

INVESTIGATION OF THERMAL STRESS CONVECTION IN NONISOTHERMAL GASES UNDER MICROGRAVITY CONDITIONS

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1. INTRODUCTION

The continuum description of momentum and energy transport in gases, based upon Newton–Stokes–Fourier constitutive relations, can become inaccurate in rarefied or highly nonequilibrium regimes, i.e., regimes in which the Knudsen number $K\bar{n}$ ($= \lambda/L$, where λ is the gas mean free path and L is the characteristic system or gradient length) is no longer small. The Burnett equations, which represent the order- $K\bar{n}^2$ solution to the Boltzmann equation, ostensibly provide a means of extending continuum formulations into the transitional Knudsen regimes ($\sim K\bar{n} < 1$).

The accuracy and validity of the Burnett equations, however, have not been firmly established. As has been noted by several authors, the asymptotic series expansion of the molecular distribution function – from which the Burnett equations are derived – has unknown convergence properties for finite $K\bar{n}$.^{1,2} The Burnett equations can also lead to Second-law impossibilities, such as heat flux in an isothermal gas.³ Furthermore, the Burnett equations increase the order of the differential equations that govern momentum and heat transport in the gas. Additional boundary condition information is required to fully close the problem – yet such information is generally not available from physical principles alone.

Because of these issues, it is generally held that the Burnett equations are valid only in regimes in which the Navier–Stokes–Fourier level of approximation already provides an adequate description of transport, i.e., regimes in which the Burnett contributions represent a small perturbation to heat and momentum transport. Such conditions can be representative of high–Mach number flows, for which application of the Burnett equations appears to have been the most successful.^{4–7} On the other hand, there is not a broad understanding of the accuracy of the Burnett equations when applied to slow–moving, nonisothermal flow (SNIF) conditions. As noted by Kogan, ‘thermal stresses’ (fluid stresses resulting from temperature gradients – which are predicted by the Burnett equations) could become a significant convection mechanism in buoyancy–free, nonisothermal gases.^{8,9} Indeed, it has been recently suggested that thermal stress convection could affect the growth of crystals in microgravity physical vapor transport experiments.^{10,11}

The work presented here consists of a theoretic

cal and numerical examination of thermally–induced stresses and flows in enclosed, highly nonisothermal gases under buoyancy–free conditions. A central objective has been to identify a strategy in which stress and/or convection effects, as predicted by the Burnett equations, could be isolated and measured in microgravity–based experiments. Because of the questionable veracity of the Burnett equations, a second objective has been to test Burnett predictions of nonisothermal gas stress and convection with the exact description provided by the direct simulation Monte Carlo (DSMC) method.

2. PREDICTION OF THERMAL STRESS CONVECTION

The initial phase of the project was aimed at calculation, using continuum and DSMC methods, of gas convection in two dimensional nonuniformly heated rectangular enclosures. Typically, two adjacent surfaces of the enclosure were modeled as adiabatic, zero–stress surfaces (i.e., planes of symmetry), and the other two adjacent surfaces were maintained at specified temperature distributions with one surface transferring a net amount of heat to the gas, and the other transferring the heat from the gas.

The continuum formulations of momentum and energy transport are identical to Navier–Stokes–Fourier models, with the exception of the Burnett stress tensor in the momentum equations and the creep and jump boundary conditions. For the conditions examined here (i.e., slow–moving flow, with $Re_L \ll 1$) the only significant terms in the Burnett stress tensor relations will be those involving temperature gradients. This thermal stress component appears as^{8,11}

$$\boldsymbol{\tau}_T = -\frac{\mu^2 R}{P} \left[\omega_3 \left(\nabla \nabla T - \frac{1}{3} (\nabla^2 T) \mathbf{I} \right) + \frac{\omega_5}{2T} \left((\nabla T)(\nabla T) - \frac{1}{3} (\nabla T \cdot \nabla T) \mathbf{I} \right) \right] \quad (1)$$

in which μ is the dynamic viscosity, R is the gas constant, and ω_3 and ω_5 are dimensionless, order–unity coefficients which depend on the interaction potential of the molecules. The creep and jump boundary conditions appear

$$\mathbf{u} = \frac{c_S \mu R}{P} \left(\nabla T - \hat{n} \frac{\partial T}{\partial n} \right) \quad (2)$$

$$T = T_w + \frac{c_T \lambda}{T} \frac{\partial T}{\partial n} \quad (3)$$

INVESTIGATION OF THERMAL STRESS CONVECTION, D. W. Mackowski

where n is the outward normal and the dimensionless coefficients c_S and c_T depend on the thermal and momentum accommodation properties of the surface.¹² Numerical solution of the governing equations was accomplished using the SIMPLER algorithm of Patankar.¹³ Coefficients corresponding to hard-sphere molecules, which gives a temperature-dependent viscosity of $\mu \sim T^{1/2}$, were used in the computations.

