Eleven Species High-Temperature Air Plasma Kinetics for Earth Entry Flows

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Table 1.
Dunn-Kang (1973) 11-species 31-reaction high-temperature air model [1, 2].

	Reaction	A, $cm^3 \cdot (mole \cdot s)^{-1} \cdot K^{-n}$	n	E, cal/mole
(1)	$O_2 + N \rightleftarrows 2O + N$	3.6×10^{18}	-1	118,800
(2)	$O_2 + NO \rightleftarrows 2O + NO$	3.6×10^{18}	-1	118,800
(3)	$N_2 + O \rightleftarrows 2N + O$	1.9×10^{17}	-0.5	226,000
(4)	$N_2 + NO \rightleftarrows 2N + NO$	1.9×10^{17}	-0.5	226,000
(5)	$N_2 + O_2 \rightleftarrows 2N + O_2$	1.9×10^{17}	-0.5	226,000
(6)	$NO + O_2 \rightleftarrows N + O + O_2$	3.9×10^{20}	-1.5	151,000
(7)	$NO + N_2 \rightleftarrows N + O + N_2$	3.9×10^{20}	-1.5	151,000
(8)	$O + NO \rightleftarrows N + O_2$	3.2×10^{9}	1	39,400
(9)	$O + N_2 \rightleftarrows N + NO$	7×10^{13}	0	76,000
(10)	$N + N_2 \rightleftarrows 2N + N$	4.085×10^{22}	-1.5	226,000
(11)	$O + N \rightleftarrows NO^+ + e^-$	1.4×10^{6}	1.5	63,800
(12)	$O + e^- \rightleftarrows O^+ + 2e^-$	3.6×10^{31}	-2.91	316,000
(13)	$N + e^- \rightleftarrows N^+ + 2e^-$	1.1×10^{32}	-3.14	338,000
(14)	$O + O \rightleftarrows O_2^+ + e^-$	1.6×10^{17}	-0.98	161,600
(15)	$O + O_2^+ \rightleftarrows O_2 + O^+$	2.92×10^{18}	-1.11	56,000
(16)	$N_2 + N^+ \rightleftarrows N + N_2^+$	2.02×10^{11}	0.81	26,000
(17)	$N + N \rightleftarrows N_2^+ + e^-$	1.4×10^{13}	0	135,600
(18)	$O + NO^+ \rightleftarrows NO + O^+$	3.63×10^{15}	-0.6	101,600
(19)	$N_2 + O^+ \rightleftarrows O + N_2^+$	3.4×10^{19}	-2	46,000
(20)	$N + NO^+ \rightleftarrows NO + N^+$	1×10^{19}	-0.93	122,000
(21)	$O_2 + NO^+ \rightleftarrows NO + O_2^+$	1.8×10^{15}	0.17	66,000
(22)	$O + NO^+ \rightleftarrows O_2 + N^+$	1.34×10^{13}	0.31	154,540
(23)	$O_2 + O \rightleftarrows 2O + O$	9×10^{19}	-1	119,000
(24)	$O_2 + O_2 \rightleftarrows 2O + O_2$	3.24×10^{19}	-1	119,000
(25)	$O_2 + N_2 \rightleftarrows 2O + N_2$	7.2×10^{18}	-1	119,000
(26)	$N_2 + N_2 \rightleftarrows 2N + N_2$	4.7×10^{17}	-0.5	226,000
(27)	$NO + O \rightleftarrows N + 2O$	7.8×10^{20}	-1.5	151,000
(28)	$NO + N \rightleftarrows O + 2N$	7.8×10^{20}	-1.5	151,000
(29)	$NO + NO \rightleftarrows N + O + NO$	7.8×10^{20}	-1.5	151,000
(30)	$O2 + N2 \rightleftarrows NO + NO^+ + e^-$	1.38×10^{20}	-1.84	282,000
(31)	$NO + N2 \rightleftarrows NO^+ + e^- + N_2$	2.2×10^{15}	-0.35	216,000

TABLE 2.
Park (1993) 11-species high-temperature air model [5].

