THE G-SCHEME OF APPROXIMATIONS TO THE THERMAL DIFFUSION FACTORS : EXPLICIT FORMULAE

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ABSTRACT

A new scheme of approximations to the thermal diffusion factors, the so-called G-scheme, has been recently introduced. But it contained an implicit equation to be solved by trials and errors, an unpleasant and tedious way to run. This paper is mainly concerned with new developments of the G-scheme, where explicit formulae are derived for the first and second approximations, considerably increasing the ease of computations. Numerical calculations are carried out for an He/K gaseous mixture and discussed.

INTRODUCTION

In the CHAPMAN-ENSKOG mathematical theory of non-uniform gases (1), the thermal diffusion factor is obtained from the solution of an infinite set of linear equations. Two ways of obtaining successive approximations to this solution have been developed by CHAPMAN and COWLING (CC-Scheme), then by KIHARA (K-scheme, see reference 2 for instance). Unfortunately, the rigorous CHAPMAN-COWLING series of approximations is slowly converging and the computations become drastically more and more tedious as the order of approximation increases. On the other hand, the K-scheme is too much based on a peculiar intermolecular force model, the so-called maxwellian one, to be easily trusted whatever the situations.

Thus a new scheme has been recently introduced to attempt to overcome these difficulties, and was found very successful in the studied situation, namely an almost-Lorentzian He/Ar mixture (3-4). This scheme exhibited the following required properties : (i) a fast convergence of the series of approximations (ii) a converged value closed to the true one (iii) easier calculations than in the CC- or the K-schemes to obtain satisfactory numerical values of the thermal diffusion factors. But it contained an implicit equation to be solved by trials and errors, an unpleasant and fairly tedious way to do. So this scheme will be called the IG-scheme (Implicit G-scheme). This paper is concerned with new developments of the G-scheme where the

implicit equation is no longer used and explicit formulae are derived. This scheme will be called the EG-scheme (Explicit G-scheme). The EG-scheme exhibits the same accuracy as the implicit one but the ease for numerical computations is considerably increased.

I - THE G-SCHEME OF APPROXIMATIONS TO THE THERMAL DIFFUSION FACTORS

I-1. Generalities

More details concerning the G-scheme can be found elsewhere (3-4). The main features are outlined below.

The m^{th} approximation in the G-scheme is defined by :

$$\left[\alpha_T\right]_{Gm} = \phi_m \left[\alpha_T\right]_m \qquad (1)$$

where $\left[\alpha_T\right]_m$ is the m^{th} approximation in the CC-scheme. The correction factor ϕ_m is estimated with the aid of the peculiar model of a Lorentzian gas in which the species 1 and 2 are interacting according to a power law :

$$F_{12} = K_{12} / r^{\nu_{12}} \qquad (2)$$

where F_{12} is the force between the two atoms at a distance r. In this $(L\nu)$-model, the ratios $(\alpha_T / \left[\alpha_T\right]_m)_{L\nu}$ can be rigorously calculated as a function of the exponent ν_{12}. These are defined as the correction factors ϕ_m. So, the relation (1) reads :

$$\left[\alpha_T\right]_{Gm} = \left(\frac{\alpha_T}{\left[\alpha_T\right]_m}\right)_{L\nu} \left[\alpha_T\right]_m \qquad (3)$$

ϕ_1 and ϕ_2 are numerically given by CHAPMAN and COWLING (1). These numerical values have been used in previous works (3-4).

In the present work, they have been analytically expressed versus the exponent ν_{12}. For this purpose, we have to express $\left[\alpha_T\right]_1$, $\left[\alpha_T\right]_2$ and α_T in the $(L\nu)$-model. The true value $(\alpha_T)_{L\nu}$ is given by the following relation (1) :

$$(\alpha_T)_{L\nu} = \frac{1}{1-C_2} \cdot \frac{\nu_{12}-5}{2(\nu_{12}-1)} \qquad (4)$$

where c_2 is the mole fraction of the light kind. The approximations $(\alpha_T)_1$ and $(\alpha_T)_2$ in the $(L\nu)$-model are deduced from the rigorous CHAPMAN-COWLING expressions by adding the following constraints : $C_2 \to 0$, $M_2 = m_2/(m_1 + m_2) \to 0$ and $M_1 = m_1/(m_1 + m_2) \to 1$, where m_1 and m_2 are the mass of atom of the kinds 1 and 2 respectively.