Direct simulation Monte Carlo calculations of hard-sphere gas convection and heat transfer were accomplished using the standard procedure developed by Bird.^{14,15} The cell size was nominally set to $0.1\lambda_0$, where λ_0 represents the mean-free-path at the equilibrium state of the system, and 10–20 molecules were assigned per cell. Simulations were conducted for a Knudsen range of $K\bar{n} = 0.01 - 0.2$. Because thermal creep and stress flows will be on the order of $K\bar{n}$ times the mean molecular velocity, resolution of the flows using DSMC required simulation times on the order of $10^6 - 10^7$ time steps.

Our continuum and DSMC calculations to date indicate that it would be very difficult to create conditions in the enclosure that result in measurable thermal stress flows that are comparable to or larger than thermal creep flows, and simultaneously maintain the $K\bar{n} < 0.1$ regime required of the Burnett equations. With the exception of the pure continuum limit ($K\bar{n} \rightarrow 0$, under which thermal stress vanishes), elimination of thermal creep cannot be accomplished by maintaining the heated/cooled walls at uniform temperatures. Rather, the discontinuity (or jump) between the surface and adjacent gas temperatures – which will be proportional to $K\bar{n}$ and the local normal temperature gradient – will lead to nonuniform gas temperatures along the nonuniformly heated surfaces. For all realistic values of $K\bar{n}$, thermal creep flows generated by the temperature jump effects were substantially larger than those resulting from thermal stress.

To minimize the effects of creep, we performed additional simulations in which the temperature distributions along the heated/cooled surfaces were assigned to provide, for a given $K\bar{n}$, nearly uniform gas temperature adjacent to the surface. Surface temperature distributions were determined from solution of the gas conduction equation with uniform gas temperature boundary conditions along the heated/cooled surfaces, and subsequent application of the solution into Eq. (3) to predict $T_w(x)$. This approach imposed a surface temperature on the heated surface which increased towards the junction with the cooled surface, with an opposite trend along the cooled wall. The effect of this strategy resulted in thermal creep flows that were confined about the hot/cold junction, and left a bulk,

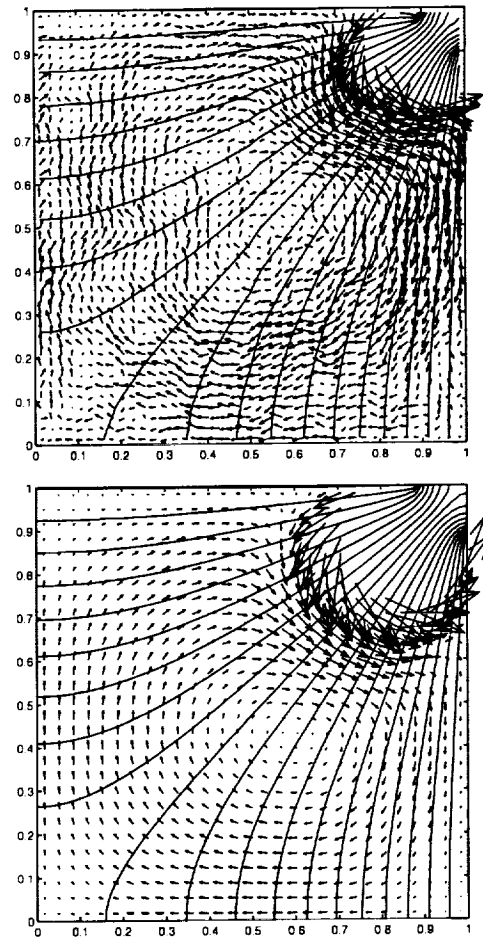


Fig. 1: DSMC (top) and continuum (bottom) results

thermal-stress driven convection pattern in the bulk of the enclosure. However, this strategy would also lead to highly nonequilibrium conditions in the vicinity of the hot/cold surface junction, for which the Burnett equations are not expected to hold.

