environments

MDPI

# Preliminary Assessment of Radiolysis for the Cooling Water System in the Rotating Target of SORGENTINA-RF

Table S1 reports the system of equations generated by Equation (3) to calculate the concentrations of each species at different times, where P*i* is the production rate of the i[th] radiolytic species.

**Table S1.** *Simulation equations.*

$$\frac{d(H_2O)}{d(t)} = k1*OH*H_2 + k3*OH*H_2O_2 + k5*OH*HO_2 + k11*H*H_2O_2 + k12*OH*H + (-1)*k15*e^-*O_2^- + (-1)*k17*e^-*H + (-2)*k20*e^{-2} + k23*H_2O_2*HO_2 + k28*OH^-*H^+ + (-1)*k29*H_2O + k30*H*OH^- + (-1)*k31*O_2^{-2} + PH_2O$$

$$\frac{d(e^-)}{d(t)} = (-1)*k7*e^-*OH + (-1)*k14*e^-*O_2 + (-1)*k15*e^-*O_2^- + (-1)*k16*e^-*HO_2 + (-1)*k17*e^-*H + (-1)*k18*e^-*H_2O_2 + (-1)*k19*e^-*H^+ + (-2)*k20*e^{-^2} + k30*H*OH^- + Pe^-$$

$$\frac{d(OH)}{d(t)} = (-1)*k1*OH*H_2 + (-1)*k2*OH*HO_2^- + (-1)*k3*OH*H_2O_2 + (-1)*k4*OH*O_2^- + (-1)*k5*OH*HO_2 + (-2)*k6*OH^2 + (-1)*k7*e^-*OH + k11*H*H_2O_2 + (-1)*k12*OH*H + k18*e^-*H_2O_2 + k23*H_2O_2*HO_2 + k32*H_2O_2*O_2^- + POH$$

$$\frac{d(H)}{d(t)} = k1*OH*H_2 + (-1)*k8*H*O_2 + (-1)*k9*H*O_2^- + (-1)*k10*H*HO_2 + (-1)*k11*H*H_2O_2 + (-1)*k12*OH*H + (-2)*k13*H^2 + (-1)*k17*e^-*H + k19*e^-*H^+ + (-1)*k30*H*OH^- + PH$$

$$\frac{d(H_2)}{d(t)} = (-1)*k1*OH*H_2 + k13*H^2 + k17*e^-*H + k20*(e^-)^2 + PH_2$$

$$\frac{d(H_2O_2)}{d(t)} = (-1)*k3*OH*H_2O_2 + k6*OH^2 + k10*H*HO_2 + (-1)*k11*H*H_2O_2 + (-1)*k18*e^-*H_2O_2 + k22*HO_2^2 + (-1)*k23*H_2O_2*HO_2 + (-1)*k26*H_2O_2 + k27*H^+*{HO_2}^- + (-1)*k32*H_2O_2*O_2 + PH_2O_2$$

$$\frac{d(HO_2)}{d(t)} = k2*OH*HO_2^- + k3*OH*H_2O_2 + (-1)*k5*OH*HO_2 + k8*H*O_2 + (-1)*k10*H*HO_2 + (-1)*k16*e^-*HO_2 + (-1)*k21*HO_2*O_2^- + (-2)*k22*HO_2^2 (-1)*k23*H_2O_2*HO_2 + (-1)*k24*HO_2 + k25*O_2^-*H^+ + PHO_2$$

$$\frac{d(O_2)}{d(t)} = k4*OH*O_2^- + k5*OH*HO_2 + (-1)*k8*H*O_2 + (-1)*k14*e^-*O_2 + k21*HO_2*O_2^- + k22*HO_2^2 + k23*H_2O_2*HO_2 + k31*(O_2^-)^2 + k32*H_2O_2*O_2^- + PO_2$$

$$\frac{d(O_2^-)}{d(t)} = (-1)*k4*OH*O_2^- + (-1)*k9*H*O_2^- + k14*e^-*O_2 + (-1)*k15*e^-*O_2^- + (-1)*k21*HO_2*O_2^- + k24*HO_2 + (-1)*k25*O_2^-*H^+ + (-2)*k31*O_2^{-2} + (-1)*k32*H_2O_2*O_2^- + PO_2^-$$

$$\frac{d(OH^-)}{d(t)} = k2*OH*HO_2^- + k4*OH*O_2^- + k7*e^-*OH + k15*e^-*O_2^- + k17*e^-*H + k18*e^-*H_2O_2 + 2*k20*e^{-2} + (-1)*k28*OH^-*H^+ + k29*H_2O + (-1)*k30*H*OH^- + k31*{O_2}^{-2} + k32*H_2O_2*{O_2}^- + POH^-$$

$$\frac{d(H^+)}{d(t)} = (-1)*k19*e^-*H^+ + k24*HO_2 + (-1)*k25*{O_2}^-*H^+ + k26*H_2O_2 + (-1)*k27*H^+*{HO_2}^- + k + (-1)*k28*OH^-*H^+ + k29*H_2O + PH^+$$

$$\frac{d({HO_2}^-)}{d(t)} = (-1)*k2*OH*HO_2^- + k9*H*O_2^- + k15*e^-*O_2^- + k16*e^-*HO_2 + k21*HO_2*O_2^- + k26*H_2O_2 + (-1)*k27*H^+*HO_2^- + k31*(O_2^-)^2 + PHO_2^-$$

This sets a relation between the energy deposition by neutrons and gammas in the water and the concentration of each species. The Monte Carlo code is used to calculate the energy deposition values, transport neutrons and photons in the given geometry. The output is the energy deposition which is calculated by a track length estimator in a given volume which is calculated as follows:

$$Energy\ deposition = W \times T_l \times \sigma_{t(E)} \times H(E) \times \frac{\rho_a}{m}$$

where

$W$: particle statistical weight

$T_l$: track length

$\sigma_{t(E)}$: microscopic total cross-section

*H(E)*: Heating number
$\rho_a$: atom density
*m*: mass of the given volume.