82a_0$ and thus an average bulk gas speed of $\bar{v} \sim 0.62a_0$ during the first transit time. After reflection, the weaker wave predicted by DSMC travels through the relatively cooler gas at a slightly slower speed.



FIGURE 7. Effect of Knudsen number Kn_0 on transient pressure at wall 1, case I: ----, $Kn_0 = 0.033; ----, Kn_0 = 0.075; ----, Kn_0 = 0.399.$

In the free-molecular limit, the bulk gas motion which develops is smaller in magnitude and the system reaches steady state more rapidly. The head of the pressure disturbance consists of molecules with speeds corresponding to a Maxwellian distribution initially at n_0 and T_{w_2} . The peak pressure occurs at a time comparable to h/v_{mp_0} where $v_{mp_0} = (2/\gamma)^{\frac{1}{2}} a_0$ is the most probable speed. For this Knudsen number the free-molecular solution actually gives a better estimate of the peak magnitude of the initial pressure disturbance reaching wall 1 than the continuum result. This is somewhat fortuitous (see figure 7), but is still a useful limiting value.

Figure 5 compares in detail the wall heat flux (q_{w_1}, q_{w_2}) transients as predicted by the NS and DSMC calculations at $Kn_0 = 0.033$. The heat flux q_w has been normalized by the steady-state DSMC value (table 1). The effect of limiting the heat flux from the heated wall (wall 2) is clearly seen in the NS result. The limiting occurs during approximately one-third of one acoustic time, or ten collision times $(t_{\nu} \sim Kn_0 t_a)$. The DSMC results show an immediate decrease in q_{w_2} from the free-molecular value. The relative differences between the peak values of wall 1 heat flux predicted by the two solutions are larger than those for pressure (figure 5).

Figure 6 quantifies the effect of the heat-flux-limited boundary condition on the NS results. Compared to the unlimited values, these qualitatively improve agreement with the DSMC results (see figure 5) by reducing the strength of the initial disturbance. All of the NS results shown utilize the limited boundary condition.

Figure 7 shows the effect of bulk rarefaction $(Kn_0 = 0.033, 0.075, 0.399)$ on pressure response at wall 1. As presaged by the limiting free-molecular results (figure 4), the effect of increased rarefaction is to decrease the time at which the initial disturbance reaches at the wall. The results for $Kn_0 = 0.399$ differ only slightly from the free-molecular values. The magnitude of the pressure wave depends in a complex manner on the rarefaction. In the continuum analysis Clarke *et al.* (1984*a,b*) find a reduction in nominal pressure (i.e. an increase in Kn_0) to increase the relative



FIGURE 8. Comparison of NS and DSMC velocity, pressure and temperature at y/h = 0.1, case I, $Kn_0 = 0.033$.



FIGURE 9. Transient pressure response at wall 2, case II, $Kn_0 = 0.033$; ---, NS; ---, DSMC;, free molecule.

strength of the pressure disturbance due to decreased inertia in the bulk gas. Though increasing rarefaction tends to accelerate the local (figure 5) and bulk (figure 3) response of the system, this gain is offset by the increased slip effects between the gas and the wall. As the Knudsen number increases, wall heating is a less efficient means of depositing energy into the gas.



FIGURE 10. Effect of Knudsen number Kn_0 on transient properties at wall 2, case II. ----, $Kn_0 = 0.033$; ----, $Kn_0 = 0.075$; ----, $Kn_0 = 0.399$.

Figure 8 compares NS and DSMC predictions of pressure, temperature, and velocity at a position $\hat{y} = 0.1h$ for $Kn_0 = 0.033$. This point is approximately five mean free paths from the (cool) wall at steady state. As is clear from the previous figures, the NS results overpredict the strength of the pressure disturbance and thus the induced gas motion, though the transient events are qualitatively similar to the DSMC results. The compression pulse initiated at the heated wall at time zero reaches \hat{y} in approximately one acoustic time, and induces a bulk gas motion downwards, toward the cool wall. The gas speed corresponds to roughly 15% of the local speed of sound. The pressure wave is then reflected off the wall and, as it again passes this position, induces a slightly positive velocity in the gas. After two more transit times ($< 2t_a$, due to heating of the interior gas), the disturbance is smaller in magnitude than that for pressure. For reference, the normal Mach number estimated by compressible flow theory (Liepmann & Roshko 1957) which leads to this initial pressure rise ($p_2/p_1 = 1.85$) is M = 1.3.

The general results for the case of wall cooling (of wall 1) are similar to those for the wall heating case above. Here, the relaxation process consists of a series of expansion waves generated at wall 1 which subsequently cross the gas.

Figure 9 shows the pressure response at wall 2 for $Kn_0 = 0.033$ (compare with figure 4). Note that properties are normalized by their initial values (table 2b) rather than those used in the previous figures. Thus, t_a here is a factor of $(79/294)^{\frac{1}{2}}$ smaller than in the wall heating case. In the continuum limit the head of the initial disturbance travels at a_0 while the tail travels at $a_0 \chi^{-\frac{1}{2}}$. As rarefaction increases, the distribution of molecular speeds leads to an earlier influence at the wall. The relative difference between the NS and DSMC values is much smaller than that in the case of wall heating due to decreased transient rarefaction effects (see below). Figure 10

shows the effect of rarefaction on the pressure at wall 2 (compare with figure 7). Here the transient behaviour appears monotonic with Knudsen number.

