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Collision Integrals of High-Temperature Air Species

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Collision integrals (transport cross sections) of air species in the temperature range 50–100,000 K have been calculated by using experimental and theoretical informations on potential energy curves and cross sections. The results for the different interactions (neutral–neutral, neutral–parent ion, electron–neutral) have been compared with old and recent calculations obtaining, in general, a satisfactory agreement. Finally analytical forms for fitting and interpolating the present numerical results are reported.

Nomenclature

b	= impact parameter
C	= parameter entering in the Morse potential
C_v	= internal specific heat
D	= binary diffusion coefficient
d	= Debye length
e	= electron charge
M	= molecular weight
p	= pressure
p_n	= statistical weight
$Q(\varepsilon, \Theta)$	= differential cross section
$Q^{(l)}$	= transport cross section of l order
r_c	= classical turning point
re	= equilibrium distance
S_{ex}	= charge-transfer cross section
T	= gas temperature
v	= relative velocity
Z	= ion charge
α	= polarizability
δ_n	= phase shift
ε	= relative energy
η	= viscosity
Θ	= deflection angle
λ_{int}	= internal thermal conductivity
λ_t	= translational thermal conductivity
ρ	= mass density
σ	= parameter entering in the potentials
$\Phi(r)$	= interaction potential
ϕ_0	= parameter entering in the potentials
$\Omega^{(1,s)}$	= collision integral of l, s order (Å^2)

I. Introduction

TRANSPORT properties of high-temperature air species are of paramount importance for understanding nonequilibrium plasma flows. Many calculations have been performed in the last 30 years. These calculations that include the famous Yos tables and the refined Gupta et al. tables have been reviewed by some of us in a recent paper.[1] Here we have discussed the accuracy of old and new calculations, giving also the strategy of future improvements.

In the present paper we report our consequent recent effort to tabulate collision integrals (transport cross sections) and related transport coefficients for air species in a wide temperature range ($50 < T < 100{,}000$ K). In doing so we were aware of the existence of recent calculations performed by different groups.[2–6] The existence of these new calculations allows us also to judge the accuracy of our results as well as in general the degree of confidence of the existing tabulations.

II. Collision Integrals

Accurate calculations of transport coefficients can be obtained once the collision integrals (transport cross section) of the different interactions are known.[7]

These quantities can be obtained by performing three integrations. The first one determines the classical deflection angle $\Theta(b, E)$ as a function of impact parameter b and relative energy E:

$$\theta(b, \varepsilon) = \pi - 2b \int_{r_c}^{\infty} \mathrm{d}r \Big/ \left[F(r, b, \varepsilon)\right]^{\frac{1}{2}} / r^2 \tag{1}$$

where the classical turning point or distance of closest approach r_c is the outermost root of

$$F(r, b, \varepsilon) = 1 - b^2/r^2 - \Phi(r)/\varepsilon \tag{2}$$

where $V(r)$ is the interaction potential.

A further averaging over the impact parameter b yields the relevant cross section

$$Q^{(1)}(\varepsilon) = 2\pi \{1 - [1 + (-1)^1]/2/(l + 1)\}^{-1} \times \int_0^{\infty} \mathrm{d}b[b(1 - \cos^1 \theta)] \tag{3}$$

and the preceding quantities can in turn be employed for a further energy averaging that produces the collision integrals as a function of temperature:

$$\Omega^{(1,s)}(T) = \frac{4(l + 1)}{(s + 1)![2l + l - (-1)^1]} \frac{1}{2kT} \times \int_0^{\infty} \mathrm{d}\varepsilon \left(\frac{\varepsilon}{kT}\right)^{s+1} Q^{(1)}(\varepsilon) \exp\left(-\frac{\varepsilon}{kT}\right) \tag{4}$$

The problem of calculating $\Omega^{(1,s)}$ therefore reduces to the knowledge of $\Phi(r)$. For many interaction forms (Morse, exponential repulsive, Lennard–Jones) the collision integrals are tabulated so that the knowledge of relevant parameters is sufficient to obtain the collision integrals. For other important interactions (electron–atom, electron–molecule, resonant charge transfer) in general, we know the diffusion cross section so that we can directly integrate Eq. (4) to obtain the collision integrals.

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Apparently we have all of the ingredients for calculating the transport properties of high-temperature gases. Difficulties however arise for the lack of informations (both theoretical and experimental) about $\Phi(r)$ in the whole internuclear distance range r. Fortunately the collision integrals are the result of three average procedures so that their values do not dramatically depend on $\Phi(r)$. Once the collision integrals are obtained, the calculation of transport coefficients of single species is straightforward. The following equations are used[7]:

$$(\lambda_t)_{ij} = 1989.1 \times 10^{-7}[T(M_i + M_j)/(2M_iM_j)]^{\frac{1}{2}} / \Omega^{(2,2)}_{i,j} \quad (5)$$

$$(\lambda_{\text{int}})_i = \rho D_{i,i} C_{vi} / M_i \quad (6)$$

$$(\eta)_{ij} = 266.93 \times 10^{-7}[2TM_iM_j/(M_i + M_j)]^{\frac{1}{2}} / \Omega^{(2,2)}_{i,j} \quad (7)$$

$$(D)_{ij} = 0.002628\left[T^3(M_i + M_j)/(2M_iM_j)\right]^{\frac{1}{2}} / p\Omega^{(2,2)}_{i,j} \quad (8)$$

All of the collision integrals have been divided by π.

III. Main Interactions

In a high-temperature environment different species can survive depending on the considered temperature range. As an example, let us consider an atmospheric nitrogen plasma under equilibrium conditions. The following equilibria can be envisaged:

$$N_2 \leftrightarrow 2N, \qquad 5000 < T < 10{,}000\,K$$

$$N \leftrightarrow N^+ + e, \qquad 10{,}000 < T < 20{,}000\,K$$

$$N^+ \leftrightarrow N^{++} + e, \qquad 20{,}000 < T < 30{,}000\,K$$

$$N^{++} \leftrightarrow N^{+++} + e, \qquad 30{,}000 < T < 50{,}000\,K$$

$$N^{+++} \leftrightarrow N^{++++} + e, \qquad 50{,}000 < T < 100{,}000\,K$$

This means that we pass from a low-temperature system, where molecules and atoms coexist, to a high-temperature one where electron, atom, and parent ion survive ending to a temperature range in which only ions and electrons exist.

We will examine the different interactions tabulating the results for the species N_2, N_2^+, N, N^+, N^{++}, N^{+++}, N^{++++}, O_2, O_2^+, O_2^-, O, O^-, O^+, O^{++}, O^{+++}, O^{++++}, NO, NO^+, e. Special emphasis is given in this paper to the interactions between majority species.

A. Nitrogen

1. Dissociation Range

$$N_2\text{–}N_2,\ N_2\text{–}N,\ N\text{–}N$$

For the interactions N_2–N_2 and N–N_2 we use an exponential repulsive form:

$$\Phi(r) = \varphi_0 \exp(-r/\rho) \quad (9)$$

the parameters of which are essentially taken from the experimental beam studies of Leonas[8] for $T > 2000$ K and a Lennard–Jones potential

$$\Phi(r) = 4\varphi_0[(\sigma/r)^{12} - (\sigma/r)^6] \quad (10)$$

for $T < 1000$ K. Results for $1000 < T < 2000$ K are then obtained by smoothly linking the two sets of data. The parameters used for the relevant potentials, based on Refs. 6–12, as well as on combination rules (c.r.), have been reported in Tables 1 and 2.

A comparison of the present calculations with experiments for η and λ in pure nitrogen[7] is reported in Tables 3 and 4 for the low-temperature region. A good agreement is observed between calculated and experimental values for both η and λ. A similar satisfactory agreement has been found for $T > 2000$ K (Ref. 1), where the exponential repulsive potential has been used.

