Simulation of Iodine Behavior by Coupling of a Standalone Model with MELCOR

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1. Introduction

During a severe accident, a large fraction of iodine in the core can be released into the containment. Iodine is important in terms of its high activity in the early phase after a core-melt accident due to its short half-life isotopes and its serious effect on the public health, especially on the thyroid [1]. Therefore, iodine behavior has been extensively studied through the international research programs. Major research areas are iodine chemistry, surface reactions, mass transfer, modeling of iodine chemistry and its applications to severe accident assessment, and accident management.

Advanced tools for modeling these phenomena have been developed and validated by several experiments such as ISTP-EPICUR (International Source Term Program - Experimental Program on Iodine Chemistry under Radiation) and PARIS, and OECD-BIP (Behavior of Iodine Project) in which Korea Institute of Nuclear Safety (KINS) has been participating. As a result, a simple iodine model, RAIM (Radio-Active Iodine chemistry Model) was developed [2], based on the IMOD methodology [3] in order to deal with organic iodides conveniently. RAIM has been also coupled with MELCOR [4], replacing the pool chemistry model (PCM). This coupling model, MELCOR-RAIM, will be used for an integrated severe-accident assessment that takes into account the organic iodine behavior. This model is described herein, and representative simulation results of the model are presented.

2. Development of the MELCOR-RAIM Model

The MELCOR code deals with water radiolysis and reactions associated with iodine and steel using the PCM. Its version 1.8.5, which is being used by KINS, cannot treat organic iodide even though the relevant reaction formulas are included in its manual. Therefore, based on the study by KAERI (Korea Atomic Energy Research Institute) that activated these reaction formulas [5], KINS modified the reaction rate constants so that the OECD-BIP and Phebus FPT1 experimental data could be adequately simulated [6]. While this model could reasonably simulate I_2 and CH_3I concentrations for BIP experiments, those of some iodine species were significantly deviated from the measured data.

In order to improve this methodology, a stand-alone model RAIM was developed. This model treats the chemical reactions associated with iodine species such as non-volatile and volatile iodine in the containment sump, non-aqueous iodine, volatile inorganic iodine and organic iodide in the containment atmosphere. It also deals with adsorption and desorption of volatile iodine on the paint surface. The rate constants of iodine reactions have been determined through a literature survey or empirically, using the EPICUR experimental data.

Then RAIM was tried to couple with the MELCOR code in order to simply treat the iodine behavior in the sump pool. Therefore, as shown in Fig. 1, some reactions in the aqueous phase were selected from RAIM and connected to the rest of the MELCOR models for thermal-hydraulic conditions, pH and partition coefficients, etc. Thus MELCOR-RAIM receives the revised quantities of iodine in the aqueous phase from the RAIM calculation; and then MELCOR treats the adsorption and desorption on the structures in the atmosphere and the sump, reflecting them.

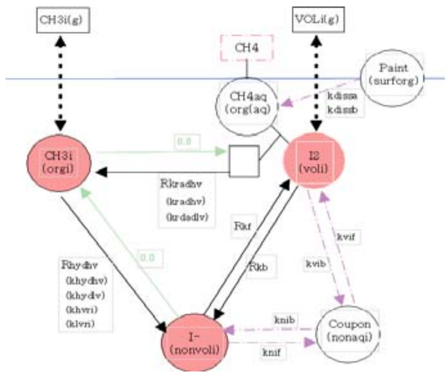

Fig. 1. The part of RAIM model applied to MELCOR-RAIM.

3. Simulation of the Iodine Experiments

In order to validate the developed iodine model, chemical behaviors of iodine species in the selected experiments are simulated with MELCOR-RAIM. In this section, the simulations of EPICUR and PHEBUS FPT1 experiments are described.

3.1 EPICUR Experiments

The EPICUR program, a part of ISTP operated by the IRSN, was set up to analyze the chemical behavior and chemical speciation of irradiated radioiodine. Fig. 2 and Fig. 3 show the simulation results of the S1-7-8 experiment, which deals with formation of organic iodide from reaction with painted coupon in the condition of pH 5 and temperature of 80 ^oC. Calculated inorganic and organic iodine concentrations using MELCOR-RAIM and MELCOR with PCM each are compared with measurements (green line). These results show that the coupling model agrees better with the measurements than MELCOR-PCM. However, Fig. 4 reveals a significant error with both calculations for the S1-3 experiment.

