

## Evaluation of the Pool Chemistry Model in MELCOR by Considering the Organic Iodine Formation within the Pool using the Phebus FPT-1 Test Data

Jong-Hwa. Park,<sup>a</sup> Dong-Ha. Kim,<sup>a</sup>

<sup>a</sup> KAERI, 150 Dukjin-dong, Yusong, Taejeon, 305-353, jhpark3@kaeri.re.kr

### 1. Introduction

In the severe accident, the understanding on the chemical form of iodine and its behavior is important for estimating the source terms because it has not only a active chemical features but also hazard to the public.

From the current understanding on the early phase of severe accident, it is known that the most of the injected iodine into the containment is the aerosol form of metal iodide such as cesium iodide and silver iodide. The remaining fraction is the gaseous form of iodine such as molecular iodine, elemental iodine or hydrogen iodide. These aerosol and gaseous iodine can be removed by the engineered safety features such as the spray system. Also the natural depletion processes like condensing, settling or deposit on the surface remove the most of the suspended aerosol and gaseous iodine and finally, cause them to accumulate within the pool on the bottom floor.

As time goes on, in the late phase of severe accident, the iodine pool chemistry phenomena starts under the strong radiation condition. The dissolved iodine within the pool can be transformed to the volatile iodine such as molecular iodine and organic iodine due to its strong chemical activity and various kind of immersed impurities such as alcohol or grease. This transformed volatile iodine can be partitioned to the atmosphere from the inside of pool. Consequently, an equilibrium concentration is reached and this suspended gaseous form of iodine becomes the main threat to the public when the containment fails or leaks in the late phase of severe accident.

Therefore, decreasing the equilibrium concentration of the suspended gaseous iodine and the trapping of iodine within the pool are the key parameters of the iodine management strategy in the late phase of severe accident. The Phebus FPT-1 showed that the silver could play an important role in trapping the iodine in the sump by forming the insoluble silver iodide from  $I_2$  or  $I^-$  [1].

The formation of volatile iodine depends on the PH, pool temperature and concentration of iodine. Generally, it showed that the high PH value could prevent the formation of volatile iodine. Therefore the addition of silver into the pool and the control of PH at high value are another important parameters for the iodine management strategy.

In this study, the pool chemistry within the sump of Phebus FPT-1 was simulated with MELCOR1.8.5. The purpose of this study is to evaluate the status of current pool chemistry model in MELCOR. The description on the input data and some assumptions will be given in section 2. Also, the evaluation results and the main findings on the pool chemistry model in MELCOR will be shown in conclusion as a summary form.

### 2. Description of the Actual Work

The current MELCOR1.8.5 code does not include the equations for the organic reactions within the pool of sump. Therefore, 43 equations were implemented into the pool chemistry model in MELCOR. Although the main focused place is confined to the containment and sump, the entire experimental circuit was modeled because the amount of injected gaseous iodine into the containment was uncertain. Therefore, this amount of injected gaseous iodine into the containment was modeled to predict by the code. The form of the injected iodine compounds, gaseous or aerosol, is dependent on their vapor pressure value. At present, no correlation is available for the vapor pressure on the methyl iodine and the silver iodine. Therefore, the vapor pressure on the methyl iodine was arbitrary modeled as the same correlation as that of the molecular iodine. For the silver iodine, the vapor pressure correlation from cesium iodide was applied. The iodine compounds that can exist in this study were predefined as cesium iodine, molecular iodine, silver iodine and methyl iodine by input.

Both the containment and the sump were modeled together as a single control volume. Therefore the mass transfer and partitioning can occur between the atmosphere of the containment and the surface of the pool. The elemental iodine and hydrogen iodide cannot be partitioned. The only iodine species that can be partitioned was assumed as molecular iodine and methyl iodine.

The un-measured cable mass and the dose rate at three places such as atmosphere, wall surface and pool were arbitrary assumed by the user. But the basic thermal hydraulic parameters such as the gas temperature, the containment pressure, the pool temperature were calculated by code. The variation of PH within the pool of sump was modeled using the tabular function option supplied from the measured data. No buffer material was modeled due to its absence in this experiment.

