CFDWARP — 8-Species Air Plasma Finite Rate Chemical Solver

THE DEGREE OF IONIZATION of the air plasma as well as its chemical composition is predicted within CFDWARP using a finite rate nonequilibrium 8-species 28-reactions model as outlined below in Table 1. The model [2] is especially suited to discharges in air at sea-level conditions. Additionally to chemical reactions related to ion-ion recombination, electron attachment, electron-ion recombination, and dissociation, the model also includes chemical reactions related to Townsend ionization (specifically reactions 1a and 1b in Table 1). Townsend ionization consists of an electron accelerated by an electric field impacting the nitrogen or oxygen molecules and releasing in the process a new electron and a positive ion. This chemical reaction is the physical phenomenon that is at the origin of sparks and lighting bolts and that occurs in a weakly-ionized plasma whenever the electric field reaches very high values. It needs to be included in the chemical model when solving plasma aerodynamics or plasma-assisted combustion in order to predict correctly the voltage drop within the cathode sheaths. Cathode sheaths are thin regions near the cathodes where the electric field is particularly high due to the current being mostly ionic.

TABLE 1.

Typical chemical reactions occurring within weakly-ionized air while using an electron-beam ionizer [2]. The species consist of e^-, O_2, N_2, O, N, O_2^+, N_2^+, O_2^-. The rate coefficients depend on the reduced electric field $E^\star$, the bulk gas temperature T (in Kelvin), and the electron temperature T^e (in Kelvin).

No.	Reaction	Rate Coefficient	Reference
1a	$e^- + N_2 \rightarrow N_2^+ + e^- + e^-$	$\exp(-0.010581 \ln^2 E^\star - 2.40411 \cdot 10^{-75} \ln^{46} E^\star)$ cm^3/s	Ref. [30]
1b	$e^- + O_2 \rightarrow O_2^+ + e^- + e^-$	$\exp(-0.010279 \ln^2 E^\star - 2.4226 \cdot 10^{-75} \ln^{46} E^\star)$ cm^3/s	Ref. [30]
2a	$e^- + O_2^+ \rightarrow O + O$	$2.0 \times 10^{-7}(300/T^e)^{0.7}$ cm^3/s	Ref. [31]
2b	$e^- + N_2^+ \rightarrow N + N$	$2.8 \times 10^{-7}(300/T^e)^{0.5}$ cm^3/s	Ref. [32]
3a	$O_2^- + N_2^+ \rightarrow O_2 + N_2$	$2.0 \times 10^{-7}(300/T)^{0.5}$ cm^3/s	Ref. [32]
3b	$O_2^- + O_2^+ \rightarrow O_2 + O_2$	$2.0 \times 10^{-7}(300/T)^{0.5}$ cm^3/s	Ref. [32]
4a	$O_2^- + N_2^+ + N_2 \rightarrow O_2 + N_2 + N_2$	$2.0 \times 10^{-25}(300/T)^{2.5}$ cm^6/s	Ref. [32]
4b	$O_2^- + O_2^+ + N_2 \rightarrow O_2 + O_2 + N_2$	$2.0 \times 10^{-25}(300/T)^{2.5}$ cm^6/s	Ref. [32]
4c	$O_2^- + N_2^+ + O_2 \rightarrow O_2 + N_2 + O_2$	$2.0 \times 10^{-25}(300/T)^{2.5}$ cm^6/s	Ref. [32]
4d	$O_2^- + O_2^+ + O_2 \rightarrow O_2 + O_2 + O_2$	$2.0 \times 10^{-25}(300/T)^{2.5}$ cm^6/s	Ref. [32]
5a	$e^- + O_2 + O_2 \rightarrow O_2^- + O_2$	$1.4 \times 10^{-29} \frac{300}{T^e} \exp\left(\frac{-600}{T}\right) \times \exp\left(\frac{700(T^e - T)}{T^e T}\right)$ cm^6/s	Ref. [32]
5b	$e^- + O_2 + N_2 \rightarrow O_2^- + N_2$	$1.07 \times 10^{-31} \left(\frac{300}{T^e}\right)^2 \exp\left(\frac{-70}{T}\right) \times \exp\left(\frac{1500(T^e - T)}{T^e T}\right)$ cm^6/s	Ref. [32]
6	$O_2^- + O_2 \rightarrow e + O_2 + O_2$	$8.6 \times 10^{-10} \exp\left(\frac{-6030}{T}\right) \times \left[1 - \exp\left(\frac{-1570}{T}\right)\right]$ cm^3/s	Ref. [33], Ch. 2
7a	$O_2 \rightarrow e^- + O_2^+$	$2.0 \times 10^{17}\ Q_b/N$ 1/s	Ref. [34]
7b	$N_2 \rightarrow e^- + N_2^+$	$1.8 \times 10^{17}\ Q_b/N$ 1/s	Ref. [34]
8a	$O_2 + O_2 \rightarrow 2O + O_2$	$3.7 \times 10^{-8} \exp(-59380/T) \times[1 - \exp(-2240/T)]$ cm^3/s	Refs. [35] and [31]
8b	$O_2 + N_2 \rightarrow 2O + N_2$	$9.3 \times 10^{-9} \exp(-59380/T) \times[1 - \exp(-2240/T)]$ cm^3/s	Refs. [35] and [31]
8c	$O_2 + O \rightarrow 3O$	$1.3 \times 10^{-7} \exp(-59380/T) \times[1 - \exp(-2240/T)]$ cm^3/s	Refs. [35] and [31]
8d	$N_2 + O_2 \rightarrow 2N + O_2$	$5.0 \times 10^{-8} \exp(-113200/T) \times[1 - \exp(-3354/T)]$ cm^3/s	Refs. [35] and [31]
8e	$N_2 + N_2 \rightarrow 2N + N_2$	$5.0 \times 10^{-8} \exp(-113200/T) \times[1 - \exp(-3354/T)]$ cm^3/s	Refs. [35] and [31]
8f	$N_2 + O \rightarrow 2N + O$	$1.1 \times 10^{-7} \exp(-113200/T) \times[1 - \exp(-3354/T)]$ cm^3/s	Refs. [35] and [31]
9a	$O + O + O_2 \rightarrow 2O_2$	$2.45 \times 10^{-31} T^{-0.63}$ cm^6/s	Refs. [35] and [31]
9b	$O + O + N_2 \rightarrow O_2 + N_2$	$2.76 \times 10^{-34} \exp(720/T)$ cm^6/s	Refs. [35] and [31]
9c	$O + O + O \rightarrow O_2 + O$	$8.8 \times 10^{-31} T^{-0.63}$ cm^6/s	Refs. [35] and [31]
9d	$N + N + O_2 \rightarrow N_2 + O_2$	$8.27 \times 10^{-34} \exp(500/T)$ cm^6/s	Refs. [35] and [31]
9e	$N + N + N_2 \rightarrow 2N_2$	$8.27 \times 10^{-34} \exp(500/T)$ cm^6/s	Refs. [35] and [31]
9f	$N + N + O \rightarrow N_2 + O$	$8.27 \times 10^{-34} \exp(500/T)$ cm^6/s	Refs. [35] and [31]
9g	$N + N + N \rightarrow N_2 + N$	$8.27 \times 10^{-34} \exp(500/T)$ cm^6/s	Refs. [35] and [31]

Additionally to being capable to well predict low-temperature air plasmas ionized by electron beams, CFDWARP is also capable of solving finite rate hydrogen-air chemical reactions through the Jachimowsky model [53], kerosene-air chemical reactions through the Kundu model, and methane-air chemical reactions through the Yungster model [54].

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