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Conductive heat transfer in rarefied binary gas mixtures confined between parallel plates based on kinetic modeling

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ABSTRACT

The kinetic model introduced by Kosuge (2009) is implemented to solve heat transfer through rarefied binary gas mixtures confined between two parallel plates maintained at different temperatures. The results have been found to be in very good agreement with corresponding ones obtained by the Boltzmann equation, the DSMC method and the Chapman-Enskog analysis. The efficiency of the Kosuge model for this problem is clearly demonstrated in the whole range of the Knudsen number for various heat flow setups, even when the temperature difference between the plates is large. The following three intermolecular models have been implemented: Hard Sphere (HS), Lennard Jones (LJ), Realistic Potential (RP). The computed HS heat fluxes in the transition and viscous regimes vary significantly with the corresponding ones of the LJ and RP models, which are close to each other. Also, the intermolecular model has a significant effect on the distribution of the mole fraction between the plates, while it has a minor effect on the density and temperature distributions. Concerning the partial heat flux distributions of the light and heavy species it has been found that moving from the hot towards the cold plate the former one is decreasing, while the latter one is increasing with the total heat flux being always constant. Heat fluxes with partial thermal accommodation at the walls are reported for He-Ne and He-Xe. For the same mixtures dimensional heat fluxes in terms of the reference pressure are plotted indicating that the total heat fluxes of the mixture with various mole fractions are always bounded from below and above by the heat flux of the heavy and light species respectively. These data may be useful for comparisons with experiments. Applying the equivalent single gas approach, it is deduced that this concept is not useful in rarefied binary gas mixture heat flow problems, which should be treated by two coupled kinetic equations. Finally, the effective thermal conductivity approximation has been successfully applied, provided that the system Knudsen number remains adequately small.

1. Introduction

The steady-state conductive heat transfer through rarefied gases confined between solid surfaces is a classical problem and, in the case of monatomic single gases, has been extensively investigated. The available research work includes heat transfer between parallel plates [1–4], coaxial cylinders [5–9] and concentric spheres [10–14] under small and large temperature differences. Since the solution of the Boltzmann equation is computationally very demanding, most of the research is based on the numerical solution of the Bhatnagar-Gross-Krook (BGK) [15], Ellipsoidal (ES) [16] and Shakhov (S) [17] kinetic models [18]. In [3,6,7,9,10–12] small values of the temperature difference between the surfaces are considered and the computed heat fluxes are obtained solving the linearized form of the corresponding kinetic model equations, while in [1,4,5,8,13,14] large temperature differences are maintained between the walls and the results are based on the nonlinear form of the model equations. In all cases, provided that the thermal conductivity coefficient is properly recovered, reliable results have been reported in the whole range of the Knudsen number. The Direct Simulation Monte Carlo (DSMC) method [19] has been also implemented to simulate this classical problem and to test various molecular interaction models [20] as well as to validate new approaches and numerical methods [21–24]. In addition, based on the Holway [16] and Rykov [25] models, as well as on the DSMC method, the problem of heat conduction through polyatomic gases has been recently tackled pointing out the effect of the rotational and vibrational degrees of freedom of the molecules [26–28]. In addition, unsteady heat conduction through monatomic and polyatomic rarefied gases in plane

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and cylindrical geometries caused by a sudden change of the wall temperature has been considered in [29–31].

The corresponding research work in the case of gas mixtures, although in practice gaseous mixtures are used more frequently than single gases, is not as extensive. In the case of small temperature differences the McCormack model [32] has been proven to be a reliable model [33–36], properly recovering simultaneously all transport coefficients and it has been applied to simulate steady [36,37] and transient [38] heat flow between plates. Recently, a detailed evaluation of the McCormack model is presented in [39] by comparing its solutions for the Couette and Fourier flows of binary gas mixtures with corresponding results of the linearized Boltzmann equation. Furthermore, the McCormack model allows the implementation of any type of intermolecular model and as reported in [36] the computed heat fluxes, particularly near the hydrodynamic regime, strongly depend on the molecular interaction law. In the case of large temperature differences however, as far as the authors are aware off, corresponding work based on kinetic models is not available in the literature. The nonlinear heat transfer through binary gas mixtures has been solved by the Boltzmann equation with the assumption of hard sphere molecules [40] and by the DSMC method supplemented by the Ab-initio potential [41], while the transient behavior has been analyzed via the DSMC method in [42]. The required computational effort in both methodologies, particularly under the assumption of general intermolecular models, is very large and it is rather evident that the search for a kinetic model simulating the specific problem with modest computational effort, allowing in parallel an in depth investigation of all involved parameters, will be very useful.

