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A Tractable Method for Estimating Atomic and Molecular Transport Coefficients

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TO calculate the flow in the vicinity of an ablating or transpiration cooled surface, one often requires the values of the transport coefficients of the various species injected into the boundary layer. Sufficient experimental data does not exist to obtain parameters needed for a semiempirical determination of these transport coefficients. A method of obtaining transport coefficients without recourse to experimental data would thus be of great value. Such methods have been studied in the past by other investigators.[1]

The purpose of this Note is to present a method of calculating transport coefficients, which is simple enough to be carried out quickly and without the use of a computer. Comparison of transport coefficients obtained using this method with experimental data show agreement which is generally as good as those obtained from more elaborate computation.

The interaction between two neutral molecules is taken to be of the form of a dispersion potential $V(r) = -A/r^6$,[2a] where r is the interparticle separation, and A is a constant for a given set of molecules. The apparent collision radius for the interaction is obtained by letting the potential be proportional to the gas temperature T. The constant of proportionality has previously been studied,[3] where it has been shown that transport coefficients depend weakly on the proportionality constant. As shown below, the present method is independent of the proportionality constant, but introduces another parameter which will be discussed later.

It is assumed that for some gas temperature T_1 the collision radius equals the root mean square radius of the outer shell electrons in the molecule, r_{ms}. With this assumption, the collision cross section σ becomes

$$\sigma = \pi \bar{r}^2 (T_1/T)^{1/3} \tag{1}$$

The transport coefficients can be written in terms of the mean square radius as

$$\mu \times 10^7 = 133.46 T^{5/6}(M^*)/(T_1^{1/3} r_{ms}) \tag{2}$$

$$D \times 10^7 = 3285 T^{11/6}/(r_{ms} p T_1^{1/3} M^*) \tag{3}$$

and

$$K \times 10^7 = 248.6 T^{5/6}/(M^* r_{ms} T_1^{1/3}) \tag{4}$$

where μ is the viscosity in g/cm sec, D is the diffusion coefficient in cm²/sec, K is the translational thermal conductivity in cal/cm sec °K, p is the pressure in atmospheres,

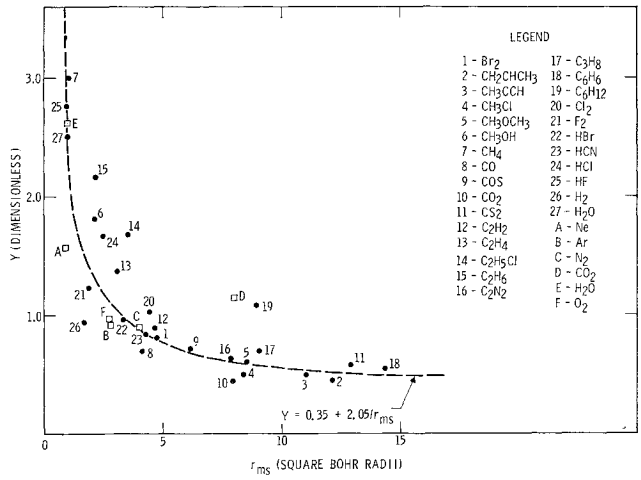

Fig. 1 Data used to obtain T_1 as a function of r_{ms}.

M^* is the reduced molecular mass in a.m.u., T_1 and T are in °K, and r_{ms} is in square Bohr radii, where the Bohr radius is 0.529 angstroms.

Calculation of the mean square radius for a single component monatomic gas using screening constants is straightforward.[2b] For a single component polyatomic gas the mean square radius can be obtained by averaging the screening constants and effective principal quantum numbers of the electron in the molecule's far field and near field. The far-field values are obtained by considering the molecule as an atom of nuclear charge equal to the sum of the atomic nuclear charges. The near-field values are obtained by averaging the effective quantum numbers and effective nuclear charges of all the atoms in the molecule.

This method of obtaining mean square molecular radii neglects the effects of inelastic processes and interactions caused by polar molecules. These effects are important in developing a rigorous theory, but can be neglected for the range of accuracies expected from the method developed in this Note.

The extension to multicomponent mixtures can be carried out by applying the approximate relation between the interaction coefficients of unlike molecules with the coefficients for like molecules.[2c] When this relation is applied, an expression relating the mean square radii is obtained. For molecules of type γ and β this relation is $(r_{ms})^2_{\gamma\beta} = (r_{ms})_\gamma (r_{ms})_\beta$.

