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Proposed Computational Method for Transport Properties of Ablation Products

Louis Biolsi*
Cooperative Institute for Research in Environmental Sciences, University of Colorado/NOAA, Boulder, Colo.

Abstract

MOST of the ablation products obtained from a carbon-phenolic ablator are polyatomic and the accurate estimation of interaction energies and transport properties for interactions involving polyatomic species is difficult. The peripheral force method for obtaining atom-molecule potentials has been applied to an interaction involving an ablation product and one of the major components of the Jovian atmosphere, the He-C_2H interaction. The results obtained for the transport properties are in good agreement with results obtained using other, less detailed, methods. Thus it is suggested that the peripheral force method is useful for the calculation of transport properties for interactions involving ablation products.

Contents

Measurements of transport properties for most interactions involving ablation products have not been made, particularly at the extremes of temperature and pressure encountered during planetary entry. Thus transport properties must be calculated theoretically. However, most ablation products are polyatomic species and it is difficult to estimate accurately the transport properties for interactions involving polyatomic gases since the interaction potentials are usually either not known or must be crudely estimated.

The peripheral force model has been proposed[1] as a method for obtaining accurate orientation-averaged potentials for interactions involving polyatomic species. This method has been tested[2] for a variety of linear, nonlinear, symmetric, and unsymmetric molecules by comparison with molecular beam data.

The purpose of this synoptic is to demonstrate that the peripheral force method is a useful method for the calculation of ablative transport properties. Other methods are available[3,4] for the estimation of transport properties for interactions involving polyatomic species. However, these methods are either based on the use of universal (nonspecific) collision integrals[3] or assume that all interactions can be accurately represented by the same empirical potential.[4] The advantage of the peripheral force model is that many of the unique properties of a given interaction (such as geometry, bond lengths, and the form of the potential) enter into the calculations. However, the calculations are not significantly more complicated than those required if the less specific methods[3,4] are used.

The transport properties have been calculated for the He–C_2H interaction, using the peripheral force model. Helium is a major constituent of the outer planets and C_2H is an important ablation product. The C_2H species is linear with the geometry[5] C-C-H. This interaction has been chosen to study since there is experimental evidence[1,6] to support the form of the He-C and He-H potentials used in the calculation.

The peripheral force method incorporates the assumption that the interactions between the "free" atom and each atom in the molecule are additive. Also, since the molecule is rotating, the potential should be averaged over all orientations; i.e.,[1]

$$V(\text{atom-molecule})_{av} = \sum V(\text{atom-atom}_m)_{av} \tag{1}$$

where V denotes potential energy, the subscript m indicates that the atom is in the molecule, the subscript av denotes orientation averaging, and the sum is over all atom-atom$_m$ interactions. The averaging procedure takes the form[1]

$$V(\text{atom-atom}_m)_{av} = \frac{1}{4\Pi}\int_0^{\Pi} V(R)2\Pi\sin\theta d\theta \tag{2}$$

where $V(R)$ is the unaveraged atom-atom potential and R is the distance between the atoms. For a repulsive inverse power (RIP) potential; i.e.,

$$V(R) = K/R^s \tag{3}$$

where K and s are empirical parameters, Eq. (2) becomes[1]

$$V(\text{atom-atom}_m)_{av} = \frac{K}{r^s}\frac{[(1+a/r)^{s-2}-(1-a/r)^{s-2}]}{(2a/r)(s-2)(1-a^2/r^2)^{s-2}} \tag{4}$$

where a is the distance from the center of geometry of the molecule to atom$_m$ and r is the distance from the free atom to the center of geometry.

It has been shown[6] that good agreement with molecular beam data is obtained by taking

$$V(R)_{\text{He-H}} = \frac{2.60}{R^{6.80}}\ (\text{ev})$$

$$V(R)_{\text{He-C}} = \frac{13.73}{R^{6.23}}\ (\text{ev}) \tag{5}$$

These results have been used in Eq. (4) along with the values of a determined from the C_2H bond lengths[5] to calculate $V(\text{atom-molecule})_{av}$, which in this case will be denoted $V(r;\text{He-}C_2H)_{av}$, using Eq. (1). The calculation has been done for three cases: 1) It was assumed that He interacts with H and the terminal C atom but not with the central C atom. 2) It was assumed that He interacts with all three atoms in C_2H. 3) It was assumed that He interacts with all three atoms but that interactions with the central C atom are half as frequent as interactions with the two other atoms. The geometry and bond lengths of C_2H lead to a small contribution to V from the interaction of He with the central C atom. Thus the results for V are nearly the same for the three cases. The geometry

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*Visiting Fellow.

