

Technical Notes

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Analytical Fits for the Determination of the Transport Properties of Air

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Nomenclature

A	= coefficient of $(\ell n T)^3$ in Eq. (1)
$A_n, B_n, b_n, C_n, c_n, D_n$	= parameters for $\Omega_{n,n}^{sc}$
B	= coefficient of $(\ell n T)^2$ in Eq. (1)
C	= coefficient of $(\ell n T)$ in Eq. (1)
D	= zeroth-order term of Eq. (1)
$\log T_n$	= parameter for $\Delta\Omega_{n,n}$
T	= temperature, K
T^*	= reduced temperature, Eq. (4)
t	= temperature variable, Eq. (6b)
U_n, u_n	= parameters for $\Delta\Omega_{n,n}$
X	= $\pi\Omega_{1,1}$, $\pi\Omega_{2,2}$, or B^*
Y_n, W_n, w_n	= parameters for $\Delta\Omega_{n,n}$
$\Delta\Omega_{n,n}(T)$	= partial collision integral, Å ²
λ	= shielding parameter, Bohr
$\Omega_{n,n}(T)$	= transport collision integral, Å ²
$\Omega_{n,n}^{sc}(T)$	= shielded coulomb collision integral, Å ²

Introduction

WE have combined the ab initio results of large-scale molecular structure calculations and measured data to construct accurate potential energy curves^{1–6} for all of the interactions of the atoms and ions of nitrogen and oxygen. The proper long-range interaction forces have been included to allow the calculation of collision integrals^{3–6} for a broad range of temperatures. The scattering phase shifts for the determination of the transport cross sections were calculated from a uniform semiclassical approximation^{3,5} that accounts for the quantum mechanical effects arising from a potential energy barrier.

More recently, we have developed computational methods⁷ to determine the scattering phase shifts from a direct solution of Schroedinger's equation for low-energy applications involving a light collision partner. For collisions involving a hydrogen atom, we have found that corrections to the diffusion and viscosity collision integrals from a full quantum mechanical treatment of the scattering can be appreciable; e.g., rising to about 8 and 4%, respectively, as the temperature decreases

to 100 K. On the other hand, one can conclude from the results of this study,⁷ that the corresponding corrections for collision partners as heavy as the air species of this work would not be significant, i.e., less than the error introduced by the uncertainty in the calculated potential energy data.

Atom–Atom and Atom–Ion Interactions

To facilitate application of our tabulated results for the collision integrals to the determination of transport properties, we have constructed analytical approximations. We have chosen a form used in codes^{8,9} developed for NASA applications; i.e., we adopt the expansion

$$\ell n X = D + C(\ell n T) + B(\ell n T)^2 + A(\ell n T)^3 \quad (1)$$

where X represents the collision integral for diffusion $\Omega_{1,1}$ or viscosity $\Omega_{2,2}$ (multiplied by π as in Refs. 8 and 9) in Å² (10^{-16} cm²), or the quantity B^* obtained from^{10,11}

$$B^* = (5\Omega_{1,2} - 4\Omega_{1,3})/\Omega_{1,1} \quad (2)$$

[In this case, as in Refs. 8 and 9, the last term of Eq. (1) is not used.] The coefficients A – D have been determined from a least-squares fit to the calculated data of Refs. 3–5. Values of coefficients are listed in Tables 1 and 2 for the collision inte-

Table 1 Coefficients of $\ell n(\pi\Omega_{n,n})$ for atom/ion pairs

Pair	n	D	C	B	A
100 K $\leq T \leq 5,000$ K					
N–N	1	7.0962	–1.3024	0.14784	–0.006737
	2	7.0037	–1.2278	0.14039	–0.006538
O–O	1	5.2411	–0.3636	0.00247	0.000232
	2	5.1694	–0.3399	0.00612	–0.000151
N–O	1	5.8428	–0.7601	0.07445	–0.003545
	2	6.0843	–0.9288	0.11270	–0.005863
N ⁺ –N	1	8.0674	–1.0579	0.11346	–0.004534
	2	10.4911	–2.2835	0.27995	–0.013210
O ⁺ –O	1	10.7127	–2.3235	0.29455	–0.012993
	2	13.2224	–3.1600	0.36120	–0.015395
N ⁺ –O	1	11.9930	–2.5881	0.28166	–0.012171
	2	10.1841	–1.7557	0.15359	–0.005525
O ⁺ –N	1	9.3839	–1.3148	0.08011	–0.001514
	2	5.5984	0.4113	–0.17796	0.011150
1,000 K $\leq T \leq 30,000$ K					
N–N	1	5.8357	–0.9011	0.10789	–0.005544
	2	7.2135	–1.2781	0.14276	–0.006464
O–O	1	9.4075	–2.0005	0.21628	–0.009051
	2	10.1214	–2.1995	0.23745	–0.009691
N–O	1	9.3209	–2.0865	0.24250	–0.010620
	2	10.1745	–2.3145	0.26472	–0.011223
N ⁺ –N	1	6.7850	–0.5684	0.05154	–0.001936
	2	16.4097	–4.4319	0.53728	–0.023378
O ⁺ –O	1	6.5348	–0.5757	0.05288	–0.001950
	2	5.7079	–0.4402	0.03706	–0.002682
N ⁺ –O	1	1.2270	1.2238	–0.16112	0.004677
	2	3.6578	0.2917	–0.04636	0.000269
O ⁺ –N	1	12.4370	–2.9705	0.35528	–0.015950
	2	21.4600	–6.1340	0.71601	–0.029254