The choice of a value for T_1 will now be discussed. The value of the temperature at which the collision cross section is equal to πr_{ms}, i.e., T_1, should decrease with increasing r_{ms} due to the increased volume over which the valence electrons are distributed in the latter case. The dependence of T_1 on r_{ms} was obtained by calculating the transport coefficient assuming $T_1 = 1000$°K for a variety of atomic and molecular gases for which experimental data exist. The ratio of the theoretical to the experimental values for each coefficient were plotting against r_{ms}. Figure 1 is a plot of this ratio Y

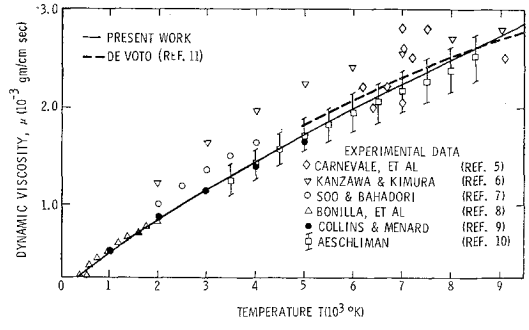

Fig. 2 Comparison of theoretical and experimental viscosities of monatomic argon.

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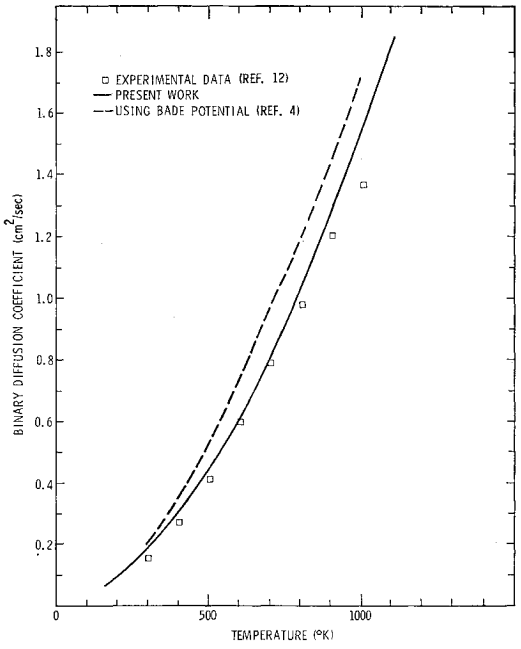

Fig. 3 Comparison of theoretical and experimental binary diffusion coefficients for carbon dioxide and molecular oxygen (at one atmosphere).

for viscosity from which $T_1(r_{ms})$ was determined. It shows the value of $T_1^{1/3}$ required in Eqs. (2–4) to be $10/Y$. A similar plot for diffusion demonstrated the same dependence on r_{ms} as for viscosity except that Y(for diffusion) $= 0.6Y$(viscosity).

Figures 2 and 3 contain the values of the transport coefficients obtained using the method described in this Note. Figures 2 and 3 also contain results obtained using other theoretical calculations by Bade[4] and Devoto.[11] Both of these calculations use a somewhat more complicated potential (exponential repulsive) and handle gas mixtures in a different manner. The relative decrease in the viscosity of argon for temperatures above 9000° K obtained by Devoto is due to the effects of ionization which are not included in the calculations contained in this Note. As is shown in the figures, coefficients obtained from the method given in this Note are close enough to experimental results to be useful in most flowfield calculations.

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Spectrum of MPD Arc Oscillations at Low-Magnetic Field

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Introduction

IN MPD thruster operation, one has a critical magnetic field below which the discharge is quiet and axisymmetric.[1–3] Above this field the discharge is concentrated into a rotating current spoke. The plasma rotates whether the spoke is present or not.[3] One would expect some sort of transition region where the discharge varies in a continuous way from the spoke to the no-spoke mode. Previous experiments[2] indicate that there is no such region.

Measurements with segmented anodes[3,5] indicate that the current spoke is a highly nonlinear phenomenon. Most of the current is concentrated in the rotating spoke. In analysis, however, it is often necessary to treat the disturbances as small perturbations.[6,7] It seemed desirable, therefore, to look for a region where the disturbances really were small. Further investigation at magnetic fields just below threshold seemed appropriate.

Apparatus

The thruster used (Fig. 1) is a McDonnell-Douglas X-7 and is described in Ref. 4. The discharge was probed with a

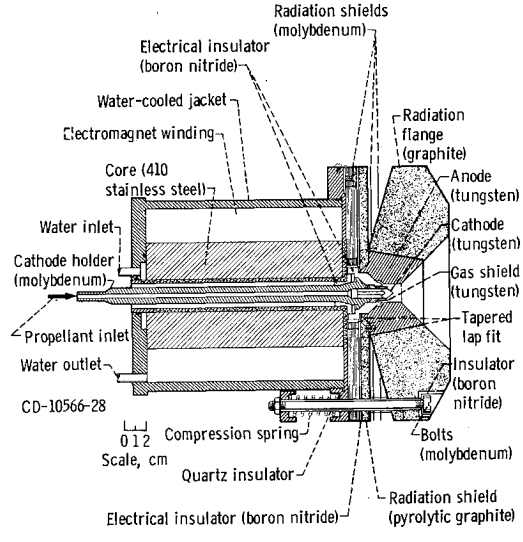

Fig. 1 Schematic drawing of McDonnell-Douglas X-7 thruster.

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