The experimental situation for N–N_2 is very scanty. For $T > 2000$ K the collision integrals calculated in the present work are in satisfactory agreement with other selection of potentials.[1] The diffusion coefficient calculated in the present work for $T = 300$ K ($D_{N\text{–}N_2} = 0.30$ cm^2 s^{-1}) is not so far from the experimental value of Ref. 13 at $T = 298$ K ($D_{N\text{–}N_2} = 0.37$ cm^2 s^{-1}). Collision integrals and transport coefficients for the interaction N–N have been obtained by averaging the contributions coming from the $^1\Sigma$, $^3\Sigma$, $^5\Sigma$, and $^7\Sigma$ potentials (bound and repulsive). The collision integrals of multipotential interaction are an average of the different potentials with statistical weights p_n equal to the spin multiplicity for Σ states and to two times the spin multiplicity for Π, Δ, ... states

Table 1 Parameters (ϕ_0, eV; σ, Å) appearing in the Lennard–Jones potentials of neutral–neutral interactions

Process	$10^2\ \phi_0$, eV	σ, Å	Reference
N–N	1.027	2.980	c.r.
O–O	1.009	2.800	9
N_2–N_2	0.7884	3.681	6
N_2–N	0.900	3.330	10
N_2–O_2	0.8776	3.557	6
N_2–O	0.9183	3.050	11
N_2–NO	0.9405	3.600	6
N–O_2	1.001	3.206	c.r.
N–O	1.017	2.884	c.r.
N–NO	1.017	3.236	c.r.
O_2–O_2	0.9759	3.433	7
O_2–O	0.9246	3.011	11
O_2–NO	0.9621	3.479	12
O–NO	1.0384	3.150	9
NO–NO	1.006	3.492	12

Table 2 Parameters (ϕ_0, eV; ρ, Å) appearing in the repulsive potentials of neutral–neutral interactions

Process	$10^4\ \phi_0$, eV	ρ, Å	Reference
N_2–N_2	0.2290	3.160	8
N_2–N	0.062	3.310	8
N_2–O_2	0.1430	3.020	8
N_2–O	1.135	5.120	8
N_2–NO	0.5780	3.610	8
N–O_2	0.387	4.130	8
N–O	0.0348	3.41	6
N–NO	0.5333	4.21	8
O_2–O_2	0.0820	2.850	8
O_2–O	1.025	4.850	8
O_2–NO	0.762	3.780	8
O–NO	0.314	3.950	8
NO–NO	0.216	3.260	8

Table 3 Comparison between calculated and experimental[7] viscosities ($\eta \times 10^7$ g cm^{-1} s^{-1}) in pure nitrogen

T, K	η (calculated)	η (experimental)*
100	686	698
200	1293	1295
300	1778	1786
800	3503	3493
1000	4055	4011

Table 4 Comparison between calculated and experimental[31] total thermal conductivity ($\lambda \times 10^5$ cal cm^{-1} s^{-1} K^{-1}) of pure nitrogen

T, K	λ (calculated)	λ (experimental)*
300	6.39	6.13
500	9.34	9.16
1000	16.3	15.7
2000	30.3	26.3

Table 5 Parameters for potentials for atom–atom interaction N (^{4}S)+N (^{4}S)

State	C	ϕ_0, eV	ρ (or σ), Å	p_n	Reference
$^1\Sigma g^+$	2.33	9.904	0.837	1	13
$^3\Sigma g^+$	2.92	3.679	1.046	3	13
$^5\Sigma g^+$	9.10	0.1362	1.44	5	13
$^7\Sigma g^+$	——	5572.0	0.240	7	14

Table 6 Collision integrals diffusion type calculated in the present work (column a) and in Refs. 2 and 3 (column b)

T, K	N–N (a)	N–N (b)	100[(a − b)/a]
250	9.39	8.49	9.6
500	7.76	7.03	9.4
1,000	6.79	5.96	12.2
2,000	5.25	5.15	1.9
5,000	4.27	4.14	3.0
10,000	3.55	3.37	5.1
15,000	3.11	2.92	6.1
20,000	2.81	2.62	6.8
50,000	2.00	1.77	11.5
100,000	1.58	1.27	19.6

$$\langle \Omega^{(1,s)} \rangle = \frac{\sum_n p_n \Omega_n^{(1,s)}}{\sum_n p_n} \tag{11}$$

The bound states have been treated according to a Morse potential

$$\Phi(r) = \varphi_0\{\exp[-2(C/\sigma)(r - r_e)] - 2\exp[-(C/\sigma)(r - r_e)]\} \tag{12}$$

whereas the repulsive ones have been treated according to Eq. (9). The parameters of the different potentials have been reported in Table 5.

For $T < 1000$ K we have used a Lennard–Jones potential, with parameters estimated using the combination rules between the values of N_2–N_2 and N–N_2 reported in Table 1. Large discrepancies still exist in the Lennard–Jones parameters for N–N interaction as can be understood by comparing the relevant values from different sources.[9,14–16] A comparison of the present results with those of Levin et al.[2,3] (see Table 6) shows a good agreement particularly in the temperature range (5000–20,000 K; pressure: 1 atm) in which N atoms are the predominant species.

2. Partial Ionization Range

Ion–neutral nonresonant collisions. Collision integrals for these interactions have been calculated by using a polarizability model. In this case the collision integrals assume a closed form given by

$$\Omega^{(1,1)}(T) = 425.4Z(\alpha)^{\frac{1}{2}}/T^{\frac{1}{2}} \tag{13}$$

$$\Omega^{(1,2)}(T) = 0.8333\Omega^{(1,1)}(T) \tag{14}$$

$$\Omega^{(1,3)}(T) = 0.7292\Omega^{(1,1)}(T) \tag{15}$$

$$\Omega^{(2,2)}(T) = 0.8710\Omega^{(1,1)}(T) \tag{16}$$

where $Z = 1$ for monocharged ions and so on and α is the polarizability. The values of polarizibilities (A^3) of the different neutral species[17] are as follows: N_2, 1.76; O_2, 1.60; NO, 1.70; N, 1.13; and O, 0.77.

Equations (13–16) have been used for all ion-nonparent neutral interactions but for N^+–O and N–O^+ interactions. In this case the recent results of Refs. 18 and 19 can be confidently used. The transport coefficients assume the closed form

$$(\lambda_t)_{ij} = 5.37 \times 10^{-7} T[(M_i + M_j)/(2M_iM_j)]^{\frac{1}{2}}/Z/(\alpha)^{\frac{1}{2}} \tag{17}$$

$$(\eta)_{ij} = 1.02 \times 10^{-7} T[(M_iM_j)/(M_i + M_j)]^{\frac{1}{2}}/Z/(\alpha)^{\frac{1}{2}} \tag{18}$$

$$(D)_{ij} = 6.177 \times 10^{-6} T^2[(M_i + M_j)/(2M_iM_j)]^{\frac{1}{2}}/p/Z/(\alpha)^{\frac{1}{2}} \tag{19}$$

Table 7 Parameters of the potentials for atom–ion interaction N(^{4}S)–N^+(^{2}P)

State	C	ϕ_0, eV	ρ (or σ), Å	p_n
$^2\Sigma g^+$	2.30	8.73	0.85	2
$^2\Sigma u^+$	3.26	5.56	0.887	2
$^2\Pi g$	2.94	2.35	1.186	4
$^2\Pi u$	2.24	7.61	0.904	4
$^4\Sigma g^+$	0.00	302.0	0.365	4
$^4\Sigma u^+$	4.60	3.4	1.000	4
$^4\Pi g$	2.32	1.0	1.054	8
$^4\Pi u$	0.00	199.0	0.408	8
$^6\Sigma g^+$	0.00	367.0	0.406	6
$^6\Sigma u^+$	0.00	894.0	0.380	6
$^6\Pi g$	0.00	693.0	0.415	12
$^6\Pi u$	0.00	341.0	0.429	12

Table 8 Collision integrals viscosity type calculated in the present paper (column a) and in Refs. 18 and 19 (column b)

T, K	N–N^+ (a)	N–N^+ (b)	100[(a − b)/a]
250	15.3	20.7	−35.3
2,000	9.55	10.55	−10.5
5,000	6.90	7.75	−12.3
10,000	5.79	5.86	−1.2
15,000	4.99	4.67	6.4
20,000	4.46	3.88	13.0
50,000	2.93	2.04	30.3
100,000	2.07	1.33	35.7

Ion–neutral resonant collisions.

