Time-dependent conductive heat transfer in rarefied polyatomic gases confined between parallel plates

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Abstract. The transient conductive heat transfer through a rarefied gas confined between two infinite parallel plates due to a sudden jump in the temperature of one of the plates is investigated in the whole range of the Knudsen number via kinetic theory. More specifically, the time-dependent heat transfer flow is modelled by the Holway kinetic model subject to diffuse boundary conditions. The governing integro-differential equation is numerically solved using the discrete velocity method in the molecular velocity space and typical finite control volume schemes in time and physical spaces. The time evolution of the density and temperature distributions as well as of the translational and rotational heat fluxes in terms of the two parameters characterizing the heat flow, namely the Knudsen number and the imposed temperature ratio between the plates is provided. The investigation is focused on the effect of the rotational degrees of freedom and a comparison between monatomic and polyatomic gases is performed. It is found that the time needed to reach the steady-state conditions varies between monatomic and polyatomic gases. In all cases the total time to recover the stationary solution in terms of the rarefaction parameter exhibits a minimum close to the well-known Knudsen minimum.

1. Introduction

Heat transfer through stationary rarefied gases confined between parallel plates is a fundamental problem in rarefied gas dynamics. This heat transfer configuration is very common in several technological applications including vacuum solar collectors [1], micro heat exchangers and microsensors [2,3]. Heat transfer modeling in rarefied gases is commonly based on kinetic theory [4] in order to yield reliable solutions in the whole range of the Knudsen number. The case of plane and cylindrical heat conduction through monatomic gases has been examined in [5,6], while the corresponding more complex heat flow setups in polyatomic gases in [7,8] based on the Holway model and the DSMC method. All above work refers to steady-state conditions, while the corresponding work in the case of transient conditions is limited to monatomic gases [9].

The present work is devoted to the kinetic solution of time-dependent conductive heat transfer through rarefied polyatomic gases confined between parallel plates by numerically solving the time dependent Holway kinetic equation [10] subject to diffuse boundary conditions. The time evolution of all macroscopic quantities including the translational and rotational heat fluxes is obtained. The response time to reach steady-state conditions is computed. The effect of the number of rotational degrees of freedom is investigated and the differences (and similarities) compared to the corresponding monatomic gas transient heat transfer problem are pointed out.
2. Plane heat flow configuration

Consider the state of a rarefied stationary nonpolar polyatomic gas confined between two infinite parallel plates fixed at $y' = \pm H / 2$, which initially are in the same temperature $T_C$. Then, at time $t' = 0$, the temperature of the plate at $y' = -H / 2$ is suddenly increased at $T_H$, with $T_H > T_C$ and then for $t' > 0$ the temperature of the two plates are maintained constant (figure 1). As a result 1D transient heat flow from the hot towards the cold plate will commence, which will gradually grow and as $t' \to \infty$, it will asymptotically approach the corresponding steady-state heat flow. The present analysis treats only the translational and rotational energy modes ignoring the vibrational ones.

![Figure 1. Heat flow configuration.](image)

In the temperature range where the effects of vibrational degrees of freedom can be neglected, the problem may be modelled by kinetic theory for a gas of rigid rotors. When intrinsic molecular angular momenta has no preferential alignment, the gas may be described by the distribution function $f(t', y', \mathbf{v}, \mathbf{I}')$, where $\mathbf{v} = (\xi_x, \xi_y, \xi_z)$ is the molecular velocity vector and $I'$ is the internal energy, describing the molecular internal states \[11\]. In polyatomic gases the internal energy is divided in the energy of the translational motion and the energy associated to the internal structure. These energies are related to the corresponding translational and rotational temperatures and heat fluxes.

Then, the macroscopic quantities of practical interest are obtained by the moments of $f'$ as

$$n(t', y') = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(t', y', \mathbf{v}, \mathbf{I}') \, d\xi_x \, d\xi_y \, d\xi_z,$$

$$u_y(t', y') = \frac{1}{n(t', y')} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \xi_y \, f(t', y', \mathbf{v}, \mathbf{I}') \, d\xi_x \, d\xi_y \, d\xi_z$$

$$T_{tr}(t', y') = \frac{m}{3k_B n(t', y')} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[ \xi_y^2 - u_y \xi_y \right] \, f(t', y', \mathbf{v}, \mathbf{I}') \, d\xi_x \, d\xi_y \, d\xi_z$$

$$T_{rot}(t', y') = \frac{2}{jk_B n(t', y')} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left( \xi_y^2 + \xi_x^2 + \xi_z^2 \right) \, f(t', y', \mathbf{v}, \mathbf{I}') \, d\xi_x \, d\xi_y \, d\xi_z$$