### 3. Conclusion

Concerning the organic iodine formation in the containment on the wall and sump, the current MELCOR1.8.5 does not have a capability to predict the important phenomena about organic iodine behavior. Therefore, 43 equations for the organic iodine reaction within the pool under the radiation condition were implemented and link to the MELCOR1.8.5. The pool chemistry phenomena of Phebus FPT-1 were simulated with this MELCOR (Refer to Figure 1.).

Although Figure 1 showed so small amount of methyl iodine with order of minus 28, the Phebus FPT-1 experiment showed an equilibrium concentration of gaseous iodine of 0.063% based on the initial core inventory after 3.5 days from the reactor scram. This measured value corresponds to about 12 kg for the typical PWR plant. As shown in Figure 1, the updated organic iodine model largely underestimated the produced amount of methyl iodine both in the pool and atmosphere. Therefore, it is necessary to improve the testing model on the organic iodine formation. On the contrary, the current MELCOR1.8.5 estimated that no organic iodine appeared from either the pool or atmosphere.

The evaluation results on the pool chemistry model in MELCOR were summarized as bellows;

- The MELCOR considers only the formation of organic iodine within the pool. But Phebus FP results showed that the organic iodine could be formed not only from the pool but also from the iodine deposited on the paint surface. Therefore, in addition to the model for the formation of organic iodine from the pool, other type of the organic formation needs to be examined and modeled.

- Also, concerning the formation of organic iodine within the pool, some reaction equations and their reaction coefficients should be verified. For the time being, the arbitrary user-defined equation form was applied to some undefined equations among the organic reaction equation set in MELCOR.

- The partition coefficient in MELCOR was calculated by the correlation, which was only a function of pool temperature. But the level of PH is the more influencing parameter on the partition coefficient. It is necessary that the current correlation for the partition coefficient should be modified to include the effect of PH in addition to the pool temperature.

- Regarding the importance of silver in trapping the iodine within the sump, the equation concerning the reaction between the silver and the iodine should be implemented in the pool chemistry model of MELCOR.

- The vapor pressure correlations on the methyl iodine and silver iodine should be included.

- The cable mass and dose value were too sensitive to predict the PH variation in the sump exactly. Therefore, it is necessary that a sensitivity study on the PH variation should be accompanied for the plant application.

In conclusion, it was found that the current model is insufficient to describe the organic iodine behavior. Although the complicated equations were implemented into the code, still coefficients or products used in the equation are unavailable or uncertain at present. More research is needed to track the iodine formation in the containment.

### ACKNOWLEDGMENTS

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### REFERENCES

- [1] B. Clement, N. Hanniet-Girault, G. Repetto, D. Jacquemain, A.V.Jones, M.P. Kissane, P.von der Hardt, LWR severe accident simulation: synthesis of the results and interpretation of the first Phebus FP experiment FPT-0", Nuclear Engineering and Design, 226(2003) 5-82.

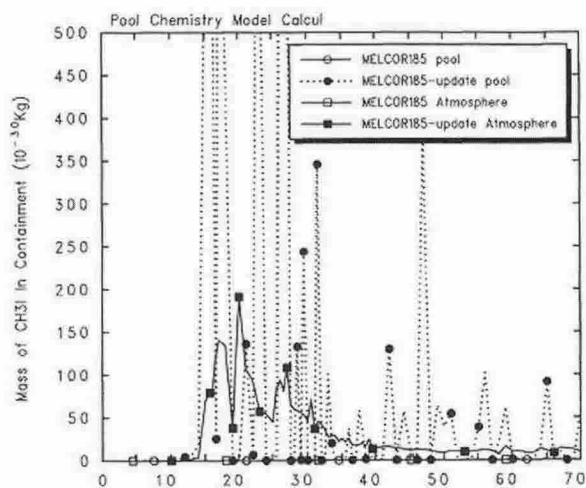


Figure 1. Methyl Iodine Mass in Containment