A Description of Enceladus' Plume Sources and Chemical Reactions Significant to the Plume-Magnetosphere Interaction

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Contents

Abstract

This document is an overview of the physical properties and locations of the jets on Enceladus' surface as well as the important chemical reactions, rates, and cross-sections needed by BATS-R-US in order to simulate the Enceladus plume and its interaction with Saturn's magnetosphere.

1 Description of Sources

1.1 Location / description of sources on Enceladus

These values are not terribly well constrained however they provide a good starting point for this simulation. The idea isn't to reproduce exactly every little blip seen by Cassini, but to get a general idea of what Cassini might see as it passes through certain features of the plume.

Table 1: There are 8 known sources (as of 2007) with the following locations [*Spitale and Porco*, 2007].

Source	Tiger Stripe	Latitude [°]	Longitude [°]	Azimuth [°]	Zenith [°]
I	Baghdad	-81.5	32.8	228.7	9.7
II	Damascus	-79.4	315.5	93.8	6.8
III	Damascus	-81.3	292.8	83.2	30.2
IV	Alexandria	-72.9	148.7	110.0	3.7
V	Cairo	-78.6	72.3	229.8	6.0
VI	Baghdad	-87.1	231.4	187.6	10.2
VII	Baghdad	-74.6	29.8	352.5	20.8
VIII	Cairo	-82.1	115.5	127.7	6.8

1.2 Properties of H_2O gas for each source

According to *Hansen et al.* [2011], the EUV spectral signature of the plume seen during a solar occultation was dominated by H_2O gas with negligible amounts of N_2.

1.3 Dust outflow

! This section is incomplete - I will come back to this !

Hedman et al. [2013] says "This can be interpreted as a difference in the maximum launch velocity of the observed particles, with $v_{max} = 200 \pm 3$ m s^{-1} when Enceladus is near pericentre and $v_{max} = 190 \pm 2$ m s^{-1} when Enceladus is near apocentre. Hence the particles visible at 0.88-1.56 μm seem to be launched with a slightly larger maximum speed"

Table 2: These values are for the plume as a whole, as we do not have a way of measuring/estimating the rate for individual jets. The values in this table come from [*Hansen et al.*, 2011]. We have no estimate for the gas temperature.

Velocity	Line-of-site Column Density	Production Rate	Temperature
Exceeding 1000 [m s^{-1}]	$0.90 \pm 0.23 \times 10^{16}$ [cm^{-2}]	~200 kg s^{-1}	?

2 Chemistry

$$\frac{\partial n_\alpha}{\partial t} = \mathcal{S}_\alpha - \mathcal{L}_\alpha \tag{1}$$

$$\begin{aligned}
\mathcal{S}_\alpha^{\text{neut}} = \; & N_{\text{src},\alpha}\delta_\alpha \\
& + \sum_{\beta,j} \left(D_{\beta(j)} n_{\text{e}} + D^{\text{h}}_{\beta(j)} n_{\text{eh}}\right) n_\beta \\
& + \sum_{\beta,j} \left(I^{\text{diss}}_{\beta(j)} n_{\text{e}} + I^{\text{diss,h}}_{\beta(j)} n_{\text{eh}}\right) n_\beta \\
& + \left(R_{\alpha_+} n_{\text{e}} + R^{\text{h}}_{\alpha_+} n_{\text{eh}}\right) n_{\alpha_+} \\
& + \sum_{\beta,j} \left(R^{\text{diss}}_{\beta(j)} n_{\text{e}} + R^{\text{diss,h}}_{\beta(j)} n_{\text{eh}}\right) n_\beta \\
& + \sum_{\beta,j} \left(\kappa^{\text{diss}}_{\beta(j)} + \kappa^{\text{diss,ion}}_{\beta(j)}\right) n_\beta \\
& + \sum_{\gamma,\beta,j} k_{\gamma\beta(j)} n_\gamma n_\beta
\end{aligned} \tag{2}$$