$$Q_{tr}(t', y') = \frac{m}{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left( \xi_y^2 - u_y \xi_y \right) \, f(t', y', \mathbf{v}, \mathbf{I}') \, d\xi_x \, d\xi_y \, d\xi_z$$

$$Q_{rot}(t', y') = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left( \xi_y^2 + \xi_x^2 + \xi_z^2 \right) \, f(t', y', \mathbf{v}, \mathbf{I}') \, d\xi_x \, d\xi_y \, d\xi_z$$

$$Q = Q_{tr} + Q_{rot}$$

where $n$, $T$, $Q$, and $u_y$ are the number density, total (thermodynamic) temperature, total heat flux and velocity respectively, while $k_B$ is the Boltzmann constant and $m$ the molecular mass. The subscripts $tr$ and $rot$ denote the translational and rotational parts. The parameter $j$ is the number of rotational degrees of freedom, with $j = 2$ in diatomic and linear molecules and $j = 3$ in all other cases ($j = 0$ refers to monoatomic molecules).
The two parameters characterizing the problem are the normalized temperature difference $\beta$ and the reference gas rarefaction parameter $\delta$

$$\beta = \frac{T_H - T_C}{2T_0}, \quad \delta = \frac{P_0 H}{\mu_0 T_0} \sim \frac{1}{Kn}$$

where $T_0 = (T_H + T_C)/2$ is the reference temperature, $\mu_0$ is the gas viscosity at $T_0$, $\tau_0 = \sqrt{2k_B T_0 / m}$ is the most probable molecular speed and $P_0 = n_0 k_B T_0$ is a reference pressure. The gas rarefaction parameter is proportional to the inverse Knudsen number and it is used for practical purposes.

3. Polyatomic kinetic modelling

The kinetic model introduced by Holway [10] where the collision integral consists of two components corresponding to the elastic and inelastic collisions is applied. In dimensionless form the Holway model for the present one dimensional problem is written as [8]

$$\frac{\partial \Psi}{\partial t} + c_y \frac{\partial \Psi}{\partial y} = \delta \rho \tau^{1-\omega} Pr \left( 1 - \frac{1}{Z} \right) (\Psi_{tr} - \Psi) + \frac{1}{Z} \left( \Psi_{rot} - \Psi \right)$$

where $t = (t' \tau_0) / H$, $y = y' / H$ and $c_y = \xi / \tau_0$ are the dimensionless independent variables of time, space and $y$–component of the molecular velocity, while the unknown dependent variables are in vector form as $\Psi = [F, G, S]^T$. Furthermore, $\Psi_{tr} = [F_{tr}, G_{tr}, S_{tr}]$ and $\Psi_{rot} = [F_{rot}, G_{rot}, S_{rot}]$ are the translational and rotational relaxing distributions given by

$$F_{tr} = \frac{\rho}{\pi \tau_{tr}} \exp \left[ -\frac{(c_y - u_y)^2}{\tau_{tr}} \right], \quad F_{rot} = \frac{\rho}{\pi \tau} \exp \left[ -\frac{(c_y - u_y)^2}{\tau} \right],$$

$$G_{tr} = \tau_{tr} F_{tr}, \quad G_{rot} = \tau F_{rot}, \quad S_{tr} = \frac{j}{2} \tau_{rot} F_{tr}, \quad S_{rot} = \frac{j}{2} \tau F_{rot}$$

(8)

The dimensionless macroscopic distributions of density, velocity, translational and rotational as well as total temperatures and corresponding heat fluxes are defined as

$$\rho = \frac{n}{n_0}, \quad u_y = \frac{u_y'}{\tau_0}, \quad \tau_{tr} = \frac{\tau_{tr}}{T_0}, \quad \tau_{rot} = \frac{\tau_{rot}}{T_0}, \quad \tau = \frac{3 \tau_{tr} + j \tau_{rot}}{3 + j},$$

$$q_{rot} = \frac{Q_{rot}}{(P_0 \tau_0)}, \quad q_{tr} = \frac{Q_{tr}}{(P_0 \tau_0)}, \quad q = q_{tr} + q_{rot}$$

(9)

Also, in Eq. (7), $Pr$ is the Prandtl number, while the parameter $0 \leq Z^{-1} \leq 1$ indicates the fraction of rotational collisions with regard to the total number of collisions. In the kinetic formulation of the problem the so-called inverse power law model (IPL) has been introduced with the viscosity varying as $\left( \mu / \mu_0 \right) = (T / T_0)^{2\omega}$ and $\omega$ denoting the gas collision index.

