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Chapman–Enskog solutions to arbitrary order in Sonine polynomials III: Diffusion, thermal diffusion, and thermal conductivity in a binary, rigid-sphere, gas mixture

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ABSTRACT

The Chapman–Enskog solutions of the Boltzmann equation provide a basis for the computation of important transport coefficients for both simple gases and gas mixtures. These coefficients include the viscosity, the thermal conductivity, and the diffusion coefficient. In a preceding paper (I), for simple, rigid-sphere gases (i.e. single-component, monatomic gases) we have shown that the use of higher-order Sonine polynomial expansions enables one to obtain results of arbitrary precision that are free of numerical error and, in a second paper (II), we have extended our initial simple gas work to modeling the viscosity in a binary, rigid-sphere, gas mixture. In this latter paper we reported an extensive set of order 60 results which are believed to constitute the best currently available benchmark viscosity values for binary, rigid-sphere, gas mixtures. It is our purpose in this paper to similarly report the results of our investigation of relatively high-order (order 70), standard, Sonine polynomial expansions for the diffusion- and thermal conductivity-related Chapman–Enskog solutions for binary gas mixtures of rigid-sphere molecules. We note that in this work, as in our previous work, we have retained the full dependence of the solution on the molecular masses, the molecular sizes, the mole fractions, and the intermolecular potential model via the omega integrals. For rigid-sphere gases, all of the relevant omega integrals needed for these solutions are analytically evaluated and, thus, results to any desired precision can be obtained. The values of the transport coefficients obtained using Sonine polynomial expansions for the Chapman–Enskog solutions converge and, therefore, the exact diffusion and thermal conductivity solutions to a given degree of convergence can be determined with certainty by expanding to sufficiently high an order. We have used *Mathematica*® for its versatility in permitting both symbolic and high-precision computations. Our results also establish confidence in the results reported recently by other authors who used direct numerical techniques to solve the relevant Chapman–Enskog equations. While in all of the direct numerical methods more-or-less full calculations need to be carried out with each variation in molecular parameters, our work has utilized explicit, general expressions for the necessary matrix elements that retain the complete parametric dependence of the problem and, thus, only a matrix inversion at the final step is needed as a parameter is varied. This work also indicates how similar results may be obtained for more realistic intermolecular potential models and how other gas-mixture problems may also be addressed with some additional effort.

1. Introduction

The Chapman–Enskog solutions of the Boltzmann equation provide a basis for the computation of important transport coefficients for both simple gases and gas mixtures [1–15]. The use of Sonine polynomial expansions for the Chapman–Enskog solutions was first suggested by Burnett [16] and has become the general method for obtaining the transport coefficients due to the relatively rapid convergence of this series [1–8,16]. While it has been found that relatively, low-order expansions (of order 4) can provide reasonable accuracy in computations of the transport coefficients (to about 1 part in 1000), the adequacy of the low-order expansions for computation of the slip and jump coefficients associated with gas-surface interfaces still needs to be explored. Also of importance is the fact that such low-order expansions do not provide good convergence (in velocity space) for the actual Chapman–Enskog solutions even though the transport coefficients derived from these solutions appear to be reasonable. Thus, it is of some interest to explore Sonine polynomial expansions to higher orders. In a preceding paper [17], we have shown for simple, rigid-sphere gases (i.e. single-component, monatomic gases) that, indeed, the use of higher-order Sonine polynomial expansions enables one to obtain results of arbitrary precision that are free of numerical error. In a second paper, we have extended our initial simple gas work to

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modeling the viscosity in a binary, rigid-sphere, gas mixture [18]. In this latter paper we reported an extensive set of order 60 results which are believed to constitute the best currently available benchmark viscosity values for binary, rigid-sphere, gas mixtures. It is our purpose in this paper to similarly report the results of our investigation of relatively high-order, standard, Sonine polynomial expansions for the diffusion- and thermal conductivity-related Chapman–Enskog solutions for binary gas mixtures of rigid-sphere molecules. In the following sections we describe the basic theory, the theoretical elements specific to diffusion, thermal diffusion, and thermal conductivity, the solution technique in terms of the Sonine polynomials, the bracket integrals, details related to the specific case of rigid-sphere molecules, and our results.

A part of our motivation with respect to this work has been some of the recently reported results on direct numerical solutions of the linearized Boltzmann equations for rigid-sphere, gas mixtures. In particular, results for the transport coefficients and the Chapman–Enskog solutions have been reported by Takata et al. [19]. Our work provides a benchmark for assessing the precision of some of the numerical results reported by these authors and, indeed, we report some such comparisons that we have made. Our work does have an important distinguishing feature in that, for rigid-sphere gas mixtures, we require no numerical integrations and thus, in principle, results of arbitrary precision can be obtained for any given order of the Sonine polynomial expansions. We note that the computational resources available to us at the present time have permitted expansions to order 70 given the manner in which we have implemented this technique, but even here it has been possible to obtain extrapolated results believed to be precise to 14 or more significant digits for each of the normalized gas mixture transport coefficients (depending upon the specific mass ratios, size ratios, and mole fractions considered) and it is certain that further improvements in the implementation of the technique or the availability of better computational resources will allow even higher-order expansions and greater convergence of the results. Further, we note that in this work we have retained the full dependence of the solutions on the molecular masses, the molecular sizes, the mole fractions, and the intermolecular potential model via the omega integrals, and we have obtained explicit (symbolic) expressions for the necessary matrix elements (derived from the bracket integrals) used in evaluating the coefficients in the Sonine polynomial expansions for the coupled Chapman–Enskog equations. These generalized matrix elements, once determined, need not be determined again. For rigid spheres (or for any other potential model of interest that can be represented via the omega integrals), we can then determine in a straightforward manner a set of matrix elements that are specific to the potential model being used and store them. These specific matrix elements require only the input of the appropriately computed omega integrals which, for rigid spheres, are known exactly such that no numerical integrations are needed. In this fashion, our method requires only a matrix inversion at the final step. This is important, as all that is needed for finding both the transport coefficients and the related Chapman–Enskog solutions for arbitrary, binary, rigid-sphere gas mixtures is precomputed in a general form. Thus, we are able to study parametric dependencies and convergence of our results in an economical and systematic way since, once the matrix elements up to the highest order are computed and stored, we can process results to any order up to this highest order without any new computations of matrix elements being required. Further, since our values for the transport coefficients converge with increasing order, since we can use arbitrarily high numerical precision as needed in *Mathematica*® for the final matrix inversion step, and since we can easily compare results for a given order with the results for immediately preceding orders, we can be confident in our results and the degree of convergence obtained.

