TRANSFER COEFFICIENT OF MULTICOMPONENT AIR WITH SUBLIMATION PRODUCTS OF GRAPHITE

V. V. Ryabov

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An economical method of calculating the viscosity, thermal conductivity, binary diffusion coefficient, and thermodiffusion coefficient is proposed, for a mixture of dissociated air and subliming graphite.

1. In investigating the heat transfer in a high-temperature viscous shock layer close to a graphite surface which is undergoing breakdown, the transfer coefficients (viscosity, heat conduction, diffusion) of multicomponent air with an admixture of the sublimation products of graphite must be determined.

Calculations of the characteristic parameters of molecular transfer both by kinetic theory [1] and by approximate methods [2, 3] are based on data regarding the elastic interaction potentials between the mixture components. Experimental investigation of the transfer coefficients to date has been restricted to the range T ~ 2000 K [4, 5], and, as noted in [6], rigorous quantum-mechanical calculation of elastic-interaction processes is only possible for atoms and molecules with a simple electron structure [7]. The basic sources of information on the interaction of molecules at high temperatures are experimental results on the scattering of fast molecular beams. Numerous data on the molecule-molecule and atom-molecule interaction were obtained in [8-11], for example. The first investigations [11] were based on the assumption of an inverse power dependence of the interaction potential $V = K/R^s$ on the distance between the centers of mass of the molecules. At the same time, analysis of the experimental conditions in [9] shows that $s$ is not constant. Evidently, the most preferable form of repulsive potential is the exponential approximation $V = A \exp(-\beta R)$. This approximation has been successfully used to describe the interaction of identical atoms (especially of inert gases [9]). The additive-potential method, proposed in [11] for approximate calculation of $V(R)$, gives good accuracy in calculating the parameters of the atom-molecule and molecule-molecule interaction. According to this method, the interaction potential of the molecules AB and CD is written as follows [9]

$$V(R) = V(r_{A0}) + V(r_{B0}) + V(r_{A0}) + V(r_{B0}),$$  

where $r$ is the interatomic distance.

The potential in Eq. (1), averaged over equiprobable orientations, determines the effective spherically symmetric potential corresponding to the point force center. Here, it is possible to choose parameters of the exponential function approximating cumbersome analytical expressions for the mean potential. This procedure was described in detail in [12,
13]. The combinatorial rule [9] is usually employed to make up the currently unknown data on the interaction potential

\[ V_{ij} = V_{ii}V_{jj}. \]  

(2)

Using the values of the collision integrals \( \Omega_{ij}^{(k,s)} [1, 14] \), the transfer coefficients of the multicomponent gas mixture may be calculated by the well-known method [1, 3, 15]. According to [14], the expression for the \( \Omega_{ij}^{(k,s)} \) integrals calculated for the exponential repulsive potential \( V(R) = A \exp(-\beta R) \) takes the form

\[ \Omega^{(k,s)} = 4 \left( \frac{nkT}{2} \right)^{1/2} I^{(k,s)}(\gamma) \gamma^2/\beta^2, \quad \gamma = \ln \left( \frac{A}{kT} \right). \]  

(3)

Here \( k \) is the Boltzmann constant; the function \( I^{(k,s)}(\gamma) \) for various \( k \), \( s \) and values 3.5 \( \leq s \leq 28.5 \) was tabulated in [14]. In the present work, these dependences are approximated by cubic splines of defect 1.

Using Eq. (3), it is simple to calculate the viscosity values \( \eta_i \) of the individual components and the binary-diffusion coefficient \( D_{ij}^{(2,2)} \) [1, 14]

\begin{align*}
\eta_i &= \frac{1.3346 \cdot 10^{-6}(M_iT)^{1/2}}{\gamma^2/\beta^2 I^{(2,2)}(\gamma)}, \quad \text{N\cdotsec/m}^2, \\
\rho D_{ij} &= \frac{0.40038 \cdot 10^{-6} \beta^2}{\gamma^2 I^{(1,1)}(\gamma)} \sqrt{\frac{2T(M_i + M_j)}{M_iM_j}}, \quad \text{kmole/m\cdotsec}.
\end{align*}

(4)

(5)

Note also that the viscosity and self-diffusion coefficient are simply related [1]

\begin{align*}
\frac{\rho D_{ij}}{\eta_i} &= \frac{6}{5} A^*, \quad A^* = \frac{Q^{(2,2)*}}{Q^{(1,1)*}}, \\
Q^{(l,s)*} &= \frac{\Omega^{(l,s)}}{\Omega^{(n,c)}} = \frac{8\gamma^2/\beta^2 I^{(l,s)}(\gamma)}{(s+1)^2 \left[ 1 - \frac{1}{2} \frac{1 + (-1)^s}{1 + l} \right] \sigma^2},
\end{align*}

(6)

(7)

where \( \sigma \) is the intermolecular-potential parameter of solid spheres [1].

2. Use of the additive-potential method [1] permits approximate calculation of the dependences \( V(R) \) by the above method for pairs of molecules C, O, N, O2, NO, CN, CO, CO2, C2, C3, C4, and C5 forming the gas mixture of dissociated air and breakdown products of graphite in the range 0.6 \( \leq R \leq 5.5 \) Å. The results obtained are approximated by an exponential function, using the least-square method. The basis functions adopted are the atom-atom interaction potentials, the parameters of which are taken from [6, 13]. Data on the molecular structure are taken from [16].

The values of the parameters \( A, \beta \) of the exponential repulsive potential obtained in the present work are shown in Table 1. These values are compared with the data of [9, 13]. The agreement of the results is basically good (an asterisk marks correlating values in Table 1). Most of the information on the interaction potentials (especially with the participation of C, O atoms) is complete, thanks to the additive-potential method used here.

For dissociated air with the ablation products of graphite at temperatures \( T = 2000-10,000 \text{ K} \), the values of the reduced \( \Omega_{ij}^{(k,s)*} \) integrals are calculated, as well as the viscosity and binary-diffusion coefficient, according to Eqs. (3)-(7). The best agreement of the present results on \( \Omega_{ij}^{(k,s)*} \) is with [6, 9, 13]. Here the values of the collision integrals calculated using the potentials with the parameters in Table 1 are intermediate between the results of other works; see the bibliography in [6]. These differences in the given temperature range may reach 50%.

The viscosity values \( \eta_i \) obtained by the given method for the individual components (Table 2) are compared with the data for O2, N2, CO2 from [4]. With a relative error of around 10%, the results are in good correlation. Comparison of the present data with those of [17] for \( \eta_i \), \( D_{ij}^{(2,2)} \) reveals only qualitative agreement. Note that, in [17], the Lennard–Jones potential was used; this potential is of strictly limited applicability, as noted in [15], for example. As an example, values of \( \rho D_{ij}/M \) at \( T = 4000 \text{ K} \) are shown in Table 3.