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Received June 23, 2004

Abstract—A mathematical model for the formation of main transient and final radiolysis products generated in tracks of fast electrons and positrons in water and aqueous solutions was constructed and described in terms of equations of inhomogeneous chemical kinetics in part 1 of this study. The model takes into account the reactions of a solute with epithermal electrons, thermal, and hydrated electrons; the ambipolar character of diffusion of charged intratrack particles; and new pathways of the formation of hydrogen and positronium due to the appearance of weakly bound states of electrons. In the present paper, the model was quantitatively fitted to experimental data on both time variation in the yields of radiolytic products (H₂O₂, H, OH, OH⁻, H₂O₂) in pure water and the yields of hydrogen (H₂, H), hydrated electron (e⁻aq) and positronium (Ps) in various dilute and concentrated aqueous solutions.

In the previous paper [1], we formulated the general model of chemical reactions in the tracks produced by fast electrons and positrons traveling in water and aqueous solutions. The model includes various processes involving primary, intermediate, and final radiolysis products and occurring over the wide span of time 10⁻¹³–10⁻⁶ s. The tracks of fast electrons and positrons are approximated by a set of single-type spherical clusters (spurs and blobs) that occur far from one another and are initially composed of the same number n₀ of short-lived radical cations H₃O⁺ and “hot” electrons e⁺, which interact with one another and with water and dissolved solutes to form stable products (Table 1). The intratrack processes are quantitatively described by means of the following system of differential equations of inhomogeneous chemical kinetics:

\[
\frac{\partial c_i}{\partial t} = D_i(t)\Delta c_i - k_{ie}c_i + k_{eOH}c_{OH},
\]

\[
\frac{\partial c_e}{\partial t} = D_e(t)\Delta c_e - \left( k_{ie}c_i + k_{eOH}c_{OH} \right) c_e \Theta(t > t_{th}) - k_{eS}c_e c_S,
\]

\[
c_e(r, 0) = n_0 g(r, 0, a_{th}, 0),
\]

\[
g(r, 0, a_{th}, 0) = \frac{\exp(-r^2/a_{th}^2)}{\pi^{3/2} a_{th}^3},
\]

\[
\frac{\partial \tilde{c}_S}{\partial t} = D_S(t)\Delta \tilde{c}_S + (k_{cS}c_e + k_{HS}\tilde{c}_S - k_{iS}c_i)\tilde{c}_S,
\]

\[
\frac{\partial \tilde{c}_S}{\partial t} = D_S(t)\Delta \tilde{c}_S + k_{cS}c_e + k_{HS}\tilde{c}_S - k_{iS}c_i \tilde{c}_S,
\]

\[
c_S(r, 0) = 0,
\]

\[
\frac{\partial c_h}{\partial t} = D_h(\Delta c_h + k_{hH}\tilde{c}_S - k_{hH}c_h + 2k_{HH}c_H^2 + k_{OH}\tilde{c}_S - k_{HH}c_h c_H - k_{HH}c_h c_{H₂O} - k_{HS}\tilde{c}_S,
\]

\[
c_h(r, 0) = n_0 G_{H_{th}} g(r, 0, a_{th}, 0),
\]

\[
\frac{\partial \tilde{c}_S}{\partial t} = D_S(t)\Delta \tilde{c}_S + \Theta(t > t_{th}) - (2k_{hh}c_h + k_{HS}\tilde{c}_S,
\]

\[
\tilde{c}_S(r, t \leq t_{th}) = 0
\]
ON THE MECHANISM OF FORMATION OF INTRATRACK YIELDS

Table 1. Primary radiation-chemical reactions and their rate constants [1].

<table>
<thead>
<tr>
<th>Ionization and electronic excitations</th>
<th>Rate constant, l mol⁻¹ s⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>(e^{**} + H_2O \rightarrow )</td>
<td>(t_{th} = 0.12) ps, (\tau_{e_{aq}}^{aq} = 0.3) ps</td>
</tr>
<tr>
<td>(e^{**} + H_2O^* \rightarrow )</td>
<td>(f_{H_2} = 0.165, k_{ie}^{aq} = 47–54) l mol⁻¹</td>
</tr>
<tr>
<td>(H_2O^* \rightarrow )</td>
<td>(\tau_{il\ molr} = 10^{e_{aq}})</td>
</tr>
<tr>
<td>(H + OH)</td>
<td>(k_{eOH} = 0)</td>
</tr>
<tr>
<td>(H + NO_3^{-} \rightarrow )</td>
<td>(k_{eNO_3^{-}} \times \tau_{e_{aq}}^{aq} = 2.1(2)) l mol⁻¹</td>
</tr>
<tr>
<td>(H + OH_2 \rightarrow )</td>
<td>(k_{eH_2O} \times \tau_{e_{aq}}^{aq} = 0.50(3)) l mol⁻¹</td>
</tr>
<tr>
<td>(ClO_4^{-} \rightarrow )</td>
<td>(k_{eClO_4^{-}} \times \tau_{e_{aq}}^{aq} = 0.08–0.09) l mol⁻¹</td>
</tr>
<tr>
<td>(Ac^{-} \rightarrow )</td>
<td>(k_{eAc^{-}} \times \tau_{e_{aq}}^{aq} = 0.6–0.7) l mol⁻¹</td>
</tr>
<tr>
<td>(H + Cl \rightarrow )</td>
<td>(k_{eCl^-} \times \tau_{e_{aq}}^{aq} = 36–42) l mol⁻¹</td>
</tr>
<tr>
<td>(H + Ac^{-} \rightarrow )</td>
<td>(k_{eAc^{-}} \times \tau_{e_{aq}}^{aq} = 0.04–0.06) l mol⁻¹</td>
</tr>
<tr>
<td>(H + H_2O_2 \rightarrow )</td>
<td>(k_{eH_2O_2} \times \tau_{e_{aq}}^{aq} = 0.01–0.05) l mol⁻¹</td>
</tr>
<tr>
<td>(H_2 + \ldots)</td>
<td>(k_{eAc^{-}} \times \tau_{e_{aq}}^{aq} \leq 0.01) l mol⁻¹</td>
</tr>
</tbody>
</table>

H2 + H2O  \(\rightarrow\) H2 + OH⁻

Note: The parameters relevant to the picosecond radiolysis step have been determined by fitting to the data presented in Figs. 2–4. The rate constants of the reactions occurring on the nanosecond time scale were borrowed from the Radiation Chemistry Data Center web site http://www.rcdc.nd.edu. All \(k_{ij}\) values are the rate constants of formation of one product species, not of the reactant decay (the values of the corresponding decay rate constants are twice greater).