Table 1 Potential energy for the He-C_2H interaction

r, Å	$V(r;\text{He-}C_2H)_{av}$, ev	V(RIP), ev
1.85	4.062	3.958
1.90	3.011	3.012
1.95	2.274	2.308
2.00	1.746	1.780
2.05	1.360	1.382
2.10	1.074	1.080
2.15	0.857	0.848
2.18	0.754	0.736

Table 2 Viscosity, $\eta(10^4$ kg/m/s), for the He-C_2H interaction

T, K	Peripheral force	Boushehri et. al.	Esch et. al.
1000	0.297	0.292	0.290
2000	0.481	0.468	0.454
3000	0.638	0.622	0.590
5000	0.910		0.820
10,000	1.47		1.28
15,000	1.95		1.66
20,000	2.39		2.00
25,000	2.79		2.31

corresponding to cases 2 and 3 is shown in Fig. 1 and the values of $V(r;\text{He-}C_2H)_{av}$ for case 2 are shown in the second column of Table 1.

The transport properties depend on the interaction potential. However, the transport collision integrals have been calculated for only a limited number of empirical potentials. The RIP and the exponential repulsive potentials are normally used to represent repulsive interactions such as those obtained for $V(r;\text{He-}C_2H)_{av}$. Both potentials have been best fit to the results for $V(r;\text{He-}C_2H)_{av}$. The RIP potential gives a better fit and the results for case 2 are shown in the third column of Table 1. The fit is very good, using the parameters $K=2165$ and $s=10.25$. Transport collision integrals for the RIP potential are tabulated[7] as functions of K, s, and temperature. The results obtained for the viscosity are shown in the second column of Table 2.

Viscosity (and other transport property) measurements are not available for the He-C_2H interaction. This is true for most interactions involving ablation products. However, the results obtained using the peripheral force model can be compared with the results obtained using the theoretical methods[3,4] mentioned previously. These results are shown in the third and fourth columns of Table 2. In the absence of experimental data, it is not possible to determine which method is most accurate. However, the peripheral force method has the intellectually satisfying feature that it incorporates more of the specific characteristics of the interaction of interest without being significantly more complicated than the other methods.

To recapitulate, the peripheral force method involves the following steps:

1) Choose the form of $V(R)$ that best represents each atom-atom$_m$ interaction. Usually experimental and/or theoretical information makes it possible to choose an empirical form for $V(R)$ which agrees quite well with the accepted potential.

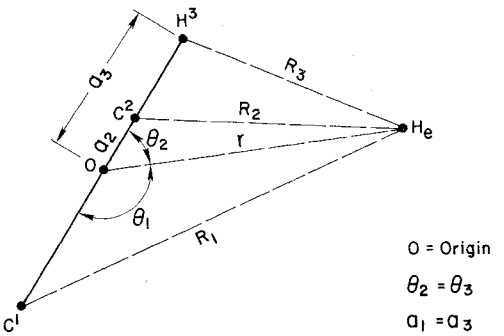

Fig. 1 Coordinate system for the He-C_2H interaction (cases 2 and 3).

2) Integrate Eq. (2) for the chosen $V(R)$ to find the orientation-averaged potential, $V(r;\text{atom-atom}_m)_{av}$.

3) Evaluate $V(r;\text{atom-atom}_m)_{av}$ for each interaction, using the known empirical potential parameters and bond lengths.

4) Sum up the results as shown in Eq. (1).

5) Best-fit the results for $V(\text{atom-molecule})_{av}$ with the most appropriate potential for which collision integrals have been calculated.

6) Evaluate the collision integrals (and the transport properties) as functions of the best-fit parameters and temperature.

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