$$\begin{aligned}
\mathcal{L}_\alpha^{\text{neut}} = \; & \left(I_\alpha n_{\text{e}} + I^{\text{h}}_\alpha n_{\text{eh}}\right) n_\alpha \\
& + \sum_{j} \left(I^{\text{diss}}_{\alpha(j)} n_{\text{e}} + I^{\text{diss,h}}_{\alpha(j)} n_{\text{eh}}\right) n_\alpha \\
& + \kappa^{\text{ion}}_\alpha n_\alpha \\
& + \sum_{j} \left(\kappa^{\text{diss}}_{\alpha(j)} + \kappa^{\text{diss,ion}}_{\alpha(j)}\right) n_\alpha \\
& + \sum_{\beta,j} k_{\alpha\beta(j)} n_\alpha n_\beta \\
& + \sum_{j} \left(D_{\alpha(j)} n_{\text{e}} + D^{\text{h}}_{\alpha(j)} n_{\text{eh}}\right) n_\alpha
\end{aligned} \tag{3}$$

$$
\begin{aligned}
\mathcal{S}_{\alpha}^{\mathrm{ion}} &= \left(I_{\alpha_-} n_{\mathrm{e}} + I_{\alpha_-}^{\mathrm{h}} n_{\mathrm{eh}}\right) n_{\alpha_-} \\
&+ \sum_{\beta,j} \left(I_{\beta(j)}^{\mathrm{diss}} n_{\mathrm{e}} + I_{\beta(j)}^{\mathrm{diss,h}} n_{\mathrm{eh}}\right) n_{\beta} \\
&+ \left(R_{\alpha_+} n_{\mathrm{e}} + R_{\alpha_+}^{\mathrm{h}} n_{\mathrm{eh}}\right) n_{\alpha_+} \\
&+ \sum_{\beta,j} \left(R_{\beta(j)}^{\mathrm{diss}} n_{\mathrm{e}} + R_{\beta(j)}^{\mathrm{diss,h}} n_{\mathrm{eh}}\right) n_{\beta} \\
&+ \kappa_{\alpha_-}^{\mathrm{ion}} n_{\alpha_-} \\
&+ \sum_{\beta,j} \left(\kappa_{\beta(j)}^{\mathrm{diss}} + \kappa_{\beta(j)}^{\mathrm{diss,ion}}\right) n_{\beta} \\
&+ \sum_{\gamma,\beta,j} k_{\gamma\beta(j)} n_{\gamma} n_{\beta} \qquad (4)
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{L}_{\alpha}^{\mathrm{ion}} &= \left(I_{\alpha} n_{\mathrm{e}} + I_{\alpha}^{\mathrm{h}} n_{\mathrm{eh}}\right) n_{\alpha} \\
&+ \sum_{j} \left(I_{\alpha(j)}^{\mathrm{diss}} n_{\mathrm{e}} + I_{\alpha(j)}^{\mathrm{diss,h}} n_{\mathrm{eh}}\right) n_{\alpha} \\
&+ \left(R_{\alpha} n_{\mathrm{e}} + R_{\alpha}^{\mathrm{h}} n_{\mathrm{eh}}\right) n_{\alpha} \\
&+ \sum_{j} \left(R_{\alpha(j)}^{\mathrm{diss}} n_{\mathrm{e}} + R_{\alpha(j)}^{\mathrm{diss,h}} n_{\mathrm{eh}}\right) n_{\alpha} \\
&+ \kappa_{\alpha}^{\mathrm{ion}} n_{\alpha} \\
&+ \sum_{j} \left(\kappa_{\alpha(j)}^{\mathrm{diss}} + \kappa_{\alpha(j)}^{\mathrm{diss,ion}}\right) n_{\alpha} \\
&+ \sum_{\beta,j} k_{\alpha\beta(j)} n_{\alpha} n_{\beta} \qquad (5)
\end{aligned}
$$

$$
\begin{aligned}
V &= \frac{1}{3}\pi r^2 h \\
&= \frac{1}{3}\pi r^2 \left(v\mathrm{d}t\right) \qquad (6)
\end{aligned}
$$

but $r = v\mathrm{d}t \tan\theta$ so

$$
V = \frac{1}{3}\pi \left(v\mathrm{d}t\right)^3 \tan^2\theta \qquad (7)
$$

and assume $\theta = \frac{\pi}{6}$.