N–N^+

In this case we must distinguish the collision integrals diffusion type from the corresponding viscosity one. The firsts are dominated by the charge exchange process, whereas the seconds (viscosity type) are dominated by valence forces, even though at low temperature polarizability forces should be taken into account.

Let us first consider viscosity-type collision integrals for N–N^+. We should treat this interaction as in the multipotential atom–atom case. The interaction of ground state atom–ion interaction N(^{4}S)–N^+(^{3}P) occurs through 12 potential curves ($^{2,4,6}\Sigma_{g,u}$; $^{2,4,6}\Pi_{g,u}$ states). Morse and repulsive potentials for the different interactions have been used, the parameters of which, taken from Ref. 20, have been reported in Table 7.

A comparison of the present results with those calculated by Stallcop et al.[21] (see Table 8) shows a satisfactory agreement (differences not exceeding 15%) in the temperature range (5000–20,000 K) in which the concentration of these species is important. Larger differences (up to 35%) are observed outside this temperature range when nitrogen atoms become a minority species.

The collision integrals diffusion type has been obtained by the usual approximation on the diffusion cross section Q^1 dominated by charge transfer. We write

$$Q^1 = 2S_{ex} \tag{20}$$

where S_{ex} is the cross section relative to the process

$$A + A^+ \rightarrow A^+ + A$$

The collision integrals diffusion type therefore assumes the following form:

$$\Omega^{(1,1)}(T) = (kT)^{-3} \int_0^\infty d\varepsilon Q^{(1)}(\varepsilon)\varepsilon^2 \exp\left(-\frac{\varepsilon}{kT}\right) \tag{21}$$

which can be easily integrated once $S_{ex}(\varepsilon)$ is known.

Table 9 C and D values for resonant charge transfer

Process	C	D	Reference
N_2–N_2^+	24.5	1.032	47
O_2–O_2^+	24.05	1.132	47
O_2–O_2^-	14.05	0.572	47
NO–NO^+	23.61	1.095	47
N–N^+	26.61	1.27	22
O–O^+	19.5	0.832	34
O–O^-	36.22	1.744	34

Table 10 Collision integrals diffusion type calculated in the present paper (column a) and in Ref. 21 (column b)

T, K	N–N^+ (a)	N–N^+ (b)	100[(a − b)/a]
250	43.8	41.8	4.5
2,000	34.5	31.8	7.8
5,000	30.7	28.4	7.5
10,000	28.1	26.2	6.7
15,000	26.5	24.9	6.0
20,000	25.5	24.0	5.9
50,000	22.3	21.0	5.8
100,000	20.0	19.0	5.0

Numerous theoretical and experimental charge-transfer cross sections have been reported in the literature.[1] The dependence of the charge-transfer cross section on relative velocity v is given by

$$S_{ex} = (C - D \ln v)^2/2 \tag{22}$$

Tabulated values of collision integrals diffusion type (see Appendix) have been obtained by inserting Eq. (22) in Eq. (21), with parameters C and D calculated from the experimental charge-transfer measurements of Belyaev et al.[22] Table 9 reports the relevant C and D values for all resonant interactions together with the sources of charge-transfer cross sections.

A comparison of the present calculations and the theoretical ones of Stallcop et al.[21] (Table 10) shows differences not exceeding 8%.

Inclusion of the polarizability contribution in the collision integrals diffusion type, as indicated in Ref. 4, increases the relevant values in the low-temperature regime. In this case the collision integrals diffusion type assumes the following form:

$$\Omega^{(1,1)}(T) = \left[\Omega_{ct}^{(1,1)^2}(T) + \Omega_p^{(1,1)^2}(T)\right]^{\frac{1}{2}} \tag{23}$$

where subscripts ct and p refer, respectively, to charge transfer and polarizability contributions:

N_2–N_2^+

Collision integrals diffusion type for this interaction has been calculated by charge-transfer cross sections, whereas collision integrals viscosity type has been calculated by using a polarizability model (see Table 9 for the relevant parameters).

3. Electron Neutral Interaction

The e–N, e–N_2 interactions are described as follows. Collision integrals for e-atom/molecule interactions have been calculated by numerical integration of the relevant cross sections by using Eq. (4), where $Q^{(1)}$ and $Q^{(2)}$ are the $l = 1$ (momentum transfer) and $l = 2$ viscosity cross section, respectively:

$$Q^{(1)}(\varepsilon) = 2\pi \int_0^{\pi} (1 - \cos^1 \vartheta) Q(\varepsilon, \vartheta) \sin \vartheta \, d\vartheta \tag{24}$$

As concerning nitrogen molecules, we have used the momentum transfer cross section reported by Phelps and Pitchford.[23] This cross section has been linearly interpolated using a 1000-point mesh in the energy range (0 ÷ 20 kT), the same used for numerical integration.

Table 11 Comparison between collision integrals diffusion type for e–N_2 interaction calculated in the present work (column a), in Ref. 27 (column b), and in Refs. 4 and 5 (column c)

T, K	e–N_2 (a)	e–N_2 (b)	e–N_2 (c)
5,000	4.30	3.06	4.32
10,000	5.43	3.62	5.41
15,000	5.03	4.46	4.98
20,000	4.53	5.61	4.46

Table 12 Comparison between collision integrals diffusion type for e–N interaction calculated in the present work (column a), in Ref. 27 (column b), and in Refs. 4 and 5 (column c)

T, K	e–N (a)	e–N (b)	e–N (c)
5,000	0.66	1.59	0.85
10,000	0.91	1.59	1.20
15,000	1.04	1.59	1.43
20,000	1.11	1.59	1.59

To calculate $Q^{(2)}$, we have corrected for the ratio $Q^{(2)}/Q^{(1)}$ expressed in terms of coefficients of the development of the differential cross section into spherical harmonics, i.e.,

$$\frac{Q^{(2)}(\varepsilon)}{Q^{(1)}(\varepsilon)} = \frac{10a_1 - 2a_3}{15a_1 - 5a_2}, \qquad Q(\varepsilon, \vartheta) = \sum_n a_n(\varepsilon) P_n(\cos \vartheta) \tag{25}$$

The coefficients a_n as a function of energy are interpolated from the set of Chandra and Temkin.[24] An additional value of $Q^{(2)}/Q^{(1)}$ for $\varepsilon = 100$ eV has been added by integrating the corresponding differential cross section of Shyn et al.[25]

In the case of e–N, the momentum transfer cross section is the one used by Capitelli and Devoto.[16] In this case we have corrected for the ratio $Q^{(2)}/Q^{(1)}$ by using phase shifts according to

$$\frac{Q^{(2)}(\varepsilon)}{Q^{(1)}(\varepsilon)} = \frac{\sum_j [(j+1)(j+2)/(2j+3)] \sin^2(\delta_j - \delta_{j+2})}{\sum_j (j+1) \sin^2(\delta_j - \delta_{j+1})} \tag{26}$$

where the phase shifts δ_n as a function of ε are interpolated from the set calculated by Thompson.[26]

A comparison of the present results with those of Refs. 4 and 27 has been reported in Tables 11 and 12. Inspection of these tables shows an excellent agreement with the results of Murphy for e–N_2 system and a satisfactory agreement with the same author for e–N interaction. The agreement is worse with the calculations of Gupta et al., who used a rigid sphere approach. Future experimental and theoretical improvement of the momentum transfer cross section for e–N is welcome to improve the relevant collision integrals.

4. Ion–Ion and Electron–Electron

For these interactions we use the screened Coulomb potential written as

$$\Phi(r) = (e^2/r) \exp[-(r/d)] \tag{27}$$

where d is the Debye length. Collision integrals for this interaction are known either in tabular form[28] or approximated with closed forms of the type[29]

$$\Omega^{(1,s)} = [4/s(s+1)] b_0^2 \left[\ln \Lambda - \tfrac{1}{2} - 2\gamma + z(s)\right] \tag{28}$$

$$\Omega^{(2,s)} = [12/s(s+1)] b_0^2 [\ln \Lambda - 1 - 2\gamma + z(s)] \tag{29}$$

where $\Lambda = 2d/b_0$ is the ratio between the Debye length and the average closest-impact parameter:

$$b_0 = \frac{e^2}{2kT} \left[\gamma = 0.577; z(s) = \sum_{n=1}^{s-1} \frac{1}{n}\right]$$

To the predominant $\ell n\ \Lambda$ term, these formulas give the same results as those derived by Spitzer,[30] using a different approach. Equations (28) and (29) can be easily calculated once Λ is known, which in turn depends on the concentration of charged particles.