The comparison between continuum/Burnett and DSMC predictions of convective flows in the enclosure has been inconclusive. DSMC calculations have shown convective flows that are qualitatively similar than those predicted by the continuum model. As an example, we show in Fig. 1 plots of velocity vectors and isotherms, calculated using the DSMC (top) and continuum (bottom) models, for a $K\bar{n} = 0.02$ hard-sphere gas contained in an enclosure with a relative temperature difference on the hot and cold walls of $2(T_H - T_C)/(T_H + T_C) = 1$. The heated wall is on the top, and the left and bottom walls are symmetry surfaces. A strip of the walls adjacent to the hot/cold junction, equal to 0.1 of the wall length, is held adiabatic, and the remainder of the walls have temperature distributions set to give isothermal gas conditions per the procedure discussed above. Velocity vectors corresponding to ther-

INVESTIGATION OF THERMAL STRESS CONVECTION, D. W. Mackowski

mal creep along the adiabatic surfaces (seen in the tight counterclockwise rotation in the upper right corner) have been removed from the plot to allow resolution of the thermal stress flows. The stress flow – as predicted by the continuum model – results in a clockwise rotation in the main body of the gas for the given conditions. A similar pattern is seen in the DSMC results. We cannot establish, however, whether the observed DSMC flows result from thermal stress, or are due to slip effects at the walls. As mentioned above, the veracity of the Burnett relations is also questionable for the highly nonequilibrium conditions of the simulations. On the other hand, temperature profiles calculated via DSMC and continuum models show significant agreement.

3. THERMAL STRESS IN 1-D HEAT TRANSFER

A simpler situation in which to compare continuum/Burnett and DSMC predictions of thermal stress effects is offered by 1-D heat transfer in a stationary gas. In this situation, the effects of thermal stress would be seen in the pressure distribution and normal stress in the gas.¹⁶

The computational domain was now taken to be a slab of gas contained between two parallel surfaces, separated by a distance L , with the surfaces at $x = 0$ and L maintained at uniform temperatures of T_{CS} and T_{HS} (with $T_{HS} > T_{CS}$), respectively. In nondimensional form (with pressure and stress normalized with the equilibrium pressure P_m and temperature by the equilibrium temperature T_m), the Burnett equation for the x -directed, normal component of the stress tensor is^{7,17}

$$\tau^* = \phi + \frac{c_1 K\bar{n}^2 \theta}{\phi} \left[\omega_1 \frac{\theta' \phi'}{\phi} - \omega_2 \left(\frac{\theta \phi'}{\phi} \right)' + \omega_3 \theta'' + \omega_5 \frac{\theta'^2}{\theta} \right] \quad (4)$$

In the above, $\phi = P/P_m$, $\tau^* = \tau/P_m$, $\theta = T/T_m$, the prime denotes differentiation with respect to $\xi = x/L$, $c_1 = (4\pi/3)(5/16)^2 = 0.4091$, and the dimensionless ω coefficients depend on the molecular interaction potential. Since the gas is stationary and buoyancy-free, the stress τ will be a constant. In the limit of $K\bar{n} \rightarrow 0$, this gives the Navier-Stokes result of $P = \tau = \text{constant}$. For finite $K\bar{n}$, however, the additional source of thermal stress can act within the nonisothermal gas. The magnitude of the thermal stress will vary with position – by virtue of the dependence of temperature and temperature gradient on position – and consequently pressure will vary to maintain a constant normal stress.

The Burnett equations make no contribution to the heat flux for a stationary gas. Consequently, the gas

temperature will be described by

$$q^* = \text{constant} = \theta^{1/2} \theta' \quad (5)$$

where q^* is the dimensionless heat flux ($= qL/kT_m$). Equation (5) can be used to combine the last two terms in Eq. (4), which results in

$$\tau^* = \phi + \frac{c_1 K\bar{n}^2}{\phi} \left[\theta \left(\omega_4 \frac{\theta' \phi'}{\phi} - \omega_2 \left(\frac{\theta \phi'}{\phi} \right)' \right) - \frac{c_2 q^{*2}}{\theta} \right] \quad (6)$$

where $c_2 = (\omega_3 - 2\omega_5)/2 = 0.9900$ for hard-sphere molecules.