Because the plume is dominantly water vapor gas we will neglect other trace molecules. This study will focus only on the dominant reactions involving water group ions ($W^+ \equiv O^+ + OH^+ + H_2O^+ + H_3O^+$).

There are 7 groups of reactions that must be considered: 1) charge exchange reactions, 2) photolytic reactions, 3) impact dissociation reactions, 4) electron impact ionization reactions,

5) electron impact ionization-dissociation reactions, 6) electron recombination reactions, and 7) dissociative electronic recombination reactions. In addition, for electron impact ionization and dissociation one must account for a "hot electron" population. The following tables of reactions were provided by [*Fleshman et al.*, 2010]. Bold facing guides the eye to the most important reactions.

Table 3: Charge exchange reactions / rates

Reaction			$k_{\alpha\beta}$ [cm^3 s^{-1}]
$H^+ + H$	$\rightarrow$	$\mathbf{H + H^+}$	9.7×10^{-9}
$H^+ + H_2$	$\rightarrow$	$H + H_2^+$	1.6×10^{-9}
$\mathbf{H^+ + O}$	$\rightarrow$	$\mathbf{H + O^+}$	3.0×10^{-9}
$\mathbf{H^+ + OH}$	$\rightarrow$	$\mathbf{H + OH^+}$	3.0×10^{-10}
$\mathbf{H^+ + H_2O}$	$\rightarrow$	$\mathbf{H + H_2O^+}$	2.0×10^{-8}
$H_2^+ + H_2$	$\rightarrow$	$H_2 + H_2^+$	3.6×10^{-9}
$H_2^+ + O$	$\rightarrow$	$H + OH^+$	1.0×10^{-9}
$H_2^+ + OH$	$\rightarrow$	$H + H_2O^+$	7.6×10^{-10}
$H_2^+ + OH$	$\rightarrow$	$H_2 + OH^+$	7.6×10^{-10}
$H_2^+ + H_2O$	$\rightarrow$	$H + H_3O^+$	3.4×10^{-9}
$H_2^+ + H_2O$	$\rightarrow$	$H_2 + H_2O^+$	3.9×10^{-9}
$\mathbf{O^+ + H}$	$\rightarrow$	$\mathbf{O + H^+}$	3.4×10^{-9}
$O^+ + H_2$	$\rightarrow$	$H + OH^+$	1.6×10^{-9}
$\mathbf{O^+ + O}$	$\rightarrow$	$\mathbf{O + O^+}$	6.2×10^{-9}
$\mathbf{O^+ + OH}$	$\rightarrow$	$\mathbf{O + OH^+}$	3.0×10^{-10}
$\mathbf{O^+ + H_2O}$	$\rightarrow$	$\mathbf{O + H_2O^+}$	2.3×10^{-9}
$O^{++} + O$	$\rightarrow$	$O^+ + O^+$	5.2×10^{-10}
$O^{++} + O$	$\rightarrow$	$O + O^{++}$	5.4×10^{-9}
$OH^+ + H_2$	$\rightarrow$	$H + H_2O^+$	1.1×10^{-9}
$\mathbf{OH^+ + OH}$	$\rightarrow$	$\mathbf{O + H_2O^+}$	7.0×10^{-10}
$\mathbf{OH^+ + H_2O}$	$\rightarrow$	$\mathbf{O + H_3O^+}$	1.3×10^{-9}
$\mathbf{OH^+ + H_2O}$	$\rightarrow$	$\mathbf{OH + H_2O^+}$	1.6×10^{-9}
$H_2O^+ + H_2$	$\rightarrow$	$H + H_3O^+$	6.1×10^{-10}
$\mathbf{H_2O^+ + H_2O}$	$\rightarrow$	$\mathbf{OH + H_3O^+}$	2.1×10^{-9}
$\mathbf{H_2O^+ + H_2O}$	$\rightarrow$	$\mathbf{H_2O + H_2O^+}$	7.9×10^{-9}

