CFD Analyses of Re-Evolved Iodine from an In-containment Water Pool

Tae Hyeon Kim[a], Woo Sung Yoon[b], Ji Hwan Jung[b*]
[a]*Central Research Institute, Korea Hydro & Nuclear Power Co. LTD., Yuseng-gu, Daejeon, Korea*
[b]*School of Mechanical Engineering, Pusan National University, Geumjeong-gu, Busan, Korea*
[*]*Corresponding author: jihwan@pusan.ac.kr*

1. Introduction

When a **l**oss **o**f **c**oolant **a**ccident (LOCA) occurs in a pressurized water reactor, fission products may be released into the atmosphere. Iodine, one of the fission products, is a major contributor to the potential atmospheric source term. A good understanding of the behavior of iodine is required to evaluate the safety and emergency procedures after a LOCA. The quantity of re-evolved iodine is related to pH level, temperature, and iodine concentration of water pool. Previous reactor safety studies have demonstrated that among all quantities affecting the iodine re-evolution, the pH of the water pool is the most important factor. In the calculation of pH for water pool, sequence calculations must consider this variable if any aqueous iodine is present, even if it is initially present in stable forms.

The present study consists of two parts: the pH evaluation and the evaluation of the iodine re-evolution. The current paper focuses on the pH evaluation method, the development of a **u**ser-**d**efined **f**unction (UDF) and the iodine re-evolution from the water pool. CFD that incorporates the UDF was used in this study to calculate the local pH level in the transient condition. The amount of re-evolved iodine was calculated based on the iodine concentration, temperature, and pH. The transportation and resulting distribution of the iodine concentration, temperature, and pH were calculated using transient analyses with CFD. The quantity of re-evolved iodine was obtained with several assumptions. In addition, the effects of the evaluation method on the estimated amount of re-evolved iodine are compared and discussed.

2. Methods and Results

The quantitative evaluation of re-evolved iodine during a LOCA in a nuclear power plants is done in two stages. The first stage is to calculate the pH in the water pool, and the second stage is to calculate the quantity of re-evolved iodine. Evaporated iodine, from the water pool to the containment atmosphere, can be estimated from characteristic iodine behaviors and pH calculations.

2.1 The pH Calculation Program

In order to predict iodine re-evolution from water pool after a LOCA, a pH evaluation program named **e**valuation of **pH** **i**n **c**ontainment building (EPHIC) was developed, and can consider the contributions from various acidic and basic materials. This program calculates the equilibrium concentrations of acidic and basic chemicals at their minimum of Gibbs free energy using their thermodynamic properties. EPHIC also calculates pH, using the equilibrium ion concentration and activity of hydrogen. This program was verified against acid-base titration experiments. Figure 1 illustrates validation test results for EPHIC calculations and experimental data. The calculated pHs for the various solutions were in good agreement with their measured values. Thus, EPHIC is considered to be suitable for the evaluation of pH in water pool and for the evaluation of iodine re-evolution, when it is incorporated into a CFD package.

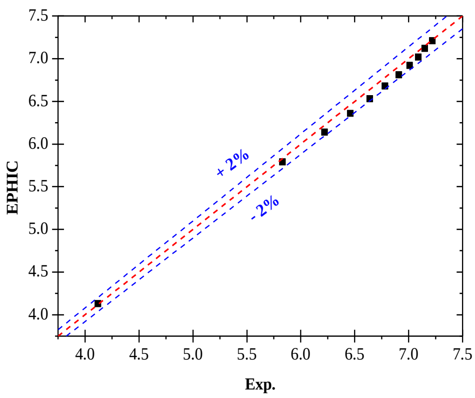


Fig. 1. Validation test results for EPHIC.

2.2 CFD Analysis of pH in Water Pool

The initial coolant of the water pool contains boric acid and nitric acid. Coolant containing TSP flows into the water pool through the HVT, causing chemical reaction. The pH in the water pool increases, due to the increase in TSP concentration, as a function of time. A three-dimensional (3D) CFD analysis with UDF that modified of EPHIC was utilized to evaluate the transport of acidic and basic materials, as well as temperature and pH distribution in the water pool after a LOCA. A 3D CAD model for the water pool of APR1400 was constructed and a 3D CFD analysis was conducted. Boundary conditions were determined in consideration of the design of APR1400. The recirculation mode was analyzed, assuming that the water level of the water pool is maintained at a quasi-steady state and that the recirculation pump operates.

