

APPENDIX A

CONSTANTS USED IN AIR MODEL

In this section the various constants that were introduced in the discussion of the physical model of air. The heats of formation of the seven chemical species used are listed below.

Table A.1 Heats of formation.

Species	h_s°
N ₂	0.0
O ₂	0.0
NO	2.996123×10^6
NO ⁺	3.283480×10^7
N	3.362161×10^7
O	1.543119×10^7
e^-	0.0

The coefficients required for the viscosity model of Blottner *et al.* (1971) are given in the following table.

Table A.2 Viscosity Coefficients for Blottner Model

Species	A_s	B_s	C_s
N ₂	0.0268142	0.3177838	-11.3155513
O ₂	0.0449290	-0.0826158	-9.2019475
NO	0.0436378	-0.0335511	-9.5767430
NO ⁺	0.3020141	-3.5039791	-3.7355157
N	0.0115572	0.6031679	-12.4327495
O	0.0203144	0.4294404	-11.6031403

The Arrhenius coefficients required for the calculation of the forward reaction rates for the six reactions and the possible collision partners are given in the following table. These were taken from Park (1985a) and Bussing and Eberhardt (1987).

Table A.3 Arrhenius coefficients for forward reaction rates.

Reaction	Partner	C_m (m ³ /kg s)	η_m	θ_{dm} (K)
1	N ₂	3.700×10^{18}	-1.600	113200
	O ₂	3.700×10^{18}	-1.600	113200
	NO	3.700×10^{18}	-1.600	113200
	NO ⁺	3.700×10^{18}	-1.600	113200
	N	1.110×10^{19}	-1.600	113200
	O	1.110×10^{19}	-1.600	113200
	e^-	1.110×10^{21}	-1.600	113200
2	N ₂	2.750×10^{16}	-1.000	59500
	O ₂	2.750×10^{16}	-1.000	59500
	NO	2.750×10^{16}	-1.000	59500
	NO ⁺	2.750×10^{16}	-1.000	59500
	N	8.250×10^{16}	-1.000	59500
	O	8.250×10^{16}	-1.000	59500
	e^-	1.320×10^{19}	-1.000	59500
3	N ₂	2.300×10^{14}	-0.500	75500
	O ₂	2.300×10^{14}	-0.500	75500
	NO	2.300×10^{14}	-0.500	75500
	NO ⁺	2.300×10^{14}	-0.500	75500
	N	4.600×10^{14}	-0.500	75500
	O	4.600×10^{14}	-0.500	75500
	e^-	7.360×10^{16}	-0.500	75500
4	—	3.180×10^{10}	0.100	37700
5	—	2.160×10^5	1.290	19220
6	—	6.500×10^8	0.000	32000

The characteristic temperatures used in the harmonic oscillator model (equation (2.5.3)) and the diffusion model (equation (2.7.5)) are given in Table A.4. The table also includes the collision diameters for use in the vibration-vibration coupling model (equation (2.7.18)).

Table A.4 Molecular constants for use in the harmonic oscillator model for vibration, the diffusion model of vibrational excitation, and the vibration-vibration coupling model.

Species	θ_{vs} (K)	θ_s (K)	$d_s \times 10^{10}$ (m)
N ₂	3395	5000	3.709
O ₂	2239	3350	3.608
NO	2817	4040	3.534
NO ⁺	2817	4040	3.534

The equilibrium constants for the chemical reactions are computed using the expression in Park (1985a), which is a curve fit to experimental data. This is done using

$$K_{eq\,m} = \exp(A_{1m} + A_{2m}Z + A_{3m}Z^2 + A_{4m}Z^3 + A_{5m}Z^4), \quad (A.1)$$

where $Z = 10,000/T$, (T in K) and the constants are given in Table A.5.

Table A.5 Constants for computing equilibrium reaction constants.

Reaction	A_{1m}	A_{2m}	A_{3m}	A_{4m}	A_{5m}
1	3.898	-12.611	0.683	-0.118	0.006
2	1.335	-4.127	-0.616	0.093	-0.005
3	1.549	-7.784	0.228	-0.043	0.002
4	2.349	-4.828	0.455	-0.075	0.004
5	0.215	-3.652	0.843	-0.136	0.007
6	-6.234	-5.536	0.494	-0.058	0.003