Table 4: Photolytic reactions / rates

Reaction			$\kappa_\alpha^{\rm ion}$ [cm^3 s^{-1}]
$H + \gamma$	$\rightarrow$	$H^+ + e$	8.0×10^{-10}
$H_2 + \gamma$	$\rightarrow$	$H_2^+ + e$	5.9×10^{-10}
$\mathbf{O} + \gamma$	$\rightarrow$	$\mathbf{O^+ + e}$	2.3×10^{-9}
$\mathbf{OH} + \gamma$	$\rightarrow$	$\mathbf{OH^+ + e}$	3.7×10^{-9}
$H_2O + \gamma$	$\rightarrow$	$H_2O^+ + e$	3.7×10^{-9}
			$\kappa_\alpha^{\rm diss}$ [cm^3 s^{-1}]
$H_2 + \gamma$	$\rightarrow$	$H + H$	4.9×10^{-10}
$\mathbf{OH} + \gamma$	$\rightarrow$	$\mathbf{O + H}$	5.5×10^{-8}
$\mathbf{H_2O} + \gamma$	$\rightarrow$	$\mathbf{H + OH}$	1.1×10^{-7}
$\mathbf{H_2O} + \gamma$	$\rightarrow$	$\mathbf{H_2 + O}$	1.5×10^{-8}
			$\kappa_\alpha^{\rm diss,ion}$ [cm^3 s^{-1}]
$H_2 + \gamma$	$\rightarrow$	$H^+ + H + e$	1.0×10^{-10}
$H_2O + \gamma$	$\rightarrow$	$H^+ + OH + e$	1.4×10^{-10}
$H_2O + \gamma$	$\rightarrow$	$O^+ + H_2 + e$	6.4×10^{-11}
$H_2O + \gamma$	$\rightarrow$	$OH^+ + H + e$	6.1×10^{-10}

Table 5: Impact dissociation reactions / rates

Reaction			D_α [cm^3 s^{-1}]
$H_2 + e$	$\rightarrow$	$H + H + e$	1.9×10^{-9}
$\mathbf{OH + e}$	$\rightarrow$	$\mathbf{O + H + e}$	6.7×10^{-11}
$\mathbf{H_2O + e}$	$\rightarrow$	$\mathbf{OH + H + e}$	1.2×10^{-9}
			$D_\alpha^{\rm h}$ [cm^3 s^{-1}]
$H_2 + e_h$	$\rightarrow$	$H + H + e$	2.3×10^{-6}
$\mathbf{OH + e_h}$	$\rightarrow$	$\mathbf{O + H + e}$	8.4×10^{-8}
$\mathbf{H_2O + e_h}$	$\rightarrow$	$\mathbf{OH + H + e}$	1.5×10^{-6}

Table 6: Electron impact ionization reactions / rates

Reaction			I_α [cm^3 s^{-1}]
$H + e$	$\rightarrow$	$H^+ + 2e$	1.1×10^{-11}
$O + e$	$\rightarrow$	$O^+ + 2e$	1.3×10^{-11}
$O^+ + e$	$\rightarrow$	$O^{++} + 2e$	2.4×10^{-16}
$\mathbf{OH} + \mathbf{e}$	$\rightarrow$	$\mathbf{OH}^+ + \mathbf{2e}$	5.3×10^{-11}
$H_2O + e$	$\rightarrow$	$H_2O^+ + 2e$	7.0×10^{-12}
			I_α^{h} [cm^3 s^{-1}]
$\mathbf{H} + \mathbf{e}_h$	$\rightarrow$	$\mathbf{H}^+ + \mathbf{2e}$	3.2×10^{-8}
$\mathbf{O} + \mathbf{e}_h$	$\rightarrow$	$\mathbf{O}^+ + \mathbf{2e}$	9.0×10^{-8}
$O^+ + e_h$	$\rightarrow$	$O^{++} + 2e$	2.7×10^{-8}
$\mathbf{OH} + \mathbf{e}_h$	$\rightarrow$	$\mathbf{OH}^+ + \mathbf{2e}$	1.2×10^{-7}
$\mathbf{H_2O} + \mathbf{e}_h$	$\rightarrow$	$\mathbf{H_2O}^+ + \mathbf{2e}$	9.1×10^{-8}