Two separate effects – or regimes – on ϕ can be anticipated from inspection of Eq. (6). One effect, which is discussed by Kogan¹⁸ and Makashev¹⁹, derives from the fact that the derivatives of ϕ will be multiplied by the small parameter (for near-continuum conditions) of $K\bar{n}^2$. The solution to Eq. (6) could therefore exhibit ‘boundary layers’ of width $\Delta\xi \sim K\bar{n}$. It is shown below that this property, combined with appropriate boundary conditions, will allow for a limited description of the Knudsen layers adjacent to the surfaces.

A second characteristic regime, as indicated by Eq. (6), would occur outside the Knudsen layers. By expanding ϕ in a power series of $K\bar{n}^2$, and neglecting all terms higher than $K\bar{n}^2$, the pressure distribution in the bulk gas would be given approximately by

$$\phi \approx \tau^* + \frac{c_1 c_2 (K\bar{n} q^*)^2}{\tau^* \theta} \quad (7)$$

As is evident from inspection of Eq. (7), thermal stress would create a pressure gradient in the gas, with pressure increasing towards the cooler regions in the gas. The gradient would be proportional to the square of $K\bar{n} q^* \sim \sqrt{\theta} d\theta/d(x/\lambda)$ – which can be interpreted as a Knudsen number based on the characteristic length of the temperature gradient (note that this quantity is independent of L). It should be emphasized that the effect predicted from Eq. (7) is fundamentally different than the pressure gradient created by ‘thermal transpiration’ of a gas in a tube with an imposed axial temperature gradient.^{20,21} The latter is a result of thermal slip at the walls of the tube, and leads to a pressure that increases in the direction of increasing temperature. Thermal stress, on the other hand, results from the effect of temperature gradients on the molecular velocity distribution function within the gas.

Although the thermal stress pressure gradient can be labeled ‘hydrostatic’ – since the gas is at rest – it

INVESTIGATION OF THERMAL STRESS CONVECTION, D. W. Mackowski

is distinctly different than that resulting from a gravitational acceleration in the x -direction. Unlike the latter, thermal stress would not result in a difference between the normal forces acting on the hot and cold surfaces. In other words, the 'pressure' measured at the surfaces – which would physically represent the normal stress τ – would be identical for both surfaces.

Thermal stress, however, will result in a different value of the normal stress than that predicted from the Navier–Stokes level of approximation. This follows from conservation of energy requirements. In particular, the average pressure in the gas represents the equilibrium pressure that would be attained if the walls were instantaneously made adiabatic. Since the equilibrium pressure is used to normalize the dimensional pressure P , this statement is equivalent to

$$\int_0^1 \phi \, d\xi = 1 \quad (8)$$

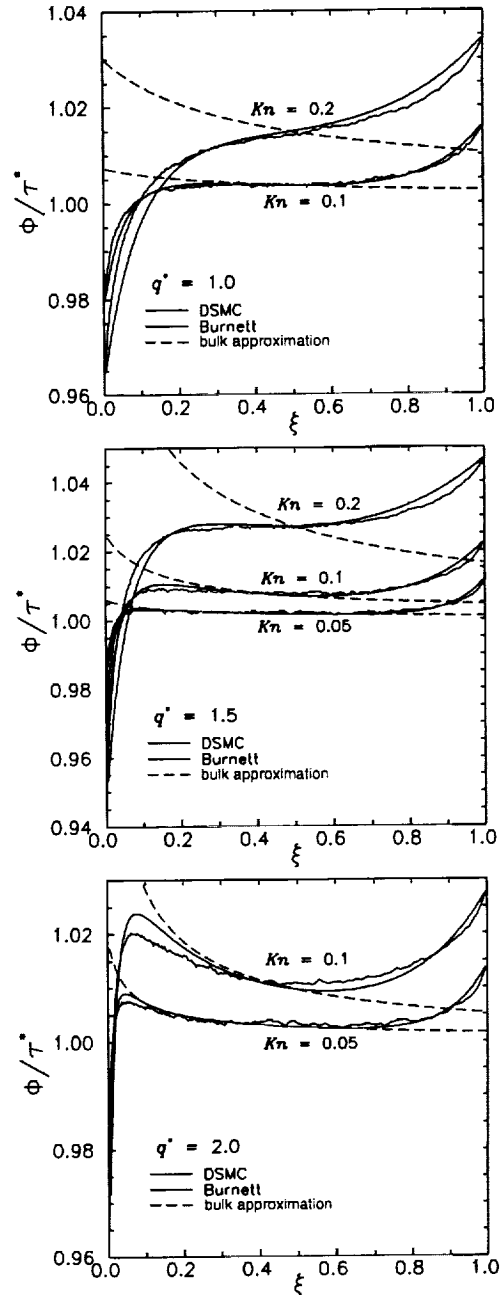
Regardless of the values of q^* and $K\bar{n}$, the pressure distribution in the gas must satisfy the energy conservation constraint implied by Eq. (8). Consequently, the normal stress τ^* would be obtained as the eigenvalue to Eq. (6) such that the solution (for specified boundary conditions) satisfies Eq. (8). In general, this value will be different than the Navier–Stokes result of $\tau^* = 1$.