A relatively large number of binary gas mixture kinetic models, has been proposed in the literature. As the most typical and commonly applied ones, the models of Gross and Krook [43], Sirovich [44], Hamel [45], Holway [46], Ogushi [47], McCormack [32], Garzo, Santos and Brey [48] and Andries, Aoki and Perthame [49], as well as the more recent model of Kosuge [50], which is of particular interest in the present work, are cited. All above models, except the ones by McCormack and Kosuge, suffer one or both of the following two important constrains [50,51]: (a) the parameters introduced in the molecular interactions cannot be accordingly adjusted to correctly produce all transport coefficients and (b) they are suitable only for the pseudo Maxwell molecules.

The McCormack kinetic model [32], as pointed above, circumvents both pitfalls, but it is a linear model and it is restricted to conditions close to local equilibrium. The recently introduced Kosuge model [50] has been derived, following the same polynomial expansion approach in the molecular velocity space as in the McCormack model, which now however, is applied into the nonlinear (instead of the linearized) collision term of the Boltzmann equation. The expansion coefficients are determined by the equivalence of moment method (Grad's 13-moment approximation). The resulting model equations are not restricted to pseudo Maxwell molecules and can fit to various molecular models (hard sphere, Lennard-Jones, realistic, etc.), while the transport coefficients obtained by the Chapman-Enskog analysis coincide with those of the Boltzmann equation at the first or second approximation. More precisely, the thermal conductivity, the viscosity, and the thermal diffusion coefficients coincide at the first approximation, while the diffusion coefficient up to the second approximation. Furthermore, its linearization yields the third order McCormack model [50], while there is no proof that the model (in its nonlinear form) fulfills the H-theorem.

The model has been applied in [50] for half-space and two-surface problems of a vapor in the presence of a non-condensable gas reproducing well the corresponding solutions of the Boltzmann equation. However, it has been also found that it does not work well in strongly nonequilibrium flow and this is contributed to the positivity of the velocity distribution function which is not always assured. In spite this deficiency it is recommended as an effective tool for the investigation of gas mixtures [50]. It is noted that in the Shakhov model for single gases the positivity of the velocity distribution function is also not assured but the model has been effectively applied in many rarefied flow and heat transfer setups [52–56].

Based on the above it is evident that further investigation of the validity of the Kosuge model in simulating rarefied gas dynamics problems is important. Within this framework, in the present work, the conductive heat flow through various binary gas mixtures confined between two parallel plates is computationally investigated. All macroscopic quantities (number densities, temperatures and heat fluxes) of practical interest are calculated in a wide range for all involved parameters (gas rarefaction, mole fraction, molecular mass ratio, temperature difference, etc.). A systematic comparison between the present results obtained by the Kosuge model and the corresponding ones obtained by the Boltzmann equation [40] and the DSMC method [41] is performed. The model validation is supplemented by comparing the computed thermal conductivity and thermal diffusion ratio coefficients with the ones obtained by the Chapman-Enskog theory [57]. The influence of various intermolecular potentials on the computed quantities is examined. The work is extended to partial thermal gas-surface accommodation and its effect on the computed heat fluxes is presented. The validity of the equivalent single gas approach [58] is analyzed in terms of the binary gas mixture composition and its mole fraction in a wide range of gas rarefaction. Furthermore, the effective thermal conductivity approximation, which has been successfully applied in single monatomic [21] and polyatomic [28] gases, is introduced here in the case of nobble gas mixtures.

2. Formulation of the heat transfer problem

Consider a stationary rarefied mixture of two monatomic gases, say components 1 and 2, confined between two infinite parallel plates, fixed at $\hat{y} = 0$ and $\hat{y} = L$, which are maintained at constant temperatures T_H and T_C respectively, with $T_H > T_C$. Then, due to the temperature difference, a steady one-dimensional heat flow is established in the direction normal to the plates and directed from the hot towards the cold plate. It is noted that indexes 1 and 2 always refer to the light and heavy species respectively. The objective is to investigate the validity of the Kosuge kinetic model in solving this heat flow problem and then, examine the steady behavior of the mixture in terms of (a) the mixture composition, (b) the mole fraction of the mixture, (c) the temperature difference between the plates, (d) the degree of gas rarefaction, (e) the intermolecular potential model and (f) the thermal accommodation coefficients (not necessarily in that order).

The temperature difference is introduced in dimensionless form as

$$\beta = \frac{T_H - T_C}{2T_0}, \tag{1}$$

where $T_0 = (T_H + T_C)/2$. The temperature ratio in terms of β is given by $T_H/T_C = (1+\beta)/(1-\beta)$. The degree of gas rarefaction is determined by the reference Knudsen number defined as

$$Kn_0 = \frac{l_0}{L}, \tag{2}$$

where $l_0 = [\sqrt{2}\pi d_1^2 n_0]^{-1}$ is the reference mean free path and corresponds to the mean free path of the molecules of species 1, having diameter d_1, when the gas mixture is in the equilibrium state at rest, with number density determined as