5. Minor Interactions

Minor interactions such as N–N^{++}, N–N^{+++}, N_2–N^+, N_2–N^{++}, N_2–N^{+++} N_2–N^{++++}, N–N^{++}, N–N^{+++}, N_2–N^{++++} occur very seldom so that their calculation can be done according to the polarizability model for both collision integrals diffusion and viscosity type. Equations (13–19) can therefore be used.

B. Oxygen

We are considering the following species O_2, O_2^+, O, O^+, O^{++}, O^{+++}, O^{++++} and e, like in the nitrogen system, plus the negative species O_2^- and O^-.

1. Dissociating Range

$$O_2\text{–}O_2,\ O_2\text{–}O,\ O\text{–}O$$

For the interactions O_2–O_2 and O–O_2 we use, as in the nitrogen case, an exponential repulsive potential for $T > 2000$ K and a Lennard–Jones potential for $T < 1000$ K. Results for $1000 < T < 2000$ K are then obtained by smoothly linking the two sets of data. The parameters used for the relevant potentials have been reported in Tables 1 and 2.

A comparison of the present calculations with corresponding results from Refs. 4 and 5 is reported in Table 13. Differences up to 10 and 30% are respectively found for O_2–O_2 and O_2–O interactions. The diffusion coefficient of O–O_2 calculated in the present work (0.34 $cm^2\ s^{-1}$) is in good agreement with the experimental value (0.30 $cm^2\ s^{-1}$) reported in Ref. 31 for $T = 300$ K.

Collision integrals for the interaction O–O have been obtained by averaging the contributions coming from the different potentials (bound and repulsive) as in the nitrogen case. The parameters of the 18 different potentials arising in the interaction $O(^3P)$–$O(^3P)$, taken from Ref. 32, have been reported in Table 14. For $T < 1000$ K we have used a Lennard–Jones potential. Table 15 shows a comparison with the recent calculations of Levin et al.[2,3] The agreement is rather satisfactory.

Table 13 Collision integrals viscosity type calculated in the present work (columns a) and in Refs. 4 and 5 (columns b) for O_2–O_2 and O_2–O interactions

	O_2–O_2		O_2–O	
T, K	a	b	a	b
300	12.67	13.79	9.6	9.78
500	11.20	11.93	8.52	9.00
1,000	9.90	10.33	7.55	7.98
2,000	9.15	9.12	5.31	7.02
5,000	7.28	7.72	4.47	5.85
10,000	6.00	6.62	3.88	5.04

Table 14 Parameters for potentials for atom–atom interaction: $O(^3P)$–$O(^3S)$

State	C	ϕ_0, eV	ρ (or σ), Å	p_n
$X\ ^3\Sigma g^-I$	3.346	3.810	1.077	3
$a^1\Delta g$	3.582	2.81	1.115	2
$b^1\Sigma g^+I$	3.636	2.44	1.126	1
$c^1\Sigma u^-I$	5.105	0.90	1.374	1
$C^3\Delta uI$	7.798	0.67	1.424	6
$A^3\Sigma u^+I$	6.523	0.61	1.411	3
$^1\Sigma g^+II$	0.000	1040.0	0.300	1
$^3\Sigma u^+II$	0.000	803.0	0.312	3
$^5\Sigma g^+I$	0.000	3414.0	0.235	5
$^5\Sigma g^+II$	0.000	4856.0	0.243	5
$^5\Sigma u^-$	0.000	1649.0	0.251	5
$^1\Pi gI$	0.000	587.0	0.296	2
$^1\Pi uI$	0.000	821.0	0.273	2
$^3\Pi gI$	0.000	158.0	0.365	6
$^3\Pi uI$	0.000	427.0	0.289	6
$^5\Pi g$	0.000	5367.0	0.197	10
$^5\Pi u$	0.000	4551.0	0.226	10
$^5\Delta g$	0.000	3527.0	0.233	10

2. Partial Ionization Range

Ion–parent atom is

$$O\text{–}O^+$$

Again we distinguish the collision integrals diffusion type from the corresponding viscosity one. The firsts are dominated by the charge exchange process, whereas the seconds (viscosity-type) are dominated by valence forces, even though at low temperature polarizability forces should be taken into account.

Let us first consider viscosity-type collision integrals for O–O^+. We should treat this interaction as in the multipotential atom–atom case. The interaction of ground state atoms $O(^3P)$–$O^+(^4S)$ occurs through 12 potential curves ($^{2,4,6}\Sigma\, g,u$; $^{2,4,6}\Pi g,u$ states). Morse and repulsive potentials for the different interactions have been used. The relevant parameters, obtained from the potentials of Ref. 33, have been reported in Table 16.

The collision integrals diffusion type has been obtained by the usual approximation on the diffusion cross section Q^1 dominated by charge transfer. The parameters C and D, necessary for the calculations, have been obtained by fitting the experimental charge transfer cross sections of Ref. 34.

A good agreement for both collision integrals diffusion and viscosity type has been found with the calculations of Refs. 18 and 19

Table 15 Comparison between collision integrals diffusion type for O–O interaction calculated in the present work (column a) and in Refs. 2 and 3 (column b)

T, K	(a)	(b)	(a − b)/a
250	8.23	9.03	9.7
500	6.82	7.28	6.7
1,000	5.98	5.89	1.5
2,000	4.76	4.84	1.7
5,000	3.81	3.76	1.3
10,000	3.12	3.05	2.2
15,000	2.74	2.65	3.3
20,000	2.50	2.39	4.8
50,000	1.82	1.64	9.8
100,000	1.42	1.17	17.6

Table 16 Parameters for potentials for atom–ion interaction: $O(^3P)$–$O^+(^4S)$

State	C	ϕ_0, eV	ρ (or σ), Å	p_n
$^2\Sigma g^+$	0.00	512.2	0.224	2
$^6\Sigma g^+$	0.00	695.6	0.361	6
$^4\Sigma u^+$	0.00	1433.3	0.215	4
$^6\Pi g$	0.00	3123.0	0.219	12
$^6\Pi u$	0.00	853.8	0.307	12
$^2\Pi g$	1.83	6.21	0.880	4
$^4\Pi g$	4.86	1.09	1.460	8
$^2\Pi u$	1.78	1.61	1.020	8
$^4\Pi u$	3.50	2.60	1.150	8
$^6\Sigma\ ^+g$	3.30	0.83	1.45	4
$^2\Sigma u^+$	3.17	0.39	1.430	2
$^6\Sigma\ ^+u$	3.44	1.15	1.480	6

Table 17 Comparison between collision integrals diffusion and viscosity type for O–O^+ interaction calculated in the present work (columns a) and in Refs. 18 and 19 (columns b)

T, K	$\Omega^{(1,1)}$ (a)	$\Omega^{(1,1)}$ (b)	$\Omega^{(2,2)}$ (a)	$\Omega^{(2,2)}$ (b)
5,000	23.36	22.6	5.65	6.39
10,000	21.82	21.13	4.31	4.75
20,000	20.33	19.72	3.17	3.41
30,000	19.48	18.90	2.65	2.81
100,000	17.06	16.47	1.60	1.65