No.	Reaction[b]	Forward Control. Temp.	Backward Control. Temp.[c]	A, $cm^3 \cdot (mole \cdot s)^{-1} \cdot K^{-n}$	n	E, cal/mole [a]	Ref.
1	$N_2 + M_1 \rightleftarrows N + N + M_1$	$\sqrt{TT_v}$	T	3.0×10^{22}	−1.6	$113200 \cdot R$	[3]
2	$N_2 + M_2 \rightleftarrows N + N + M_2$	$\sqrt{TT_v}$	T	7.0×10^{21}	−1.6	$113200 \cdot R$	[3]
3	$N_2 + e^- \rightleftarrows N + N + e^-$	$\sqrt{T_e T_v}$	$\sqrt{TT_e}$	1.2×10^{25}	−1.6	$113200 \cdot R$	[4]
4	$O_2 + M_1 \rightleftarrows O + O + M_1$	$\sqrt{TT_v}$	T	1.0×10^{22}	−1.5	$59500 \cdot R$	[3]
5	$O_2 + M_2 \rightleftarrows O + O + M_2$	$\sqrt{TT_v}$	T	2.0×10^{21}	−1.5	$59500 \cdot R$	[3]
6	$NO + M_3 \rightleftarrows N + O + M_3$	$\sqrt{TT_v}$	T	1.1×10^{17}	0.0	$75500 \cdot R$	[3]
7	$NO + M_4 \rightleftarrows N + O + M_4$	$\sqrt{TT_v}$	T	5.0×10^{15}	0.0	$75500 \cdot R$	[3]
8	$NO + O \rightleftarrows N + O_2$	T	T	8.4×10^{12}	0.0	$19450 \cdot R$	[3]
9	$N_2 + O \rightleftarrows NO + N$	T	T	6.4×10^{17}	−1.0	$38400 \cdot R$	[3]
10	$N + O \rightleftarrows NO^+ + e^-$	T	$\sqrt{T_v T_e}$	8.8×10^{8}	1.0	$31900 \cdot R$	[5]
11	$O + O \rightleftarrows O_2^+ + e^-$	T	$\sqrt{T_v T_e}$	7.1×10^{2}	2.7	$80600 \cdot R$	[5]
12	$N + N \rightleftarrows N_2^+ + e^-$	T	$\sqrt{T_v T_e}$	4.4×10^{7}	1.5	$67500 \cdot R$	[5]
13	$NO^+ + O \rightleftarrows N^+ + O_2$	T	T	1.0×10^{12}	0.5	$77200 \cdot R$	[3]
14	$N^+ + N_2 \rightleftarrows N_2^+ + N$	T	T	1.0×10^{12}	0.5	$12200 \cdot R$	[3]
15	$O_2^+ + N \rightleftarrows N^+ + O_2$	T	T	8.7×10^{13}	0.14	$28600 \cdot R$	[3]
16	$O^+ + NO \rightleftarrows N^+ + O_2$	T	T	1.4×10^{5}	1.90	$26600 \cdot R$	[3]
17	$O_2^+ + N_2 \rightleftarrows N_2^+ + O_2$	T	T	9.9×10^{12}	0.00	$40700 \cdot R$	[3]
18	$O_2^+ + O \rightleftarrows O^+ + O_2$	T	T	4.0×10^{12}	−0.09	$18000 \cdot R$	[3]
19	$NO^+ + N \rightleftarrows O^+ + N_2$	T	T	3.4×10^{13}	−1.08	$12800 \cdot R$	[3]
20	$NO^+ + O_2 \rightleftarrows O_2^+ + NO$	T	T	2.4×10^{13}	0.41	$32600 \cdot R$	[3]
21	$NO^+ + O \rightleftarrows O_2^+ + N$	T	T	7.2×10^{12}	0.29	$48600 \cdot R$	[3]
22	$O^+ + N_2 \rightleftarrows N_2^+ + O$	T	T	9.1×10^{11}	0.36	$22800 \cdot R$	[3]
23	$NO^+ + N \rightleftarrows N_2^+ + O$	T	T	7.2×10^{13}	0.00	$35500 \cdot R$	[3]
24	$O + e^- \rightleftarrows O^+ + e^- + e^-$	T_e	T_e	3.9×10^{33}	−3.78	$158500 \cdot R$	[3]
25	$N + e^- \rightleftarrows N^+ + e^- + e^-$	T_e	T_e	2.5×10^{34}	−3.82	$168600 \cdot R$	[3]
26	$O^+ + e^- \rightarrow O + h\nu$	T_e	–	1.07×10^{11}	−0.52	0	[5]
27	$N^+ + e^- \rightarrow N + h\nu$	T_e	–	1.52×10^{11}	−0.48	0	[5]

