# Analysis of mass transfer effect on chemically produced iodine release from aqueous phase

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To investigate the mass transfer effect on the overall iodine release to the environment, we propose a chemical-process-reduced mass transfer (CPR-MT) model for iodine that is based on two-film theory and includes an effective mass transfer coefficient ($\tilde{k}_{\mathrm{mt}}$). By formally decomposing $\tilde{k}_{\mathrm{mt}}$ into iodine chemistry and mass transfer contributions, we discuss their impact for a variety of severe accident conditions of nuclear power station.

**Keywords:** Iodine chemistry, KICHE, mass transfer coefficient, two-film theory

**1. Introduction** In the source term evaluation of iodine during a severe accident in nuclear power station, a combination model between iodine chemistry and mass transfer is usually employed to describe the transferring behavior from the aqueous phase to the gas phase as the re-volatilization. In general, it is difficult to separately evaluate the contributions from chemical and mass-transfer processes in the overall iodine release. Therefore, in this study, we attempt it by proposing a chemical-process-reduced mass transfer (CPR-MT) model for iodine. The model is based on the two-film theory and, instead of the conventional mass transfer coefficient ($k_{\mathrm{mt}}$), it includes an effective mass transfer coefficient of iodine ($\tilde{k}_{\mathrm{mt}}$) as a single and optimized parameter. Here, $\tilde{k}_{\mathrm{mt}}$ involves the both contributions and is determined by fitting to the time-dependent concentrations of several iodine species. By regarding this coefficient as a function of pH and $k_{\mathrm{mt}}$, we formally separate their contributions ($F_{\mathrm{pH}}$ and $F_{\mathrm{mt}}$) from $\tilde{k}_{\mathrm{mt}}$,

$$\tilde{k}_{\mathrm{mt}}(\mathrm{pH}, k_{\mathrm{mt}}) = F_{\mathrm{pH}} F_{\mathrm{mt}} \tilde{k}^{0}_{\mathrm{mt}}, \quad (1)$$

where $\tilde{k}^{0}_{\mathrm{mt}}$ is the value of $\tilde{k}_{\mathrm{mt}}$ under pH and $k_{\mathrm{mt}}$ set to 7 and $10^{-5}$ m/s, respectively.

**2. Computational details** KICHE code [1] with LIRIC 3.2 [2] reaction database was utilized to evaluate the time-dependent concentrations of iodine species at room temperature. Analytical system was set to the real-size torus-shaped suppression chamber in Fukushima Daiichi Unit 3. The initial iodine anion concentration and γ-ray dose rate are 1.0E-5 mol/L and 3 kGy/h, respectively. The gas phase is swept by nitrogen gas with 300 $m^3$/s.

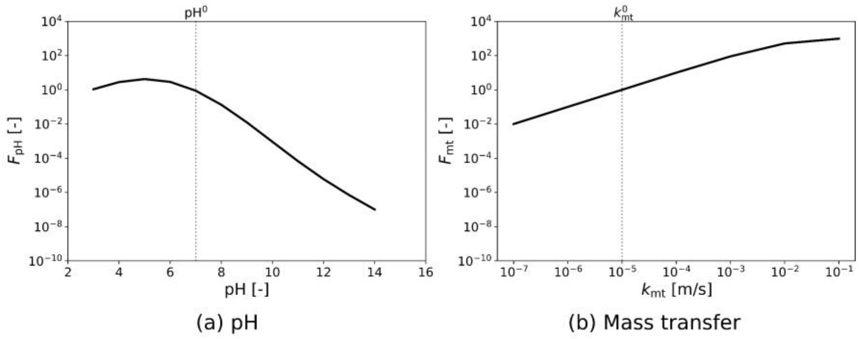


Figure 1 pH (a) and mass transfer (b) contributions defined in Eq.(1).

**3. Results and discussion** Figure 1 plots $F_{\mathrm{pH}}$ and $F_{\mathrm{mt}}$ as functions of pH and $k_{\mathrm{mt}}$, respectively. In this case, $\tilde{k}^{0}_{\mathrm{mt}}$ is 2.26 m/s. Even though there is a very broad peak at pH = 5, the $F_{\mathrm{pH}}$ change is small in the acidic range (pH < 7). Hence, in this range, the contribution of mass transfer is significant. Not shown here, the curvature of $F_{\mathrm{pH}}$ is dominated by the amount of molecular iodine ($I_2$) in aqueous phase. Interestingly, in the logarithmic scale, $F_{\mathrm{mt}}$ is nearly linear except for a very high rate range. These results show that the uncertainty of $k_{\mathrm{mt}}$ (or its product with gas-liquid interfacial area) has a large impact on the source term evaluation for iodine, as well as iodine chemistry.

**References** [1] Moriyama, K., et al. JAEA-Data/Code 2021-034 (2011). [2] Wren, J.C., et al. Radiat. Phys. Chem., 60, 577-596 (2001).