Table 18 Parameters for potentials for atom–ion interaction: $O(^3P)$–$O^-(^2P)$

State	C	ϕ_0, eV	ρ (or σ), Å	p_n
$^4\Delta u$	0.00	187.1	0.507	8
$^4\Pi g$	0.00	811.5	0.314	8
$^4\Pi g(2)$	0.00	100.1	0.680	8
$^4\Pi u(2)$	0.00	1,500.0	0.288	8
$^4\Sigma u^+$	0.00	274.5	0.467	4
$^4\Sigma g^-(2)$	0.00	159.7	0.588	4
$^4\Sigma u^-(2)$	0.00	46.2	0.617	4
$^2\Delta g$	0.00	3,860,000	0.111	4
$^2\Pi g(2)$	0.00	77.3	0.523	4
$^2\Pi u(2)$	0.00	67.60	0.581	4
$^2\Sigma g^-$	0.00	153.2	0.473	2
$^2\Sigma u^-$	0.00	47.90	0.826	2
$^4\Delta g$	3.55	0.70	1.640	8
$^4\Sigma g^+$	3.55	0.70	1.640	4
$^4\Pi u(1)$	2.77	0.35	1.904	8
$^4\Sigma g^-(1)$	4.33	0.04	2.730	4
$^4\Sigma u^-(1)$	1.42	2.00	1.243	4
$^2\Delta u$	2.75	1.25	1.534	4
$^2\Pi g(1)$	1.42	1.25	1.243	4
$^2\Pi u(1)$	1.00	2.83	0.780	4
$^2\Sigma g^+(2)$	2.17	0.35	1.825	2
$^2\Sigma u^+$	2.89	1.25	1.530	2
$^2\Sigma g^-(1)$	3.31	1.00	1.706	2
$^2\Sigma u^-(1)$	3.55	0.70	1.640	2

(see Table 17). The differences between the two sets of values do not exceed 3 and 13% for diffusion- and viscosity-type collision integrals:

$$O\text{–}O^-$$

We have treated the interaction O–O^- as for ion–atom–parent case. The viscosity-type collision integrals have been calculated by averaging all of the contributions coming from the whole potential manifold,[35] whereas the collision integrals diffusion type has been calculated by allowing charge-transfer cross sections. Potential parameters, derived from the quantum mechanical values of Ref. 35, have been reported in Table 18:

$$O_2\text{–}O_2^+;\ O_2\text{–}O_2^-$$

We have used the same method discussed for N_2–N_2^+ with parameters reported in Table 7.

3. Electron–Neutral e–O_2, e–O

We have integrated the momentum transfer cross sections of Phelps and Pitchford[36] for e–O_2 system, whereas the correction $Q^{(2)}/Q^{(1)}$ has been obtained by integrating the differential cross section of Shyn and Sharp.[37]

For e–O cross sections we have used the $Q^{(2)}$ and $Q^{(1)}$ cross sections of Thomas and Nesbet.[38] An additional point at 100 eV has been obtained by using the differential cross sections of Blaha and Davis.[39]

Table A1 Parameters used to fit the collision integrals for interactions between two molecules [see Eq. (A1)]

Process	$\Omega^{(i,j)}$	$a1$	$a2$	$a3$	$a4$	$a5$	$a6$
N_2–N_2	$\Omega^{(1,1)}$	4.2447E+02	2.5868E+04	−1.0330E+00	2.7547E+01	1.0000E+00	4.2785E−01
	$\Omega^{(1,2)}$	2.7590E+02	4.6513E+04	−1.4489E+00	1.5340E+01	8.8021E−01	4.1708E−01
	$\Omega^{(1,3)}$	1.3522E+02	6.1370E+04	−1.8121E+00	7.5032E+00	4.3667E−01	4.2663E−01
	$\Omega^{(2,2)}$	7.5032E+02	4.3769E+04	−9.6115E−01	5.5575E+01	7.3450E−01	4.7747E−01
O_2–O_2	$\Omega^{(1,1)}$	4.1068E+02	2.4065E+04	−8.8536E−01	4.3180E+01	1.4356E−01	6.1155E−01
	$\Omega^{(1,2)}$	2.8255E+02	2.6422E+04	−1.1429E+00	2.5231E+01	2.0801E−01	5.6608E−01
	$\Omega^{(1,3)}$	2.1907E+02	3.3527E+04	−1.3774E+00	1.8137E+01	2.2481E−01	5.5076E−01
	$\Omega^{(2,2)}$	5.3367E+02	2.8676E+04	−8.3866E−01	5.6127E+01	6.1295E−02	6.8066E−01
NO–NO	$\Omega^{(1,1)}$	3.5215E+02	1.7562E+04	−8.8485E−01	2.9253E+01	6.3570E−01	4.5570E−01
	$\Omega^{(1,2)}$	1.1494E+02	1.2389E+04	−1.2491E+00	7.3328E+00	3.4827E−01	4.2860E−01
	$\Omega^{(1,3)}$	1.9167E+02	5.3633E+04	−1.6030E+00	1.1561E+01	6.3881E−01	4.3160E−01
	$\Omega^{(2,2)}$	3.7951E+02	1.7383E+04	−7.9157E−01	3.7919E+01	1.8054E−01	5.4195E−01
N_2–O_2	$\Omega^{(1,1)}$	2.9109E+02	1.6995E+04	−9.4388E−01	2.4968E+01	2.8136E−01	5.1156E−01
	$\Omega^{(1,2)}$	2.3289E+02	2.6336E+04	−1.2642E+00	1.6690E+01	3.9632E−01	4.8003E−01
	$\Omega^{(1,3)}$	1.3425E+02	3.0382E+04	−1.5533E+00	9.1243E+00	2.6978E−01	4.7767E−01
	$\Omega^{(2,2)}$	2.9974E+02	1.6635E+04	−8.9024E−01	2.7140E+01	1.0368E−01	5.7374E−01
N_2–NO	$\Omega^{(1,1)}$	1.6324E+02	7.2640E+03	−9.5137E−01	8.2746E+00	1.0000E+00	3.4180E−01
	$\Omega^{(1,2)}$	1.1646E+02	1.9357E+04	−1.4606E+00	4.4626E+00	8.8277E−01	3.3773E−01
	$\Omega^{(1,3)}$	2.6945E+01	1.7648E+04	−1.9074E+00	1.1168E+00	1.8471E−01	3.5476E−01
	$\Omega^{(2,2)}$	1.7855E+02	7.4922E+03	−8.3567E−01	1.3283E+01	4.0509E−01	3.9878E−01
O_2–NO	$\Omega^{(1,1)}$	1.5090E+02	6.7215E+03	−9.1171E−01	9.6404E+00	8.2038E−01	3.4903E−01
	$\Omega^{(1,2)}$	9.6359E+01	1.1890E+04	−1.3477E+00	4.4156E+00	7.4636E−01	3.3393E−01
	$\Omega^{(1,3)}$	3.2746E+01	1.4087E+04	−1.7751E+00	1.4877E+00	2.5246E−01	3.4294E−01
	$\Omega^{(2,2)}$	2.4059E+02	1.0381E+04	−8.1156E−01	2.1388E+01	3.9864E−01	4.2191E−01
N_2–N_2^+	$\Omega^{(1,1)}$	−1.5707E+02	1.6358E+02	−1.5782E−03	4.6818E−02	3.7122E−02	5.8367E−02
	$\Omega^{(1,2)}$	−1.5988E+02	1.6168E+02	−4.4121E−04	1.2796E−02	1.0896E−02	5.7820E−02
	$\Omega^{(1,3)}$	−1.5655E+02	1.6306E+02	−1.6250E−03	4.7258E−02	3.9996E−02	5.7329E−02
	$\Omega^{(2,2)}$	−6.1066E+01	1.0830E+02	1.6620E−05	1.9752E−04	9.6025E−02	5.0012E−01
O_2–O_2^+	$\Omega^{(1,1)}$	−1.1575E+02	3.7386E+02	−4.8436E−02	3.6486E+00	2.6117E−01	1.4145E−01
	$\Omega^{(1,2)}$	−2.5560E+02	2.7178E+02	−2.8455E−03	1.4886E−01	1.0396E−01	7.4847E−02
	$\Omega^{(1,3)}$	−2.0496E+02	5.3410E+02	−4.3204E−02	4.7254E+00	5.0113E−01	1.1552E−01
	$\Omega^{(2,2)}$	1.4651E+03	4.5141E+02	−4.7817E−01	1.0000E+00	3.1366E+00	4.9971E−01
O_2–O_2^-	$\Omega^{(1,1)}$	−8.0988E+02	8.0994E+02	−2.8497E−06	1.1887E−03	1.1348E−03	5.1275E−02
	$\Omega^{(1,2)}$	−8.0988E+02	8.0994E+02	−2.8733E−06	1.2180E−03	1.1439E−03	5.1841E−02
	$\Omega^{(1,3)}$	−8.0987E+02	8.0993E+02	−2.8894E−06	1.2744E−03	1.1510E−03	5.4517E−02
	$\Omega^{(2,2)}$	−8.1760E+02	8.1960E+02	7.2017E−08	1.1182E−05	4.2552E−03	5.0013E−01
NO–NO^+	$\Omega^{(1,1)}$	−8.1007E+02	8.1015E+02	−4.6391E−06	7.5318E−04	5.5734E−04	7.3176E−02
	$\Omega^{(1,2)}$	−8.1015E+02	8.1023E+02	−4.9170E−06	7.6379E−04	6.2676E−04	6.9886E−02
	$\Omega^{(1,3)}$	−8.1009E+02	8.1017E+02	−4.7522E−06	7.7546E−04	5.9147E−04	7.3438E−02
	$\Omega^{(2,2)}$	−8.0815E+02	8.0826E+02	1.4346E−09	3.3750E−07	2.1668E−04	5.0007E−01