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Table 2 Coefficients of $\ell n(B^*)$ for atom/ion pairs

Pair	D	C	B
100 K $\leq T \leq 5,000$ K			
N-N	0.8161	-0.2064	0.01532
O-O	0.1772	0.0004	-0.00027
N-O	0.8181	-0.2088	0.01557
N ⁺ -N	0.4232	-0.0899	0.00562
O ⁺ -O	0.5151	-0.1208	0.00794
N ⁺ -O	1.1022	-0.2794	0.02116
O ⁺ -N	1.2316	-0.3061	0.02189
1,000 K $\leq T \leq 30,000$ K			
N-N	0.3210	-0.0595	0.00488
O-O	1.1642	-0.2390	0.01430
N-O	0.9845	-0.2089	0.01326
N ⁺ -N	0.1023	-0.0102	0.00072
O ⁺ -O	0.2386	-0.0432	0.00260
N ⁺ -O	-1.3866	0.3625	-0.01999
O ⁺ -N	-1.3265	0.3249	-0.01657

grals and B^* , respectively. The fit to the calculated collision integrals is accurate to within about 1%.

Corresponding fits to other quantities¹¹ A^*-K^* , that are obtained from the collision integrals and are needed to determine transport coefficients to second order, are available from the authors on request.

Ion-Ion Interactions

We have investigated⁶ the correction to the shielded coulomb collision integrals arising from the application of realistic potential energy curves (that are found to be considerably different than coulomb interactions at small separation distances⁶) for the interaction of the ions of nitrogen and oxygen. We have found that this correction can be significant at higher temperatures and pressures.

We have also developed analytical approximations for the ion-ion collision integrals; for convenience, we include these results here. The diffusion and viscosity collision integrals are obtained from the sum

$$\Omega_{n,n} = \Omega_{n,n}^{\text{sc}} + \Delta\Omega_{n,n} \quad (3)$$

where $\Omega_{n,n}^{\text{sc}}$ is the shielded coulomb collision integral and $\Delta\Omega_{n,n}$ is the correction resulting from the deviations of the calculated potential energies from a coulomb potential energy. Using the reduced temperature

$$T^* = a\lambda T \quad (4)$$

where a is 3.167×10^{-6} , and $\Omega_{n,n}^{\text{sc}}$ can be obtained in \AA^2 from the following expressions:

For small T^* ($0.01 \leq T^* < 4$):

$$\ell n(\Omega_{n,n}^{\text{sc}}/\lambda^2) = -A_n - B_n T^{*b_n} \ell n T^* \quad (5a)$$

For large T^* ($T^* \geq 4$):

$$\frac{\Omega_{n,n}^{\text{sc}}}{\lambda^2} = -\frac{0.140}{T^{*2}} \ell n[D_n T^*(1 - C_n e^{-c_n T^*}) + 1] \quad (5b)$$

The values of the parameters are listed in Table 3. We have found⁶ that the values of $\Omega_{n,n}^{\text{sc}}$ from relations in Eq. (5) agree with the calculated results to within about 1%. For high-temperature applications ($\log T \geq 4.5$), $\Delta\Omega_{n,n}$ can be obtained in \AA^2 from

$$\Delta\Omega_{n,n} = Y_n + W_n t^2 e^{-w_n t^2} - U_n (\lambda^{-1} - 0.05)(t - u_n) \quad (6a)$$

Table 3 Parameters of Eqs. (5) for $\Omega_{n,n}^{\text{sc}}$

n	A _n	B _n	b _n
0.01 $\leq T^* < 4$			
1	2.671	1.165	0.0860
2	2.375	1.188	0.0928
n	C _n	c _n	D _n
$T^* \geq 4$			
1	0.138	0.0106	0.765
2	0.157	0.0274	1.235

Table 4 Parameters of Eqs. (6) for $\Delta\Omega_{n,n}$ for ion-ion pairs

Pair	n	log T _n	Y _n	w _n	W _n	u _n	U _n
log T ≥ 4.5							
N ⁺ -N ⁺	1	4.2	-0.154	0.653	0.86	1.10	1.2
	2	4.3	-0.270	0.848	1.58	0.95	1.6
O ⁺ -O ⁺	1	4.2	-0.088	0.728	1.24	1.05	1.8
	2	4.3	-0.146	0.939	2.14	0.90	2.2
N ⁺ -O ⁺	1	4.4	-0.036	0.898	0.95	0.90	0.6
	2	4.5	-0.097	1.278	1.83	0.75	0.6

where

$$t = \log T - \log T_n \quad (6b)$$

The values of the parameters are listed in Table 4 for the various ion-ion interactions.