Table 7: Electron impact ionization-dissociation reactions / rates

Reaction			I_α^{diss} [cm^3 s^{-1}]
$H_2O + e$	$\rightarrow$	$H^+ + OH + 2e$	5.3×10^{-14}
$H_2O + e$	$\rightarrow$	$O^+ + 2H + 2e$	3.2×10^{-15}
$H_2O + e$	$\rightarrow$	$OH^+ + H + 2e$	1.1×10^{-12}
			$I_\alpha^{\mathrm{diss,h}}$ [cm^3 s^{-1}]
$\mathbf{H_2O} + \mathbf{e}_h$	$\rightarrow$	$\mathbf{H}^+ + \mathbf{OH} + \mathbf{2e}$	4.1×10^{-8}
$H_2O + e_h$	$\rightarrow$	$O^+ + 2H + 2e$	1.1×10^{-8}
$\mathbf{H_2O} + \mathbf{e}_h$	$\rightarrow$	$\mathbf{OH}^+ + \mathbf{H} + \mathbf{2e}$	4.5×10^{-8}

Table 8: Electron recombination reactions / rates

Reaction			R_α [cm^3 s^{-1}]
$H^+ + e$	$\rightarrow$	H	8.5×10^{-11}
$O^+ + e$	$\rightarrow$	O	3.2×10^{-13}
$O^{++} + e$	$\rightarrow$	O^+	1.9×10^{-12}
			R_α^{h} [cm^3 s^{-1}]
$H^+ + e_h$	$\rightarrow$	H	6.4×10^{-12}
$O^+ + e_h$	$\rightarrow$	O	3.0×10^{-13}
$O^{++} + e_h$	$\rightarrow$	O^+	1.5×10^{-12}

Table 9: Dissociative electronic recombination reactions / rates

Reaction			R_α^{diss} [cm^3 s^{-1}]
$H_2^+ + e$	$\rightarrow$	$H + H$	2.0×10^{-8}
$\mathbf{OH^+ + e}$	$\rightarrow$	$\mathbf{O + H}$	9.6×10^{-9}
$\mathbf{H_2O^+ + e}$	$\rightarrow$	$\mathbf{OH + H}$	2.0×10^{-8}
$\mathbf{H_3O^+ + e}$	$\rightarrow$	$\mathbf{OH + H_2}$	1.4×10^{-8}
			$R_\alpha^{\mathrm{diss,h}}$ [cm^3 s^{-1}]
$H_2^+ + e_h$	$\rightarrow$	$H + H$	2.0×10^{-8}
$OH^+ + e_h$	$\rightarrow$	$O + H$	1.1×10^{-9}
$H_2O^+ + e_h$	$\rightarrow$	$OH + H$	8.9×10^{-11}
$H_3O^+ + e_h$	$\rightarrow$	$OH + H_2$	4.7×10^{-11}