Table A2 Parameters used to fit the collision integrals for interactions between molecules and atoms [see Eq. (A1)]

Process	$\Omega^{(i,j)}$	$a1$	$a2$	$a3$	$a4$	$a5$	$a6$
O_2–O	$\Omega^{(1,1)}$	5.4824E+01	2.6124E+03	−1.2756E+00	−1.0000E+00	1.7971E+00	2.4756E−01
	$\Omega^{(1,2)}$	1.1271E+01	5.9978E+03	−1.8948E+00	2.1033E−01	2.2547E−01	2.9521E−01
	$\Omega^{(1,3)}$	3.0924E+00	3.1551E+04	−2.7099E+00	1.1433E−01	4.6291E−02	3.2618E−01
	$\Omega^{(2,2)}$	6.4059E+01	1.6075E+03	−9.2241E−01	1.0000E+00	1.5258E+00	2.5189E−01
N_2–O	$\Omega^{(1,1)}$	4.2411E−11	7.0283E−09	−1.7738E+00	−1.3666E−12	1.4068E−12	2.5682E−01
	$\Omega^{(1,2)}$	9.3078E+01	3.7746E+05	−2.4904E+00	1.0000E+00	1.8012E+00	3.0818E−01
	$\Omega^{(1,3)}$	7.1865E+01	8.4650E+06	−3.3838E+00	2.3305E+00	1.0000E+00	3.4250E−01
	$\Omega^{(2,2)}$	4.8434E−11	1.3958E−09	−1.3115E+00	−2.0696E−12	1.9493E−12	2.2447E−01
NO–O	$\Omega^{(1,1)}$	1.0948E+02	3.9522E+03	−9.2591E−01	5.6774E+00	1.0000E+00	3.4478E−01
	$\Omega^{(1,2)}$	4.9973E+01	6.8422E+03	−1.4022E+00	2.4320E+00	4.1518E−01	3.6638E−01
	$\Omega^{(1,3)}$	1.5346E+01	1.2856E+04	−1.9585E+00	8.1792E−01	1.1084E−01	3.8800E−01
	$\Omega^{(2,2)}$	3.4111E+02	1.2306E+04	−7.6446E−01	3.4503E+01	9.6152E−01	4.1455E−01
NO–N	$\Omega^{(1,1)}$	1.8376E+01	5.8513E+02	−1.0885E+00	2.1989E−02	3.7017E−01	2.7990E−01
	$\Omega^{(1,2)}$	1.9001E+00	6.2564E+02	−1.7235E+00	4.7035E−02	2.4421E−02	3.2671E−01
	$\Omega^{(1,3)}$	6.3924E−01	1.7922E+03	−2.3300E+00	2.4350E−02	6.2276E−03	3.5811E−01
	$\Omega^{(2,2)}$	5.2091E+00	1.2579E+02	−7.9721E−01	2.2715E−01	6.0530E−02	2.9981E−01
O_2–N	$\Omega^{(1,1)}$	3.4675E+01	1.3056E+03	−1.1164E+00	3.4754E−01	5.7951E−01	3.0097E−01
	$\Omega^{(1,2)}$	4.7427E+00	1.7737E+03	−1.7517E+00	1.4546E−01	5.1947E−02	3.4688E−01
	$\Omega^{(1,3)}$	1.1480E+00	3.3633E+03	−2.3376E+00	4.9886E−02	9.5303E−03	3.7913E−01
	$\Omega^{(2,2)}$	9.7073E+01	2.5179E+03	−8.2806E−01	4.4350E+00	1.0000E+00	3.1601E−01
N_2–N	$\Omega^{(1,1)}$	2.3258E+01	1.9547E+03	−1.2673E+00	9.9578E−01	1.0382E−01	4.4037E−01
	$\Omega^{(1,2)}$	2.3258E+01	1.4173E+04	−1.8460E+00	1.2542E+00	7.0239E−02	4.9160E−01
	$\Omega^{(1,3)}$	1.4489E−01	4.8346E+02	−2.3505E+00	9.0340E−03	3.2446E−04	5.3192E−01
	$\Omega^{(2,2)}$	2.0822E+01	9.8291E+02	−1.0120E+00	1.1670E+00	6.8362E−02	4.3962E−01

Table A3 Parameters used to fit the collision integrals for interactions between two atoms [see Eq. (A1)]