An approximate value for τ^* can be obtained by neglecting the effects of the Knudsen layers at the surfaces, for which the pressure distribution would be given by Eq. (7). To order $K\bar{n}^2$, this gives¹⁶

$$\tau^* \approx 1 - c_1 c_2 (K\bar{n} q^*)^2 \quad (9)$$

This relatively–simple approximation indicates that thermal stress will lower the normal stress in a closed system relative to that predicted from the Navier–Stokes level – although we note again that the effects of Knudsen layers have been neglected in the analysis.

The final elements required to close the problem are the boundary conditions for pressure. As is the case with the Navier–Stokes approximation, the boundary conditions for the Burnett equations should represent an extrapolation of the solution across the region, adjacent to the wall, where the solution is no longer valid. Makashev¹⁹ and Schamberg²² have proposed boundary conditions that are consistent with the order– $K\bar{n}^2$ accuracy of the Burnett equations. The accuracy of these approaches, however, has not been well established.²³ Alternatively, order– $K\bar{n}$ relations can be derived for the pressure 'slip' adjacent to a heated or cooled surface.^{12,21} However, our work at this stage is primarily concerned with determining whether there are boundary conditions which, when coupled to the



Figs. 2–4: DSMC and continuum pressure distributions

Burnett equations, can reproduce DSMC predictions of pressure distributions in a nonisothermal gas. Therefore, the pressures at the hot and cold surfaces were taken to be parameters, and were chosen to provide the best agreement between theory and DSMC results. The obvious choice for the pressure at the surfaces will be the values determined from DSMC predictions.

Comparisons of Burnett (via numerical solution of Eq. (6)) and DSMC predictions of pressure distribution appear in Figs. 2–4. Each plot shows $P/\tau = \phi/\tau^*$ vs.

INVESTIGATION OF THERMAL STRESS CONVECTION, D. W. Mackowski

$\bar{x}i = x/L$ for a fixed value of q^* , with $K\bar{n}$ a parameter. Two theoretical predictions of P/τ are shown for each set of DSMC results. The first corresponds to the numerical solution of Eq. (6), with boundary conditions obtained from extrapolation of the DSMC-derived pressures to the surfaces and temperatures predicted from Eq. (5). The second represents the bulk gas thermal stress pressure distribution predicted from Eq. (7), which does not account for boundary effects. This latter prediction has been shifted by a constant to match with the full-Burnett solution at $\xi = 0.5$.

As is evident from the results, the pressure profiles show distinct Knudsen layers at both the cooled and heated surfaces. The drop in pressure at the cooled surface, and the increase in pressure at the hot surface, are both consistent with the predictions of pressure slip relations.²¹ The pressure drop at the cold surface can be considerable for the conditions examined here – amounting to around an 8% decrease for $K\bar{n} = 0.2$ and $q^* = 1.5$.

The solutions of the Burnett equation, with DSMC derived boundary conditions, are seen to capture the essential features of the DSMC pressure distribution. In particular, the solutions provide a good description of the width and form of the Knudsen layers and the pressure distribution outside the layers. The difference between the theoretical and DSMC results is greatest at the edge of the cold-surface Knudsen layers, for which the theoretical model tends to overpredict the pressure. This is most evident for the results corresponding to $q^* = 2.0$ in Fig. 4. Nevertheless, the fact that the Burnett equations can resolve, to a reasonable accuracy, the Knudsen layers at the surface is somewhat surprising – especially when considering that the theory is based on the order- $K\bar{n}$ continuum temperature profile. We also examined solutions to Eq. (6) using boundary values of ϕ that were different than the DSMC results, and found that the exact, DSMC-derived boundary conditions provide the best overall agreement between Burnett equation predictions and DSMC results.