The following expressions are found :

$$\left(\left[\alpha_T\right]_1\right)_{L\nu} = \frac{5}{2(1-C_2)} m_2^{-1/2} \frac{a_{-1-0} - 1}{a_{-1-1}} \qquad (5)$$

$$\left(\left[\alpha_T\right]_2\right)_{L\nu} = \frac{5}{2(1-C_2)} m_2^{-1/2} \begin{vmatrix} a_{-1-0} & a_{-1-2} \\ a_{-2-0} & a_{-2-2} \end{vmatrix} \Big/ \begin{vmatrix} a_{-1-1} & a_{-1-2} \\ a_{-2-1} & a_{-2-2} \end{vmatrix} \qquad (6)$$

where the expressions for the matrix elements are given elsewhere (1) as functions of some collision integrals. Keeping in mind that we are concerned with a (Lν)-model, using the corresponding expressions for the collision integrals available from the reference (1), the following results are found after some lengthy but straightforward calculations :

$$\phi_1(\nu_{12}) = \frac{13\,\nu^2_{12} - 42\,\nu_{12} + 45}{10(\nu_{12} - 1)^2} \qquad (7)$$

$$\phi_2(\nu_{12}) = \frac{1275\,\nu^5_{12} - 9673\,\nu^4_{12} + 30934\,\nu^3_{12} - 52058\,\nu^2_{12} + 45935\,\nu_{12} - 16925}{20(\nu_{12} - 1)^2(57\,\nu^3_{12} - 281\,\nu^2_{12} + 487\,\nu_{12} - 295)} \qquad (8)$$

ν	ϕ_1^{-1}	ϕ_2^{-1}
3	1.11	1.01
4	1.06	1.01
5	1.00	1.00
6	0.96	0.99
7	0.93	0.98
8	0.91	0.97
9	0.89	0.96
10	0.88	0.95
11	0.87	0.95
12	0.86	0.94
13	0.85	0.94
14	0.84	0.94
15	0.84	0.93
16	0.83	0.93
17	0.83	0.93
18	0.83	0.93
19	0.82	0.93
20	0.82	0.92

Table I gives numerical values for ϕ_1 and ϕ_2 versus ν_{12} calculated from (7) and (8) respectively. They slightly correct the values given by CHAPMAN and COWLING (1).

The only problem to solve now is to compute realistic values of ν_{12} in order to deduce ϕ_1 and ϕ_2 from them, then $[\alpha_T]_{G1}$ and $[\alpha_T]_{G2}$.

I-2. The implicit G-scheme

Details are given elsewhere (3-4). The exponent ν_{12} is deduced from the following equation :

$$[\alpha_T]_{1\nu_{12}} = [\alpha_T]_1 \qquad (9)$$

in which $[\alpha_T]_1$ is the first approximation in the CC-scheme computed from 'real' interatomic potentials and $[\alpha_T]_{1\,\nu_{12}}$ is the first approximation in the CC-scheme computed with 'real' interatomic potentials for all interactions but the (1-2)-interaction. For the (1-2)-interaction, the inverse-power force law is used in such a way that ν_{12} remains the only unknown term in (9), that means (1) :

$$A = \frac{3\nu_{12} - 5}{5(\nu_{12} - 1)} \quad \frac{A_2(\nu_{12})}{A_1(\nu_{12})} \tag{10}$$

$$B = \frac{(3\nu_{12} - 5)(\nu_{12} + 1)}{5(\nu_{12} - 1)2} \tag{11}$$

$$C = \frac{2(3\nu_{12} - 5)}{5(\nu_{12} - 1)} \tag{12}$$

and E (CHAPMAN-COWLING notations) is calculated using the real (1-2) interatomic potential (otherwise, there would appear a second unknown term in (9), namely the constant K_{12} appearing in relation (2)). Relation (9) is solved by trials and errors, allowing to deduce a realistic value for the exponent ν_{12} and then to compute $[\alpha_T]_{G1}$ and $[\alpha_T]_{G2}$.

I-3. Explicit G-scheme

The expression for the first approximation in the CC-scheme is now recalled :

$$[\alpha_T]_1 = 5(C-1)\frac{S_1(1-C_2) - S_2C_2}{Q_1(1-C_2)^2 + Q_2C_2^2 + Q_{12}C_2(1-C_2)} \tag{13}$$

where S_1, S_2, Q_1, Q_2, Q_{12} are known functions of the mass of atoms and collision integrals (1).

It is well known that the $[\alpha_T]_1$ value is mainly determined by the C value which is the most influent term in (13). Thus the equivalent exponent ν_{12} can be estimated by the following relation, instead of (9) :

$$\frac{2(3\nu_{12} - 5)}{5(\nu_{12} - 1)} = C \tag{14}$$

thus : $$\nu_{12} = \frac{5(C-2)}{5C-6} \tag{15}$$

This expression can be substituted into (7) and (8) to express the correction factors explicitly versus C.