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Matching Solutions for Unsteady Conduction in Simple Bodies with Surface Heat Fluxes

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Nomenclature

- k = thermal conductivity
 L = slab semithickness or radius of cylinder and sphere
 q_s = uniform surface heat flux
 T = temperature
 t = temporal variable
 X, X' = dimensionless x, x' ; $x/L, x'/L$
 x = space variable measured from the center
 x' = space variable measured from the surface,
 $x + x' = L$
 α = thermal diffusivity
 τ = dimensionless $t, \alpha t/L^2$
 ϕ = dimensionless $T, k(T - T_i)/q_s L$

Introduction

AMONG the arsenal of analytical methods of solution for the treatment of unsteady state heat conduction in simple coordinate systems, the method of separation of variables is by far the most commonly adopted in literature on conduction heat transfer. However, its step-by-step implementation presents inconveniences on some occasions, especially when the partial differential equation and/or the boundary conditions involve nonhomogeneities. Under these circumstances utilization of other solution techniques are more appropriate and sometimes become indispensable. In principle, the method of separation of variables leads to an exact infinite series that is conveniently simplified to an approximate one-term of series solution for practical applications. The latter provides the so-called long-time solution and serves to generate different versions of temperature-time charts that are applicable to the cooling of simple bodies with convective surfaces.

The central objective of the present study is twofold. First, to establish a definite region of validity of the venerable one-term of series solution for simple bodies exposed to a uniform surface heat flux. Second, to supplement this simplified solution with an optional technique having physical roots, i.e., the semi-infinite body solution. The latter, supposedly may permit a faster and more precise calculation for the temperature re-

sponse of simple bodies for short times. Evaluation of the compact semi-infinite body solution involving one or two terms only may be carried out by hand. To the author's knowledge the literature does not contain information pertinent to the previously cited objectives.

Mathematical Formulation

At $t = 0$, q_s is suddenly applied at the surface $x = L$ of a simple body (slab, cylinder, sphere) with constant thermophysical properties. These bodies possess a uniform temperature T_i for $t < 0$. The one-dimensional, transient heat conduction equation, along with the initial and boundary conditions, are

$$\frac{\partial \phi}{\partial \tau} = \frac{\partial^2 \phi}{\partial X^2} + \frac{c}{X} \frac{\partial \phi}{\partial X} \quad (1)$$

where the parameter c becomes 0 (slab), 1 (cylinder), and 2 (sphere).

$$\phi(X, 0) = 0 \quad (2a)$$

$$\frac{\partial \phi}{\partial X}(0, \tau) = 0 \quad (2b)$$

$$\frac{\partial \phi}{\partial X}(1, \tau) = 1 \quad (2c)$$

Method of Separation of Variables

This method constitutes the baseline solution. As is customarily done, the superposition of functions

$$\phi(X, \tau) = f_1(\tau) + f_2(X) + f_3(X, \tau) \quad (3)$$

can eliminate the ensuing difficulty arising from the nonhomogeneous boundary condition of Eq. (2c). Thus, the series solutions, $\phi(X, \tau)$, and the characteristic values μ_n are found in Luikov¹:

Slab:

$$\phi(X, \tau) = \tau - \frac{1}{2} \left(\frac{1}{3} - X^2 \right) - 2 \sum_{n=1}^{\infty} \frac{(-1)^n}{\mu_n^2} \cos(\mu_n X) e^{-\mu_n^2 \tau} \quad (4)$$

where $\mu_n = n\pi$, $n = 1, 2, 3 \dots$

Cylinder:

$$\phi(X, \tau) = 2\tau - \frac{1}{4} (1 - 2X^2) - \sum_{n=1}^{\infty} \frac{2}{\mu_n^2 J_0(\mu_n)} J_0(\mu_n X) e^{-\mu_n^2 \tau} \quad (5)$$

where $J_0'(\mu_n) = J_1(\mu_n)$, $n = 1, 2, 3 \dots$

Sphere:

$$\phi(X, \tau) = 3\tau - \frac{1}{2} \left(\frac{3}{5} - X^2 \right) - 2 \sum_{n=1}^{\infty} \frac{1}{\mu_n \cos \mu_n} \frac{\sin(\mu_n X)}{\mu_n X} e^{-\mu_n^2 \tau} \quad (6)$$

where $\tan \mu_n = \mu_n$, $n = 1, 2, 3 \dots$

It is widely known that the pressing characteristic of the preceding infinite series is that they tend to converge rapidly for long times. The mere presence of only one term in the series suffices to produce acceptable results. On the contrary, these infinite series show severe divergence patterns for short times even when many terms are present. The behavior becomes so abnormal that the numerical evaluation of the one-term of series solution does not meet the initial condition [Eq. (2a)]. In fact, for very short times the local temperatures consistently overpredict the initial condition in contraposition with

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