2. The basic theory

Following the work and notations of Chapman and Cowling [1], we offer below an abbreviated version of the relevant theory. For an arbitrary, rarefied, gas mixture, one begins with the Boltzmann equations describing the molecular distribution functions of the constituent gases:

$$\left(\frac{\partial}{\partial t}+\mathbf{c}_i\cdot\nabla_r+\mathbf{F}_i\cdot\nabla_{c_i}\right)f_i(\mathbf{r},\mathbf{c}_i,t) = \sum_j\iiint\left(f_i'f_j'-f_if_j\right)gb\,\mathrm{d}b\,\mathrm{d}\varepsilon\,\mathrm{d}\mathbf{c}_j=\sum_j J(f_if_j), \tag{1}$$

in which the left-hand side (LHS) is known as the streaming term of the equation which contains the differential streaming operator in the brackets, the right-hand side (RHS) is a sum over what are known as the collision integrals in which $J(f_if_j)$ is called the collision operator, $f_i(\mathbf{r},\mathbf{c}_i,t)$ is the molecular distribution function of the i-th constituent, g is the magnitude of the pre-collision relative velocity, $\mathbf{g}=\mathbf{c}_j-\mathbf{c}_i$, b is the ‘impact parameter’ associated with the binary scattering events, ε is an angle corresponding to the azimuthal orientation of the scattering plane, and $\mathbf{c}$ is the molecular velocity. A prime ($'$) indicates a function of a post-collision velocity while the corresponding lack of a prime indicates a pre-collision velocity dependence, e.g. $f_i=f_i(\mathbf{r},\mathbf{c}_i,t)$ while $f_i'=f_i(\mathbf{r},\mathbf{c}_i',t)$. In the summation over the different constituents, scattering between like constituents (i.e. when $i=j$) is treated in the same way as scattering between unlike constituents with the various pre- and post-collision velocities retained as separate variables for purposes of integration. In this circumstance, for clarity, it is common practice to drop the i subscript inside the collision integral in order to facilitate the necessary discrimination between the velocities (i.e. $\mathbf{c}_i\to\mathbf{c}$ and $f_i\to f$). Of course it follows from this that, if one is dealing with a simple gas having only one constituent, one obtains from this process the single Boltzmann equation describing the gas in which $j=1$ and no subscript is necessary on the LHS:

$$\left(\frac{\partial}{\partial t}+\mathbf{c}\cdot\nabla_r+\mathbf{F}\cdot\nabla_c\right)f(\mathbf{r},\mathbf{c},t) = \iiint\left(f'f_1'-ff_1\right)gb\,\mathrm{d}b\,\mathrm{d}\varepsilon\,\mathrm{d}\mathbf{c}_1. \tag{2}$$

Equivalent expressions for the above equations are often encountered in which $b\,\mathrm{d}b\,\mathrm{d}\varepsilon$ is expressed as $\alpha_{ij}(g,\chi)\,\mathrm{d}\mathbf{e}'$ or $\sigma_{ij}(g,\chi)\,\mathrm{d}\boldsymbol{\Omega}$ where χ is the scattering angle (the angle between $\mathbf{g}$ and $\mathbf{g}'$) and $\alpha_{ij}(g,\chi)=\sigma_{ij}(g,\chi)$ is known as the differential collision cross-section which describes the probability per unit time per unit volume that two molecules colliding with velocities, $\mathbf{c}_i$ in $\mathrm{d}\mathbf{c}_i$ and $\mathbf{c}_j$ in $\mathrm{d}\mathbf{c}_j$, will have a relative velocity after collision, $\mathbf{g}'=\mathbf{c}_j'-\mathbf{c}_i'$, that lies within the solid angle, $\mathrm{d}\mathbf{e}'=\mathrm{d}\boldsymbol{\Omega}=\sin(\chi)\,\mathrm{d}\chi\,\mathrm{d}\varepsilon$.

For the specific case of a binary gas mixture, one expresses the distribution functions f_1 and f_2 in the form:

$$f_1=f_1^{(0)}+f_1^{(1)}+f_1^{(2)}+\cdots, \tag{3}$$

$$f_2=f_2^{(0)}+f_2^{(1)}+f_2^{(2)}+\cdots, \tag{4}$$

where the lowest-order approximations are chosen to be:

$$f_1^{(0)}=n_1\left(\frac{m_1}{2\pi kT}\right)^{3/2}\exp\left(-\frac{m_1}{2kT}(\mathbf{c}_1-\mathbf{c}_0)^2\right), \tag{5}$$

$$f_2^{(0)}=n_2\left(\frac{m_2}{2\pi kT}\right)^{3/2}\exp\left(-\frac{m_2}{2kT}(\mathbf{c}_2-\mathbf{c}_0)^2\right), \tag{6}$$