At the two plates the Maxwell boundary conditions with purely diffuse reflection are applied for the incoming distributions. Hereby, to distinguish between incident and reflected quantities the superscripts (−) and (+) are introduced. Following a well-known procedure the following reflected reduced distributions at the boundaries $y = \pm 1/2$ are deduced:

$$F^+ = \left( \rho_w / \sqrt{\pi \tau^{2\omega}} \right) \exp \left( -\frac{c_y^2}{\tau} \right), \quad G^+ = \tau^{2\omega} F^+, \quad S^+ = \left( \frac{j}{2} \right) \tau^{2\omega} F^+$$

(10)
where $t' = (1 + \beta)$ and the parameter $\rho_v$ is specified by the no penetration condition. The problem to be numerically solved consists of the kinetic equations (7) with the associated expressions (8) and (9) subject to boundary conditions (10).

The discretization of the kinetic equations in the molecular velocity space is based on the discrete velocity method. In the physical space a second order difference scheme is applied, while the macroscopic quantities are computed by Gauss-Legendre quadrature. Concerning the temporal discretization, a semi-implicit scheme is used as in [12]. The results presented in the next section have been obtained with $10^3$ nodes in the physical space, 96 molecular speeds and time step $\Delta t = 10^{-4}$. The evolution with respect to time is concluded at some time $t_E$, where the computed density, temperature and heat flux reach up to 99% of their corresponding steady-state values.

4. Results and discussion

In figure 2 the evolution of the translational $q_t$ and rotational $q_{rot}$ heat fluxes at the center of the gap $(y = 0)$ is presented in terms of the dimensionless time $t$ up to some certain time for typical values of $\delta = [0, 1, 50]$ and for $T_H/T_C = [1.1, 3, 10]$ corresponding to small, moderate and large temperature gradients. The relaxation times to steady-state conditions are about the same for the translational and rotational heat fluxes and they are both increased as the temperature ratio is increased. Furthermore, the time needed to reach the steady-state situation in the transition regime ($\delta = 1$) is considerably smaller than the corresponding times in the free molecular ($\delta = 0$) and hydrodynamic ($\delta = 50$) regimes.

In figure 3 the total dimensionless response time $t_E$ is shown in terms of the rarefaction parameter $\delta$ for different values of the temperature ratio $T_H/T_C$ for a diatomic gas, while corresponding results for a monoatomic gases are also included for comparison purposes. In all cases the required response time is reaching a minimum somewhere inside the transition regime at about $\delta = 1$. This behavior has some resemblance to the well-known Knudsen minimum. For values of $\delta > 1$, the time $t_E$ for a polyatomic gas is larger than for the corresponding monoatomic one and for values of $\delta < 1$, the time $t_E$ is about the same for polyatomic and monoatomic gases at small and moderate temperature ratios, while at the large temperature ratio it is larger for the monoatomic gas.

In order to obtain a more physical understanding of the required time to reach steady-state conditions and to facilitate comparisons with experiments certain dimensional times $t'$ [s] in terms of the reference pressure $P_0$ [Pa] are given in figure 4 for the monatomic gases of Ar and He, the diatomic gases of H$_2$ and N$_2$ and the polyatomic gases of CO$_2$ and SF$_6$. The distance between the plates is $H = 5$ mm with the temperature of the cold plate set at $T_C = 273$ [K] and the temperature ratio $T_H/T_C = 3$. The reference pressure $P_0$ [Pa] is easily connected to the rarefaction parameter $\delta$, via Eq. (6), once the viscosity and the most probable velocity of each gas is specified. All computations are based on the IPL interaction law with $\omega = [0.81, 0.66, 0.67, 0.74, 0.93, 0.69]$ for Ar, He, H$_2$, N$_2$, CO$_2$ and SF$_6$ respectively. It is noted that the dependency of the results on $Z$ is small and therefore in all cases $Z = 5$ is introduced [8]. The minimum response times at figure 3, are also present here in the range of 1-10 [Pa] depending on the specific gas. In the case of monatomic gases as molecular mass $m$ is increased the response time is also monotonically increased. In polyatomic gases this trend is not always valid because it also depends on the internal structure. For example the response time of N$_2$ is larger than of Ar even if N$_2$ is lighter of Ar. Of course the response times of H$_2$ and SF$_6$, which are the lightest and heaviest gases are the smallest and the largest respectively.

Closing this work it is noted that the interest of the research community in time-dependent heat transfer in rarefied gases has been lately increased mainly due to the technological applications in the field of microfluidics. It is hoped that the provided results may trigger some experimental work in time-dependent heat transfer configurations and also support the design and optimization of micro heat transfer devices.
Figure 2. Time evolution of $q_r$ (solid) and rotational $q_{rot}$ (dash dot) heat fluxes for various parameters.

Figure 3. Response time $t_E$ of diatomic (solid) and monoatomic gases (dashed) in terms of $\delta$ and $T_H/T_C = [1.1, 3, 10]$.

Figure 4. Response time $t'$ [s] in terms of reference pressure $P_0$ with $T_H/T_C = 3$ for various polyatomic and monoatomic gases.

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