Process	$\Omega^{(i,j)}$	$a1$	$a2$	$a3$	$a4$	$a5$	$a6$
O–O	$\Omega^{(1,1)}$	2.2077E+01	1.1401E+03	−8.9608E−01	2.8716E+00	4.9476E−02	4.8371E−01
	$\Omega^{(1,2)}$	1.3163E+01	1.4855E+03	−1.2581E+00	1.3503E+00	4.9169E−02	4.5654E−01
	$\Omega^{(1,3)}$	8.1273E+00	2.5461E+03	−1.6310E+00	7.8355E−01	3.4738E−02	4.5586E−01
	$\Omega^{(2,2)}$	2.3400E+01	1.0581E+03	−8.0168E−01	3.4801E+00	1.9999E−02	5.4191E−01
O–N	$\Omega^{(1,1)}$	2.2683E+01	1.2470E+03	−1.0271E+00	1.9320E+00	6.4407E−02	5.0887E−01
	$\Omega^{(1,2)}$	1.0660E+01	2.3223E+03	−1.4924E+00	9.1182E−01	2.4379E−02	5.4850E−01
	$\Omega^{(1,3)}$	5.8682E+01	5.0777E+04	−1.9247E+00	5.3712E+00	1.0570E−01	5.8600E−01
	$\Omega^{(2,2)}$	2.1163E+01	8.6509E+02	−8.1169E−01	2.6270E+00	2.2254E−02	5.6508E−01
N–N	$\Omega^{(1,1)}$	1.9939E+01	9.0652E+02	−8.4875E−01	2.3809E+00	3.8782E−02	4.8674E−01
	$\Omega^{(1,2)}$	9.3402E+00	1.0845E+03	−1.2761E+00	7.9736E−01	3.5324E−02	4.4711E−01
	$\Omega^{(1,3)}$	5.5929E+00	2.1522E+03	−1.6966E+00	4.4782E−01	2.4128E−02	4.4567E−01
	$\Omega^{(2,2)}$	2.3736E+01	9.1364E+02	−7.7981E−01	2.7874E+00	4.9002E−02	4.6224E−01
N–N^+	$\Omega^{(1,1)}$	−1.3960E+02	3.6208E+02	−4.3674E−02	2.7103E+00	3.0103E−01	1.2418E−01
	$\Omega^{(1,2)}$	−1.2812E+02	3.8252E+02	−5.0422E−02	3.2848E+00	2.4802E−01	1.4072E−01
	$\Omega^{(1,3)}$	−1.3692E+02	3.7076E+02	−4.6642E−02	3.0216E+00	3.0143E−01	1.3162E−01
	$\Omega^{(2,2)}$	−1.859E+08[a]	1.859E+08[a]	6.4006E−08	1.6400E+01	1.0000E+00	4.7003E−01
O–O^+	$\Omega^{(1,1)}$	−1.1682E+02	3.2563E+02	−3.9601E−02	4.1463E+00	3.1988E−01	1.0766E−01
	$\Omega^{(1,2)}$	−1.2217E+02	3.2403E+02	−3.6500E−02	3.9708E+00	4.5589E−01	1.0641E−01
	$\Omega^{(1,3)}$	−1.1681E+01	2.7424E+02	−6.0360E−02	5.5075E+00	3.2206E−01	1.7246E−01
	$\Omega^{(2,2)}$	3.6880E−12	9.1735E−12	−2.5404E−01	4.1706E−13	4.2236E−15	5.4721E−01
O–O^-	$\Omega^{(1,1)}$	−1.8629E+02	4.5965E+02	−4.2524E−02	1.7729E+00	2.2350E−01	1.1551E−01
	$\Omega^{(1,2)}$	−1.8573E+02	4.5401E+02	−4.2623E−02	1.7886E+00	2.2835E−01	1.1778E−01
	$\Omega^{(1,3)}$	−1.6695E+02	4.3964E+02	−4.6328E−02	1.8948E+00	1.9829E−01	1.2731E−01
	$\Omega^{(2,2)}$	7.2311E+01	4.1593E+02	−2.1377E−01	7.3743E+00	4.3752E−02	6.1938E−01
N^+–O	$\Omega^{(1,1)}$	7.0546E+00	1.5774E+03	−1.0493E+00	3.9567E−01	4.1793E−03	6.3764E−01
	$\Omega^{(1,2)}$	7.6038E+00	1.1282E+03	−1.0559E+00	4.2961E−01	5.3188E−03	6.4415E−01
	$\Omega^{(1,3)}$	8.3999E+00	9.2587E+02	−1.0601E+00	4.7469E−01	6.7752E−03	6.4716E−01
	$\Omega^{(2,2)}$	7.5016E+00	1.1305E+03	−9.0625E−01	5.6489E−01	3.5543E−03	6.3384E−01
O^+–N	$\Omega^{(1,1)}$	3.9346E−01	6.7619E+01	−8.5579E−01	3.9606E−02	3.0435E−05	7.9289E−01
	$\Omega^{(1,2)}$	4.1859E−01	5.2033E+01	−8.5611E−01	4.2620E−02	3.6537E−05	8.0866E−01
	$\Omega^{(1,3)}$	4.6966E−01	4.6150E+01	−8.5645E−01	4.8058E−02	4.6548E−05	8.1726E−01
	$\Omega^{(2,2)}$	4.9141E−01	4.7448E+01	−6.2444E−01	8.3568E−02	1.4153E−05	8.5148E−01

[a] $a1 = -1.85975093E+08$ $a2 = 1.85975492E+08$.

4. Ion–Ion and Electron–Electron

We can confidently use Eqs. (29) and (30) also for negative-positive ion interactions.

5. Minor Interactions

Minor interactions such as O–O^{++}, O–O^{+++}, O–O^{++++}, O_2–O^+, O_2–O^{++}, O_2–O^{+++}, O_2–O^{++++} occur very seldom so that their calculation can be done according to the polarizability model for both collision integrals diffusion and viscosity type. Equations (13–19) can therefore be used.

C. Nitrogen Oxide

NO–NO

In this case we use a Lennard–Jones potential up to 1000 K and an exponential repulsive potential for $T > 2000$ K.

NO–NO^+

Diffusion-type collision integrals have been obtained by using charge-transfer cross sections, whereas a polarizability model has been used for collision integrals viscosity type.

Table A4 Parameters used to fit the collision integrals for interactions between electrons and molecules [see Eq. (A2)]

Process	$\Omega^{(i,j)}$	$a1, a7$	$a2, a8$	$a3, a9$	$a4$	$a5$	$a6$
e–N_2	$\Omega^{(1,1)}$	4.4763E+00	8.9123E+00	8.6558E+01	−1.1907E+01	7.3977E−01	8.1569E−02
	$\Omega^{(1,2)}$	6.2997E+00	2.8143E+00	6.0373E+00	−6.1715E−07	5.9733E+00	−1.3242E−01
	$\Omega^{(1,3)}$	6.0853E+00	2.5330E+00	9.8515E+00	−1.1814E−10	9.2906E+00	−4.0522E−01
	$\Omega^{(1,4)}$	5.8136E+00	2.4462E+00	9.3499E+00	−1.1687E−11	1.0256E+01	−3.9827E−01
	$\Omega^{(1,5)}$	5.4329E+00	2.3732E+00	6.5229E+00	−5.6704E−11	9.6931E+00	−2.4519E−01
	$\Omega^{(2,2)}$	7.7099E+00	3.6418E+00	6.9892E+01	−2.9740E−01	1.3600E+00	−7.0673E−01
	$\Omega^{(1,1)}$	1.7704E+00	9.2013E+00	8.0978E−01			
	$\Omega^{(1,2)}$	2.1061E+00	8.9217E+00	7.2869E−01			
	$\Omega^{(1,3)}$	2.4046E+00	8.6973E+00	6.7041E−01			
	$\Omega^{(1,4)}$	2.6488E+00	8.5107E+00	6.2512E−01			
	$\Omega^{(1,5)}$	2.8589E+00	8.3525E+00	5.9211E−01			
	$\Omega^{(2,2)}$	2.1153E+00	8.9418E+00	8.3996E−01			
e–O_2	$\Omega^{(1,1)}$	8.3307E+00	2.1057E+00	1.3703E+02	1.6462E−03	2.2034E+00	−1.6638E+00
	$\Omega^{(1,2)}$	8.3440E+00	2.1878E+00	2.6005E+02	−4.7740E−02	−7.8236E−01	−1.8609E+00
	$\Omega^{(1,3)}$	8.2363E+00	2.2106E+00	3.5049E+02	−1.0523E−01	−8.9547E−01	−1.9861E+00
	$\Omega^{(1,4)}$	7.7713E+00	2.2180E+00	8.0242E+01	−2.9025E−06	4.7426E+00	−1.3707E+00
	$\Omega^{(1,5)}$	8.0580E+00	2.2437E+00	4.9008E+02	−2.0701E−01	−1.0225E+00	−2.1302E+00
	$\Omega^{(2,2)}$	8.1575E+00	2.8053E+00	9.3652E+00	−4.1748E−04	3.6655E+00	−1.8979E−01
	$\Omega^{(1,1)}$	−7.1918E−01	9.7316E+00	1.0537E+00			
	$\Omega^{(1,2)}$	−9.0948E−01	9.4672E+00	1.0447E+00			
	$\Omega^{(1,3)}$	−9.7555E−01	9.2465E+00	1.0010E+00			
	$\Omega^{(1,4)}$	−9.8561E−01	9.0635E+00	9.5788E−01			
	$\Omega^{(1,5)}$	−1.0577E+00	8.9127E+00	9.4543E−01			
	$\Omega^{(2,2)}$	−7.6150E−01	9.3932E+00	9.6517E−01			
e–NO	$\Omega^{(1,1)}$	−7.2965E−01	1.3332E+01	7.8565E+02	−1.9259E+02	2.8336E−01	−6.3703E−02
	$\Omega^{(1,2)}$	−1.4887E+01	1.8148E+01	2.5286E+03	−1.0586E+03	2.5251E−01	9.4792E−02
	$\Omega^{(1,3)}$	−9.5704E+00	1.7653E+01	1.4649E+03	−5.5148E+02	3.6509E−01	1.4218E−01
	$\Omega^{(1,4)}$	−4.8381E+00	1.6713E+01	8.8349E+02	−2.8954E+02	5.0399E−01	2.0687E−01
	$\Omega^{(1,5)}$	5.8041E−01	1.3987E+01	3.9144E+02	−9.7881E+01	7.0323E−01	2.8223E−01
	$\Omega^{(2,2)}$	3.8989E−02	1.4692E+01	6.6332E+02	−1.6621E+02	5.9703E−01	1.9528E−01
	$\Omega^{(1,1)}$	9.3029E−01	8.8086E+00	9.6216E−01			
	$\Omega^{(1,2)}$	1.0562E+00	8.5064E+00	8.7879E−01			
	$\Omega^{(1,3)}$	1.1651E+00	8.2614E+00	8.2346E−01			
	$\Omega^{(1,4)}$	1.2667E+00	8.0651E+00	7.9767E−01			
	$\Omega^{(1,5)}$	1.3560E+00	7.9087E+00	7.8024E−01			
	$\Omega^{(2,2)}$	1.0178E+00	8.6724E+00	9.6611E−01			