[a] The universal gas constant R must be set to 1.9872 cal/K·mol
[b] $M_1 = N,\ O,\ N^+,\ O^+$
$M_2 = N_2,\ O_2,\ NO,\ N_2^+,\ O_2^+,\ NO^+$
$M_3 = N,\ O,\ NO,\ N^+,\ O^+$
$M_4 = N_2, O_2, N_2^+,\ O_2^+,\ NO^+$
[c] See Ref. [6]

Table 3.
Boyd (2007) 11-species high-temperature air model.

No.	Reaction[b]	Forward Control. Temp.	Backward Control. Temp.[c]	A, $\mathrm{cm^3 \cdot (mole \cdot s)^{-1} \cdot K^{-n}}$	n	E, cal/mole [a]	Ref.
1	$N_2 + M_1 \rightleftarrows N + N + M_1$	$\sqrt{TT_v}$	T	3.0×10^{22}	−1.6	$113200 \cdot R$	[3]
2	$N_2 + M_2 \rightleftarrows N + N + M_2$	$\sqrt{TT_v}$	T	7.0×10^{21}	−1.6	$113200 \cdot R$	[3]
3	$N_2 + e^- \rightleftarrows N + N + e^-$	$\sqrt{T_e T_v}$	$\sqrt{TT_e}$	3.0×10^{24}	−1.6	$113200 \cdot R$	[3]
4	$O_2 + M_1 \rightleftarrows O + O + M_1$	$\sqrt{TT_v}$	T	1.0×10^{22}	−1.5	$59500 \cdot R$	[3]
5	$O_2 + M_2 \rightleftarrows O + O + M_2$	$\sqrt{TT_v}$	T	2.0×10^{21}	−1.5	$59500 \cdot R$	[3]
6	$NO + M_3 \rightleftarrows N + O + M_3$	$\sqrt{TT_v}$	T	1.1×10^{17}	0.0	$75500 \cdot R$	[3]
7	$NO + M_4 \rightleftarrows N + O + M_4$	$\sqrt{TT_v}$	T	5.0×10^{15}	0.0	$75500 \cdot R$	[3]
8	$NO + O \rightleftarrows N + O_2$	T	T	8.4×10^{12}	0.0	$19400 \cdot R$	[7]
9	$N_2 + O \rightleftarrows NO + N$	T	T	5.7×10^{12}	0.42	$42938 \cdot R$	[8]
10	$N + O \rightleftarrows NO^+ + e^-$	T	$\sqrt{T_e T_v}$	5.3×10^{12}	0.0	$32000 \cdot R$	[9]
11	$O + O \rightleftarrows O_2^+ + e^-$	T	$\sqrt{T_e T_v}$	1.1×10^{13}	0	$81200 \cdot R$	[9]
12	$N + N \rightleftarrows N_2^+ + e^-$	T	$\sqrt{T_e T_v}$	2.0×10^{13}	0	$67700 \cdot R$	[9]
13	$NO^+ + O \rightleftarrows N^+ + O_2$	T	T	1.0×10^{12}	0.5	$77200 \cdot R$	[3]
14	$N^+ + N_2 \rightleftarrows N_2^+ + N$	T	T	1.0×10^{12}	0.5	$12200 \cdot R$	[3]
15	$O_2^+ + N \rightleftarrows N^+ + O_2$	T	T	8.7×10^{13}	0.14	$28600 \cdot R$	[3]
16	$O^+ + NO \rightleftarrows N^+ + O_2$	T	T	1.4×10^{5}	1.90	$26600 \cdot R$	[3]
17	$O_2^+ + N_2 \rightleftarrows N_2^+ + O_2$	T	T	9.9×10^{12}	0.00	$40700 \cdot R$	[3]
18	$O_2^+ + O \rightleftarrows O^+ + O_2$	T	T	4.0×10^{12}	−0.09	$18000 \cdot R$	[3]
19	$NO^+ + N \rightleftarrows O^+ + N_2$	T	T	3.4×10^{13}	−1.08	$12800 \cdot R$	[3]
20	$NO^+ + O_2 \rightleftarrows O_2^+ + NO$	T	T	2.4×10^{13}	0.41	$32600 \cdot R$	[3]
21	$NO^+ + O \rightleftarrows O_2^+ + N$	T	T	7.2×10^{12}	0.29	$48600 \cdot R$	[3]
22	$O^+ + N_2 \rightleftarrows N_2^+ + O$	T	T	9.1×10^{11}	0.36	$22800 \cdot R$	[3]
23	$NO^+ + N \rightleftarrows N_2^+ + O$	T	T	7.2×10^{13}	0.00	$35500 \cdot R$	[3]
24	$O + e^- \rightleftarrows O^+ + e^- + e^-$	T_e	T_e	3.9×10^{33}	−3.78	$158500 \cdot R$	[3]
25	$N + e^- \rightleftarrows N^+ + e^- + e^-$	T_e	T_e	2.5×10^{34}	−3.82	$168600 \cdot R$	[3]
26	$O^+ + e^- \rightarrow O + h\nu$	T_e	–	1.07×10^{11}	−0.52	0	[5]
27	$N^+ + e^- \rightarrow N + h\nu$	T_e	–	1.52×10^{11}	−0.48	0	[5]