3 Source and Loss Equations for Each Individual Neutral Species

3.1 H_2O

$$\mathcal{S}_{\mathrm{H_2O}} = 1.2044 \times 10^{29} \left[\frac{\text{molecules}}{s}\right] + \left[(K13) \cdot n_{\mathrm{H_2O^+}}\right] \cdot n_{\mathrm{H_2O}} \tag{8}$$

$$\begin{aligned}
\mathcal{L}_{\mathrm{H_2O}} = \Big[& J04 + J05 + J10 + J11 + J12 + J13 \\
& + (D02 + I04 + ID01 + ID02 + ID03) \cdot n_{\mathrm{e}} \\
& + (K04) \cdot n_{\mathrm{H^+}} \\
& + (K08) \cdot n_{\mathrm{O^+}} \\
& + (K10 + K11) \cdot n_{\mathrm{OH^+}} \\
& + (K12 + K13) \cdot n_{\mathrm{H_2O^+}} \\
& + (K19 + K20) \cdot n_{\mathrm{H_2^+}} \Big] \cdot n_{\mathrm{H_2O}}
\end{aligned} \tag{9}$$

3.2 OH

$$\begin{aligned}
\mathcal{S}_{\mathrm{OH}} = & \left[J04 + J11 + D02 + (ID01) \cdot n_{\mathrm{e}}\right] \cdot n_{\mathrm{H_2O}} \\
& + \left[(RD02) \cdot n_{\mathrm{e}}\right] \cdot n_{\mathrm{H_2O^+}} \\
& + \left[(RD03) \cdot n_{\mathrm{e}}\right] \cdot n_{\mathrm{H_3O^+}}
\end{aligned} \tag{10}$$

$$\mathcal{L}_{\mathrm{OH}} = \left[J02 + J03 + (D01 + I01) \cdot n_e\right] \cdot n_{\mathrm{OH}} \tag{11}$$

3.3 H

$$\begin{aligned}
\mathcal{S}_{\mathrm{H}} = & \left[J04 + J13 + D02 + (2 \cdot ID02 + ID03) \cdot n_e\right] \cdot n_{\mathrm{H_2O}} \\
& + \left[J03 + D01\right] \cdot n_{\mathrm{OH}} \\
& + \left[J08 + J09 + 2 \cdot D03\right] \cdot n_{\mathrm{H_2}} \\
& + \left[(R01) \cdot n_e\right] \cdot n_{\mathrm{H^+}} \\
& + \left[(RD01) \cdot n_{\mathrm{e}}\right] \cdot n_{\mathrm{OH^+}} \\
& + \left[(RD02) \cdot n_{\mathrm{e}}\right] \cdot n_{\mathrm{H_2O^+}} \\
& + \left[(2 \cdot RD04) \cdot n_{\mathrm{e}}\right] \cdot n_{\mathrm{H_2^+}}
\end{aligned} \tag{12}$$

$$\mathcal{L}_{\mathrm{H}} = \left[J06 + (I02) \cdot n_{\mathrm{e}}\right] \cdot n_{\mathrm{H}} \tag{13}$$

3.4 H_2

$$\begin{aligned}\mathcal{S}_{\mathrm{H_2}} &= [J05 + J12] \cdot n_{\mathrm{H_2O}} \\ &\quad + [(RD03) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_3O^+}}\end{aligned} \tag{14}$$

$$\mathcal{L}_{\mathrm{H_2}} = [J07 + J08 + J09 + (D03) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_2}} \tag{15}$$

3.5 O

$$\begin{aligned}\mathcal{S}_{\mathrm{O}} &= [J05] \cdot n_{\mathrm{H_2O}} \\ &\quad + [J03 + D01] \cdot n_{\mathrm{OH}} \\ &\quad + [(R02) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{O^+}} \\ &\quad + [(RD01) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{OH^+}}\end{aligned} \tag{16}$$

$$\mathcal{L}_{\mathrm{O}} = [J01 + (I03) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{O}} \tag{17}$$

4 Source and Loss Equations for Each Individual Ion Species

4.1 H_2O^+

$$\mathcal{S}_{\mathrm{H_2O^+}} = [J10 + (I04) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_2O}} \tag{18}$$

$$\mathcal{L}_{\mathrm{H_2O^+}} = [(RD02) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_2O^+}} \tag{19}$$