Figure 2 shows boundary conditions and lumped region of the water pool.

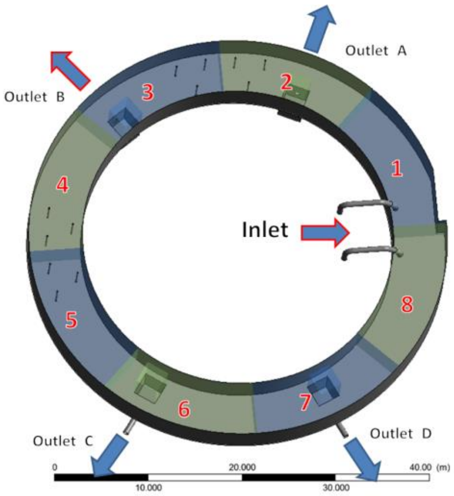
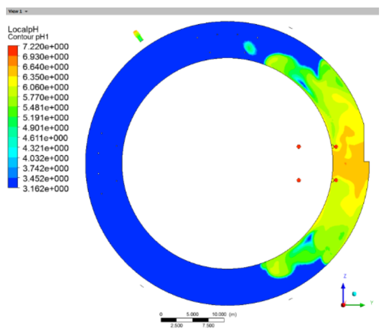
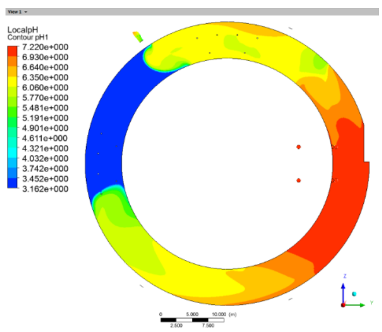


Fig. 2. Lumped calculation region of the water pool.

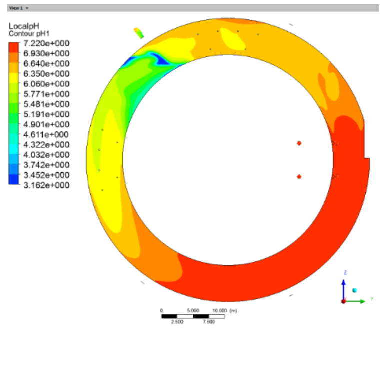
Figure 3 displays the pH contours as a function of time at the mid water level. The pH contour is analogous to the temperature or ion contours, because their energy and mass transfer equations have the same form. The pH of the water pool is 7.0 or higher if the concentrations of the acidic and basic materials exceed 70% of their maximum. Thus, the area with a pH greater than 7.0 expands with time.



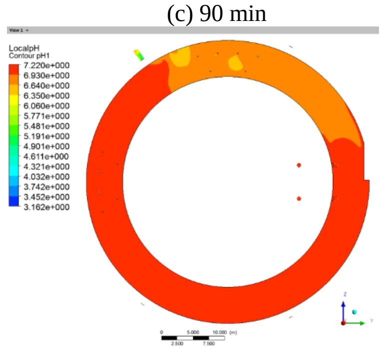
(a) 20 min



(b) 60 min



(c) 90 min



(d) 157 min

Fig. 3. pH contours as a function of time at mid-level.

The pH variation in each lumped segment is plotted in Fig. 4. The total-volume-averaged pH is also plotted, for comparison. The whole volume averaged pH reached 7.0 after 8967 s (149.5 min). The concentration distribution of the hydrogen ions revealed a transition similar to that of the temperature and ionized iodine concentration distributions. In addition, there are many consistencies among the lumped-segment average pHs, temperature distributions, and ionized iodine concentrations.

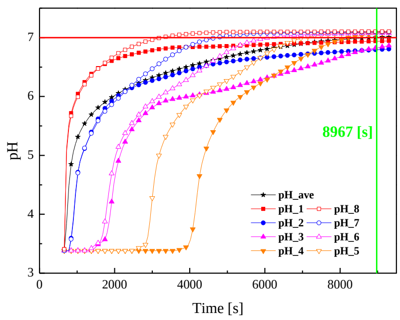


Fig. 4. Averaged pH as a function of time in the water pool.