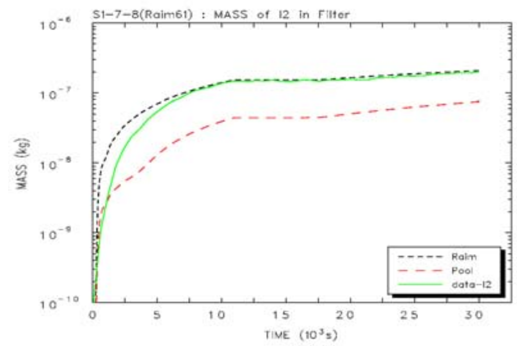

Fig. 2. Concentration of volatile inorganic iodine as a function of time for the S1-7-8 experiment.

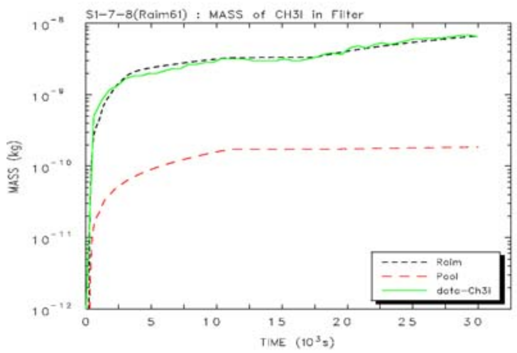

Fig. 3. Concentration of volatile organic iodide as a function of time for the S1-7-8 experiment.

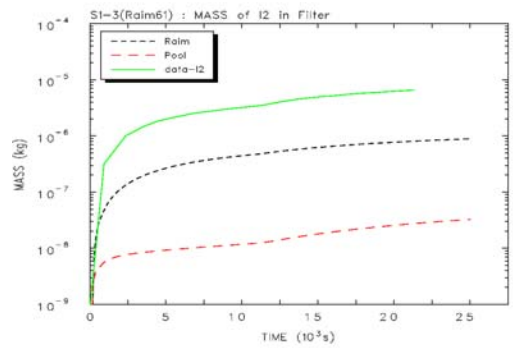

Fig. 4. Concentration of volatile inorganic iodine as a function of time for S1-3 experiment.

3.2 PHEBUS-FPT1 Experiment (ISP-46)

The PHEBUS FPT1 experiment, which simulated a SBLOCA sequence, was performed by IRSN in 1996. The test data was open for ISP-46 exercise. Fig. 5 shows that both MELCOR models agree with the total gaseous iodine concentration, but MELCOR-RAIM estimates CH_3I concentration quite higher than MELCOR with PCM.

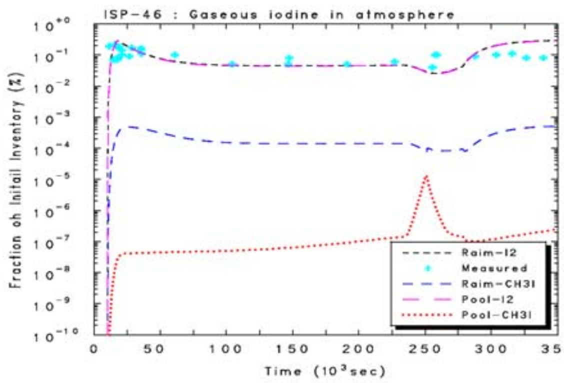

Fig. 5. Concentration of gaseous iodine in the atmosphere as a function of time for the PHEBUS FPT1 experiment.

5. Conclusions

A coupling model, MELCOR-RAIM was developed through replacing the pool chemistry model of MELCOR by the RAIM model. In order to validate the developed model, EPICUR and PHEBUS FPT1 experiments were simulated with MELCOR-RAIM. The results support the appropriateness and efficiency of this model in general, while for some cases it results in a significant error. Further study is required in the areas such as adsorption and revaporization of gaseous iodine, and the effect of iron in the sump.

Acknowledgments

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