4.2 H_3O^+

$$\mathcal{S}_{\mathrm{H_2O^+}} = 0 \tag{20}$$

$$\mathcal{L}_{\mathrm{H_2O^+}} = [(RD03) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_3O^+}} \tag{21}$$

4.3 $\mathbf{OH^+}$

$$\begin{aligned}\mathcal{S}_{\mathrm{OH^+}} &= [J13 + (ID03) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_2O}} \\ &\quad + [J02 + (I01) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{OH}} \end{aligned} \tag{22}$$

$$\mathcal{L}_{\mathrm{OH^+}} = [(RD01) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{OH^+}} \tag{23}$$

4.4 $\mathbf{H^+}$

$$\begin{aligned}\mathcal{S}_{\mathrm{H^+}} &= [J11 + (ID01) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_2O}} \\ &\quad + [J06 + (I02) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H}} \\ &\quad + [J09] \cdot n_{H_2} \end{aligned} \tag{24}$$

$$\mathcal{L}_{\mathrm{H^+}} = [(R01) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H^+}} \tag{25}$$

4.5 $\mathbf{H_2^+}$

$$\mathcal{S}_{\mathrm{H_2^+}} = [J07] \cdot n_{H_2} \tag{26}$$

$$\mathcal{L}_{\mathrm{H_2^+}} = [(RD04) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_2^+}} \tag{27}$$

4.6 $\mathbf{O^+}$

$$\begin{aligned}\mathcal{S}_{\mathrm{O^+}} &= [J12 + (ID02) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{H_2O}} \\ &\quad + [J01 + (I03) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{O}} \\ &\quad + [(R03) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{O^{++}}} \end{aligned} \tag{28}$$

$$\mathcal{L}_{\mathrm{O^+}} = [(I05 + R02) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{O^+}} \tag{29}$$

4.7 $\mathbf{O^{++}}$

$$\mathcal{S}_{\mathrm{O^{++}}} = [I05 \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{O^+}} \tag{30}$$

$$\mathcal{L}_{\mathrm{O^{++}}} = [(R03) \cdot n_{\mathrm{e}}] \cdot n_{\mathrm{O^{++}}} \tag{31}$$

5 Source and Loss Equation for Electrons

$$\begin{aligned}
\mathcal{S}_\mathrm{e} \;=\;& [J11 + J12 + J13 + D02 + 2 \cdot (I04 + ID01 + ID02 + ID03)] \cdot n_{\mathrm{H_2O}} \\
&+ [J02 + D01 + 2 \cdot I01] \cdot n_{\mathrm{OH}} \\
&+ [J06 + 2 \cdot I02] \cdot n_{\mathrm{H}} \\
&+ [J07 + J09 + D03] \cdot n_{\mathrm{H_2}} \\
&+ [J01 + 2 \cdot I03] \cdot n_{\mathrm{O}} \\
&+ [2 \cdot I05] \cdot n_{\mathrm{O+}}
\end{aligned} \tag{32}$$

$$\begin{aligned}
\mathcal{L}_\mathrm{e} \;=\;& [D02 + I04 + ID01 + ID02 + ID03] \cdot n_{\mathrm{H_2O}} \\
&+ [D01 + I01] \cdot n_{\mathrm{OH}} \\
&+ [I02] \cdot n_{\mathrm{H}} \\
&+ [D03] \cdot n_{\mathrm{H_2}} \\
&+ [I03] \cdot n_{\mathrm{O}} \\
&+ [I05 + R02] \cdot n_{\mathrm{O+}} \\
&+ [R01] \cdot n_{\mathrm{H^+}} \\
&+ [R03] \cdot n_{\mathrm{O^{++}}} \\
&+ [RD01] \, n_{\mathrm{OH^+}} \\
&+ [RD02] \, n_{\mathrm{H_2O^+}} \\
&+ [RD03] \, n_{\mathrm{H_3O^+}} \\
&+ [RD04] \, n_{\mathrm{H_2^+}}
\end{aligned} \tag{33}$$

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