The DSMC results for $q^* = 2.0$ appear to show a pressure distribution in the bulk gas that is described by Eq. (7). On the other hand, the pressure distribution for $q^* = 1.5$ and $K\bar{n} = 0.2$ (Fig. 3) – for which Eq. (7) predicts a greater effect – is dominated by the Knudsen layers extending from the surfaces. To eliminate the effects of the Knudsen layers at the hot wall, we performed additional DSMC calculations in which the velocities of the incoming molecules at the hot boundary were sampled from the Chapman-Enskog distribution function for the fixed values of q^* and $K\bar{n}$. By doing so, the hot surface now approximated an open boundary. The corresponding DSMC results showed a

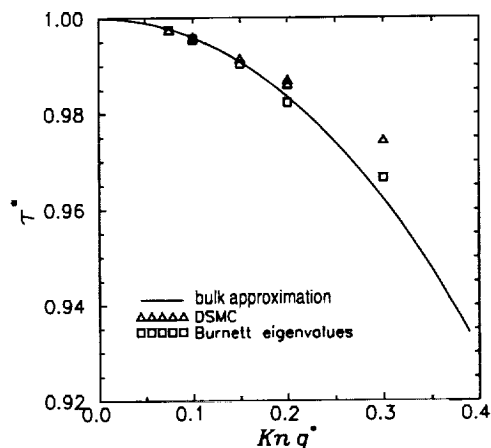


Fig. 5: DSMC and continuum normal stress

pressure distribution in the bulk gas that was accurately represented by Eq. (7).

A final comparison of theory and experiment can be obtained from the dimensionless normal stress. The simplified model of Eq. (9) indicates that τ^* should be a function primarily of $K\bar{n} q^*$. Accordingly, we plot in Fig. 5 the DSMC values of τ^* vs. $K\bar{n} q^*$ for the seven different combinations of $K\bar{n}$ and q^* that were used in the closed system calculations (results of Figs. 2–4). Theoretical results correspond to the derived eigenvalues of Eq. (6) for the DSMC-derived boundary conditions, and to the approximation given by Eq. (9).

The first point to make is that the predictions of τ^* from full solution of the Burnett differential equation are nearly equivalent to those obtained from the bulk-gas approximation of Eq. (9). Evidently, the decrease in pressure at the cold surface is compensated by the increase at the hot, so that the Knudsen layers have a small effect on the averaged pressure in the gas. Secondly, the primary dependence of τ^* on $K\bar{n} q^*$ is supported in the DSMC results at $K\bar{n} q^* = 0.1$ and 0.2 – which each correspond to two combinations of $K\bar{n}$ and q^* . As observed, the results are nearly identical at these points. Finally, the theoretical predictions are in excellent agreement with the DSMC results for $K\bar{n} q^* \leq 0.15$, beyond which the theory overpredicts the decrease in τ^* . As can be seen from the results, the relative decrease in normal stress on the surfaces is quite small, i.e., $\tau^* = 0.975$ for $q^* = 2.0$ and $K\bar{n} = 0.2$, or a 2.5% decrease in ‘measured’ pressure at the surface. We should emphasize, however, that this decrease is still significantly larger than the numerical precision of the DSMC simulations.

SUMMARY

The project has sought to ascertain the veracity of

INVESTIGATION OF THERMAL STRESS CONVECTION, D. W. Mackowski

the Burnett relations, as applied to slow moving, highly nonisothermal gases, by comparison of convection and stress predictions with those generated by the DSMC method. The Burnett equations were found to provide reasonable descriptions of the pressure distribution and normal stress in stationary gases with a 1-D temperature gradient. Continuum/Burnett predictions of thermal stress convection in 2-D heated enclosures, however, are not quantitatively supported by DSMC results. For such situations, it appears that thermal creep flows, generated at the boundaries of the enclosure, will be significantly larger than the flows resulting from thermal stress in the gas.

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