The present authors are unaware of any detailed assessments of the effect of rarefaction on a general unsteady gasdynamic problem. Some DSMC results are available regarding the simulation of vortical flows. These include forced vortex motion (Bird 1987), Oseen vortex decay (Wetzel & Oertel 1987) and periodic vortex shedding from a plate (Koura 1990) or bluff body (Koura 1991). In the latter paper, the impulsive insertion of a body into a rarefied free-stream gas is analogous to the boundary temperature rise case considered here. The development of the vortex shedding there is seen to be dependent on a bulk Knudsen number, with NS and DSMC methods predicting different values for the minimum Kn at which shedding begins. Unfortunately, detailed comparisons between the two solutions are not made. In the present paper, the continuum (NS) and DSMC results are seen to be quite different even at a relatively small nominal Knudsen number, due to transient rarefaction effects near the wall. These local differences in turn alter the bulk flow field response. The same fundamentally non-continuum behaviour is to be expected in any problem where unsteady gas motion near a boundary arises. This phenomenon may well be present in other micromachines and microelectronic devices such as accelerometers and fast-response pressure microgauges.

Clearly, the nominal Knudsen number is a poor measure of the magnitude of transient rarefaction effects. A more appropriate parameter must be based on the transient features of the problem. One possibility is a Knudsen number based on a local mean free path and the scale gradient of the temperature, i.e.

$$Kn_T = \frac{\lambda}{T} \left| \frac{\mathrm{d}T}{\mathrm{d}y} \right|$$

(Present 1958; Bird 1976). This term essentially represents the small parameter preceding the perturbation terms in the Chapman-Enskog form of the Navier-Stokes distribution function (Bird 1976). It is also present in the formula for temperature slip at a surface if it assumed that the Chapman-Enskog distribution function is appropriate at the edge of the Knudsen layer (Gupta *et al.* 1985). Assuming slip corrections are small, the temperature slip becomes

$$\frac{T_{\rm s}}{T_{\rm w}} \sim 1 + \frac{\lambda}{T} \frac{{\rm d}T}{{\rm d}n},$$

where n is the outward normal at the surface, and the right-hand side is evaluated at the edge of the Knudsen layer. The slip temperature T_s is used to replace the (known) no-slip temperature boundary condition T_w . By evaluating the local Knudsen number near the appropriate walls, we can estimate the transient degree of rarefaction and determine qualitatively the utility of the slip corrections in the continuum formulation.

Figure 11 shows results based on NS calculations at $Kn_0 = 0.033$. The solid line gives the value 0.1h from the heated wall, while the dashed line is the value at 0.1hfrom the cooled wall, and each dataset is plotted versus its acoustic time. Much greater rarefaction effects are indicated for the case of wall heating, as was apparent from the DSMC comparisons shown in figures 5 and 9. The difference is due mainly to the difference in scale lengths between the two cases, i.e. the tendency of the compression wave to steepen while the expansion wave flattens. The parameter is not a quantitative estimate of transient rarefaction.



FIGURE 11. Local Knudsen number $Kn_T = (\lambda/T) |dT/dy|$ as predicted by NS solution for $Kn_0 = 0.033$: -----, wall heating, y = 0.9 h; -----, wall cooling, y = 0.1h.

Since the local Knudsen number cannot be estimated a priori, it is not of great value as a correlation parameter. If we generalize the present problem to consider wall temperature ratio χ as a parameter, however, it is of use in a bulk sense. Here, we can rewrite it as

$$Kn_T = 2Kn_0 \chi \left| (1-\chi)/(1+\chi) \right|,$$

where for our purposes $\chi \ge 1$. Koura & Kondo (1969) confirms qualitatively that this parameter is more appropriate for the steady-state problem.

The present results and the studies of vortical motion and shock structure (Fiscko & Chapman 1988; Pham-Van-Diep *et al.* 1991; Zhong *et al.* 1991) referred to earlier all appear to show that the motion of an even slightly rarefied gas is described mathematically by a set of differential equations more diffusive in nature than the Navier–Stokes equations. The additional terms in the Burnett equations are dominantly diffusive. For the present problem, these terms may be of non-negligible magnitude during the transient phase. Though this problem has direct practical application, it also appears to be useful for theoretical analyses into the utility of the Burnett equations.

6. Conclusions

The response of a confined rarefied gas subject to rapid heating or cooling of a container wall has been studied numerically. For the rapid wall temperature changes considered here the gas response is better measured by an acoustic, rather than conduction, timescale, with steady-state conditions being achieved after roughly ten wave crossing times. For the case of wall cooling under slightly rarefied conditions, Navier–Stokes solutions agree relatively well with direct simulation Monte Carlo results. For wall heating at the same nominal Knudsen number, the continuum

solution is less accurate due to larger transient rarefaction effects. A local Knudsen number based on the scale length of the temperature gradient is found to be a qualitative measure of the transient rarefaction. The effect of increasing bulk rarefaction leads to different qualitative behaviour between the two cases. For wall cooling, transient properties such as wall pressure vary monotonically between the limiting continuum and free-molecular values. For wall heating the variation is non-monotonic due to the competition between decreasing inertia in the gas and decreasing heat flux from the wall; there exists some Knudsen number at which the maximum (relative) pressure disturbance can be generated.

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