The following expressions are obtained, after some lengthy but straightforward computations :

$$\phi_1(C) = \frac{5C^2 - 8C + 5}{2} \tag{16}$$

$$\phi_2(C) = \frac{-125\,C^4 + 300\,C^3 - 350\,C^2 + 204\,C - 85}{4(-25\,C^2 + 30\,C - 19)} \tag{17}$$

Surprisingly, the function $\phi_2(C)$ is much simpler than $\phi_2(\nu_{12})$. Thus, the two first approximations to the thermal diffusion factors in the explicit G-scheme are according to relation (3) :

$$\left[\alpha_T\right]_{G1} = \frac{5\,C^2 - 8\,C + 5}{2}\left[\alpha_T\right]_1 \qquad (18)$$

$$\left[\alpha_T\right]_{G2} = \frac{-125\,C^4 + 300\,C^3 - 350\,C^2 + 204\,C - 85}{4(-25\,C^2 + 30\,C - 19)}\left[\alpha_T\right]_2 \qquad (19)$$

Our notations $\left[\alpha_T\right]_{G1}$ and $\left[\alpha_T\right]_{G2}$ do not distinguish between the implicit and the explicit G-schemes. The reason is that the IG-scheme will be given up in further works, having now only an 'historical' interest.

II - COMPARISONS BETWEEN THE CC- and G- SCHEMES

The first and second approximations in the CC- and in the EG-schemes have been computed for an He/K gaseous mixture. Modified BUCKINGHAM potentials have been chosen :

$$\varphi_{ij}(r) = \frac{\varepsilon_{ij}}{1-\frac{6}{\alpha_{ij}}}\left[\frac{6}{\alpha_{ij}}\exp\left[\alpha_{ij}\left(1-\frac{r}{r_{m,ij}}\right)\right] - \left(\frac{r_{m,ij}}{r}\right)^6\right] \qquad (20a)$$

if $r > r_{max,ij}$, and

$$\varphi_{ij}(r) = \infty \quad , \text{ if } \quad r \leqslant r_{max,ij} \qquad (20b)$$

The subscripts i and j designate the species. The parameters ε_{ij}, $r_{m,ij}$ and α_{ij} are parameters characterizing the atomic interactions, and r is the distance of separation. Finally, $r_{max,ij}$ is a very small separation distance for which the potential given by (20a) has a spurious maximum. The values of the parameters are given by MASON and RICE (5) for the interaction (2-2) : $\alpha_{22} = 12{,}4$; $\varepsilon_{22}/k = 9{,}16$; $r_{m,22} = 0{,}3135$ nm. For the interactions (1-1) and (1-2) the parameters values are available from DARRIGO calculations (6) : $\alpha_{11} = 14$; $\alpha_{12} = 13{,}23$; $\varepsilon_{11}/k = 1666$; $\varepsilon_{12}/k = 121{,}45$; $r_{m,11} = 0{,}3602$ nm ; $r_{m,12} = 0{,}3373$ nm. The collision integrals have been computed from MASON tabulations (7).

Some examples of results are given on the figures 1 and 2 in almost-Lorentzian cases ($C_2 \leqslant 25$ %). The values of $(\alpha_T)_{L\nu}$ computed using relation (4) and the computed exponents ν_{12} are also given. It is considered that the mixture becomes non-Lorentzian when $(\alpha_T)_{L\nu} \sim 1{,}5\alpha_T$, thus for $C_2 \sim 25\%$. The Lorentzian or non-Lorentzian character of the mixture will be exhaustively discussed elsewhere. The three conditions mentioned in the introduction are obeyed : (i) the G-scheme converges faster than the CC-one. (ii) the nearly converged value $\left[\alpha_T\right]_{G2}$ is nearly equal to the true α_T. This can be easily understood since, according to relation 3, the following relation holds in the $(L\nu)$-model :

$$\left[\alpha_T\right]_{G1} = \left[\alpha_T\right]_{G2} = \alpha_T$$

Furthermore, previous experiments (3-4) agree with this conclusion. (iii) As a result of the previous discussion of the conditions (i) and (ii), it can be said than $[\alpha_T]_{G1}$ is a better approximation than $[\alpha_T]_2$, so a better approximation of α_T is obtained with much simpler computations.

The G- scheme can also be used for non-Lorentzian mixtures with some success, but results and discussion cannot be reported here because they would need too much place. It will be done elsewhere.

CONCLUSION

Explicit formulae for the G-scheme of approximations to the thermal diffusion factors have been given. Computations have been made for a He/K mixture in the almost-Lorentzian case. It is concluded that the G-scheme should be preferred to the CC-one in such situations.

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