Table A5 Parameters used to fit the collision integrals for interactions between electrons and atoms [see Eq. (A2)]

Process	$\Omega^{(i,j)}$	$a1, a7$	$a2, a8$	$a3, a9$	$a4$	$a5$	$a6$
e–N	$\Omega^{(1,1)}$	8.9279E+00	1.1613E+00	1.6494E+00	1.2796E−01	2.7394E−01	−2.7594E−01
	$\Omega^{(1,2)}$	8.6314E+00	1.0738E+00	1.8882E+00	1.2214E−01	3.3398E−01	−3.4447E−01
	$\Omega^{(1,3)}$	8.4009E+00	9.8544E−01	1.9023E+00	1.1026E−01	4.4086E−01	−3.6762E−01
	$\Omega^{(1,4)}$	8.2043E+00	9.4398E−01	1.8527E+00	1.0647E−01	4.8117E−01	−3.6661E−01
	$\Omega^{(1,5)}$	8.0388E+00	9.0527E−01	1.8833E+00	1.0051E−01	5.4116E−01	−3.8773E−01
	$\Omega^{(2,2)}$	8.2257E+00	9.5133E−01	8.7677E−01	6.8519E−02	1.6570E−01	3.4127E−02
	$\Omega^{(1,1)}$	0.0000E+00	0.0000E+00	1.0000E+00			
	$\Omega^{(1,2)}$	0.0000E+00	0.0000E+00	1.0000E+00			
	$\Omega^{(1,3)}$	0.0000E+00	0.0000E+00	1.0000E+00			
	$\Omega^{(1,4)}$	0.0000E+00	0.0000E+00	1.0000E+00			
	$\Omega^{(1,5)}$	0.0000E+00	0.0000E+00	1.0000E+00			
	$\Omega^{(2,2)}$	3.5900E−01	9.6380E+00	9.0876E−01			
e–O	$\Omega^{(1,1)}$	1.0568E+01	1.3640E+00	3.0548E+04	2.4439E−01	1.2512E−01	−4.2290E+00
	$\Omega^{(1,2)}$	1.0276E+01	1.3728E+00	7.8394E+04	2.2579E−01	2.0701E−01	−4.6626E+00
	$\Omega^{(1,3)}$	1.0069E+01	1.2781E+00	1.2008E+05	2.1584E−01	2.7462E−01	−4.9024E+00
	$\Omega^{(1,4)}$	9.9739E+00	1.3564E+00	2.7669E+05	2.2906E−01	1.7466E−01	−5.2350E+00
	$\Omega^{(1,5)}$	9.9629E+00	1.4615E+00	9.4493E+05	1.9454E−01	2.2494E−01	−5.7280E+00
	$\Omega^{(2,2)}$	9.9767E+00	1.6871E+00	2.9697E+05	5.6206E−02	1.4522E−01	−5.1321E+00
	$\Omega^{(1,1)}$	2.7943E−01	8.6407E+00	1.7624E+00			
	$\Omega^{(1,2)}$	2.4241E−01	8.1977E+00	1.5622E+00			
	$\Omega^{(1,3)}$	2.5935E−01	8.0276E+00	1.5527E+00			
	$\Omega^{(1,4)}$	2.4244E−01	7.7435E+00	1.4870E+00			
	$\Omega^{(1,5)}$	1.9924E−01	7.4822E+00	1.3722E+00			
	$\Omega^{(2,2)}$	7.1705E−02	8.4309E+00	1.3830E+00			

Neutral interactions:

$$N_2\text{–}O,\ N\text{–}O_2,\ N_2\text{–}NO,\ O_2\text{–}NO,\ O\text{–}NO,\ N\text{–}NO$$

In this case we use a Lennard–Jones potential up to 1000 K and an exponential repulsive potential for $T > 2000$ K:

Ion–neutral:

$$N_2\text{–}O^+,\ N^+\text{–}O_2,\ N_2^+\text{–}NO,\ O_2^+\text{–}NO,\ O^+\text{–}NO,\ N^+\text{–}NO$$

In this case we use a polarizability model for both collision integrals diffusion and viscosity type.

Main mixed interactions are described as follows. For N–O interaction we simplify the problem by using an exponential potential for $T > 2000$ K and a Lennard–Jones one for $T < 1000$ K. This approximation gives collision integrals in satisfactory agreement with the recent calculations of Levin et al.[2,3] For $N\text{–}O^+$, $N^+\text{–}O$ we directly use the recent calculations of Stallcop et al.[21]

IV. Comments

The present data constitute a new database for the calculation of equilibrium and nonequilibrium air plasmas. They complement already existing tabulations as those of Refs. 4, 5, 18, 19, and 27. Partial comparisons of the present collision integrals with the corresponding ones from these references have been reported in this paper.

More interesting is the comparison of the transport coefficients such as thermal conductivity, viscosity, and electrical conductivity for equilibrium air obtained by using the different sets of collision integrals. This comparison has been recently made by d'Angola et al.[40] and by Bottin et al.[41] In particular d'Angola et al.,[40] by using the present collision integrals and higher approximations of the Chapman and Enskog method, compared transport coefficients for air plasmas with the corresponding values obtained by Murphy[4,5] and by Yos.[42] He found differences with the results calculated in Refs. 4, 5, and 42 not exceeding respectively 14 and 24.2% for the total thermal conductivity and 7.5 and 16.3% for the viscosity in the temperature interval $300 < T < 30{,}000$ K.

A similar comparison is presented by Bottin et al.,[41] who used a combination of present collision integrals and those of Ref. 27. His comparison with Refs. 4, 5, and 43 closely follows that one reported by d'Angola et al.[40] The Gupta et al.[43] results are not so far from those of Yos.[42]

These comparisons[40,41,44,45] tell us that the strong progress made in the last 30 years on collision integrals and on kinetic theory of gas results in a moderate deviation of transport coefficients calculated by Yos in 1967, thus emphasizing the quality of collision integral calculations and the judicious selection of approximate formulas for calculating the transport coefficients made by this author.

Finally, we want to point out that our calculations of total thermal conductivity are also in agreement with the results of Bacri and Raffanel[46] in the dissociation (neutral) regime ($T < 7000$ K), thus implying that the different choices of potentials made in the two calculations for neutral–neutral interactions give comparable collision integrals.

V. Conclusions

In this paper we have presented a new database for calculating collision integrals of high-temperature air species in the temperature range 50–100,000 K. These data, which are in satisfactory agreement with those reported in Refs. 4, 5, 18, 19, and 27, have been already used by different authors for calculating equilibrium and nonequilibrium transport properties of air and N_2 and O_2 plasmas.

Appendix: Fitting Analytical Expressions

The following formulas are used to fit the collision integrals in interactions between heavy particles (Tables A1–A3):

$$\Omega^{(i,j)} = \frac{a1 + a2T^{a3}}{a4 + a5T^{a6}} \tag{A1}$$

and in interactions between electron and heavy particles (Tables A4 and A5):

$$\Omega^{(i,j)} = \frac{a3(\ell n\, T)^{a6} \exp[(\ell n\, T - a1)/a2]}{\exp[(\ell n\, T - a1)/a2] + \exp[-(\ell n\, T - a1)/a2]} + a7 \exp\{-[(\ell n\, T - a8)/a9]^2\} + a4[1 + (\ell n\, T)^{a5}] \tag{A2}$$

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