The 3D CFD analysis results show that a pH of 7.0 is reached after 149.5 minutes. The lumped-segment averaged pH increases, depending on location. Near the spillway, the change in the averaged pH is faster than the change in whole volume's averaged pH. Regional averaged pHs rapidly approach an asymptote in clockwise flow direction. In the counterclockwise flow direction, however, the pH changes are dependent on the path of the fluid flow. Similar to the temperature distribution, the ionized iodine concentration distribution and the lumped-segment average pH are increased by the location of the fluid.

2.3 Evaluation for Iodine Re-Evolution in Water Pool

Using the CFD analysis results described above, the amount of re-evolved iodine can be estimated. Four different methods for evaluating the amount of re-evolved iodine were examined: Method 1 was the overall volume-averaged method; Method 2 was the lumped segment volume-averaged method; Method 3 was the interfacial volatilization method; and Method 4 was the two-film model method. Figure 5 presents the accumulated quantity of the re-evolved iodine as a function of time calculated using each evaluation method. The accumulated quantity increases sharply after initiation of the event and reaches an asymptote soon. It is because the pH of the solution also increases and suppresses the re-evolution of iodine. The amount of re-evolved iodine calculated using Method 1 appeared to be significantly higher than that determined using the other methods. The amount of re-evolved iodine evaluated using Method 3, which appeared to be more realistic because the convective iodine transport through the water solution was considered, was approximately two thousandth of that evaluated using Method 1. This indicates that Method 1, which has been used for safety analyses, is very conservative compared with other realistic methods.

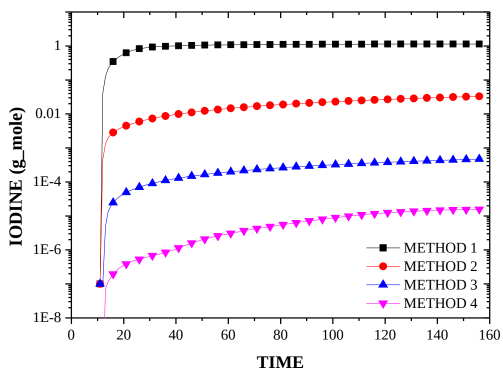


Fig. 5. Quantity of re-evolved iodine as a function of time for each evaluation method.

3. Conclusions

The quantitative evaluation of re-evolved iodine during a LOCA in a commercial nuclear power plants is done in two stages. The first stage is to calculate the pH in the water pool, and the second stage is to calculate the quantity of re-evolved iodine. Evaporated iodine, from the water pool water to the containment atmosphere, can be estimated from characteristic iodine behaviors and pH calculations. The 3D CFD analysis results show that the pH reached 7.0 after 149.5 minutes. Lumped-segment averaged pH increased, depending on location. Near the spillway, the change in averaged pH was faster than the change in whole-volume averaged pH. Evaluating the amount of re-evolved iodine were examined using four different methods. As a result of our evaluation of iodine re-evolution, the initial molecular iodine concentration of a water pool has a significant impact on the amount of gaseous iodine, more so than the pH or temperature, due to the locally similar distributions of TSP and iodine. In other words, when the local iodine concentration is increased, the local pH is simultaneously increased, although the presence of TSP mitigates the rise in pH. An increased pH obstructs the conversion of iodide ions into molecular iodine. Therefore, the evaluation of the local distributions of TSP and iodine is necessary.

REFERENCES

[1] P. Atkins and J. D. Paula, Atkins' physical chemistry. 8th ed., W.H. Freeman and Company, New York (2006)
[2] E.C. Beahm, R.A. Lorenz, C. F. Weber, Iodine Evolution and pH Control, NUREG/CR-5950 (ORNL/TM-12242), Oak Ridge National Laboratory (1992).
[3] B. Clément, L. Cantrel, G. Ducros, F. Funke, L. Herranz, A. Rydl, G. Weber, C. Wren, State of the art report on iodine chemistry. NEA/CSNI/R(2007)1, OECD, Paris (2007).
[4] Energy Operations Engineering Report for Suppression Pool pH and Iodine Re-Evolution Methodology, GGNS-98-0039, Revision 3, Entergy Operations, Inc. (2000).
[5] C.F. Weber and E.C. Beahm, Calculation of pH and Iodine volatility under reactor accident conditions, ORNL/NRC/LTR-99/3, Oak Ridge National Laboratory (1999).
[6] C.F. Weber, E.C. Beahm, T.S. Kress, Modeling of Iodine behavior in reactor containments, ORNL/TM-12202, Oak Ridge National Laboratory (1992).