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[b] $M_1 = N,\ O,\ N^+,\ O^+$
$M_2 = N_2,\ O_2,\ NO,\ N_2^+,\ O_2^+,\ NO^+$
$M_3 = N,\ O,\ NO,\ N^+,\ O^+$
$M_4 = N_2, O_2, N_2^+,\ O_2^+,\ NO^+$

[c] See Ref. [6]

References

[1] Dunn, M. G. and Kang, S. W., "Theroretical and Experimental Studies of Reentry Plasmas," *NASA CR-2232*, 1973.

[2] Bussing, T. and Eberhardt, S., "Chemistry Associated with Hypersonic Vehicles," June 1987, AIAA Paper 87-1292.

[3] Park, C., *Nonequilibrium Hypersonic Aerothermodynamics*, Wiley, New-York, 1990.

[4] Sharma, S. P., Gillespie, W. D., and Meyer, S. A., "Shock Front Radiation Measurements in Air," Jan. 1991, AIAA Paper 91-0573.

[5] Park, C., "Review of Chemical-Kinetic Problems of Future NASA Missions, I: Earth Entries," *Journal of Thermophysics and Heat Transfer*, Vol. 7, No. 3, 1993, pp. 385–398.

[6] Candler, G. V. and MacCormack, R. W., "Computation of Weakly Ionized Hypersonic Flows in Thermochemical Nonequilibrium," *Journal of Thermophysics and Heat Transfer*, Vol. 5, 1991, pp. 266–273.

[7] Bose, D. and Candler, G. V., "Thermal rate constants of the O2+N→NO+O reaction based on the A2 and A4 potential-energy surfaces," *The Journal of Chemical Physics*, Vol. 107, No. 16, 1997, pp. 6136–6145.

[8] Bose, D. and Candler, G. V., "Thermal rate constants of the N2+O→NO+N reaction using ab initio 3A and 3A potential energy surfaces," *The Journal of Chemical Physics*, Vol. 104, No. 8, 1996, pp. 2825–2833.

[9] Boyd, I. D., "Modeling of associative ionization reactions in hypersonic rarefied flows," *Physics of Fluids*, Vol. 19, No. 9, 2007, pp. 096102.