# Validation of MELCOR 1.8.5 pool chemistry model with RTF experiments

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### 1. Introduction

Understanding of iodine behaviour in the containment is essential for the evaluation of severe accident consequences because iodine is a critical source term for early fatality. Qualified tools for the calculation of the iodine source term are also needed to perform meaningful risk analyses and to make decisions in the field of accident management, mitigation measures and emergency preparedness.

The MELCOR1.8.5 code used for consequence analysis in KINS (Korea Institute of Nuclear Safety) has iodine pool chemistry models, and can simulate the formation of molecular iodine gas from containment sump in severe accident condition. But the capability of this model needs to be verified against experimental data and thus to validate the MELCOR pool chemistry model, we have evaluated the ISP-41 and the P11T1 test both of which are iodine formation experiments performed by RTF(Radioiodine Test Facility) of AECL.(fig.1)



Figure 1. Radioiodine Test Facility (RTF)

### 2. Analysis of RTF Tests

In aqueous phase, molecular  $iodine(I_2)$  is generated from iodide ion by reactions as follows.[1]

$$2I^{-} + 2H^{+} + \frac{1}{2}O_{2} \Leftrightarrow I_{2} + H_{2}O \quad (1)$$
$$2I^{-} \xleftarrow{radiation} I_{2} \quad (2)$$

Important parameters of these reactions are temperature, radiation dose, wall deposition rate and pH level.

In ISP-41 and P11T1 tests, pH is a main parameter of  $I_2(gas)$  formation. In the MELCOR pool chemistry model,  $I_2$  concentration of pool is mainly affected by pool pH. And by the partition coefficient which means ratio of concentration in atmosphere to pool,  $I_2(gas)$  concentration is calculated by  $I_2(aq)$  concentration. [2]

### 2.1. MELCOR Modeling of RTF

The RTF experiment vessel was modeled in MELCOR as a single control volume of 0.688m in diameter by 0.918m high with stainless steel walls. The experimental pool and atmosphere sampling loops were not simulated(fig.2).

Initial conditions were modeled in MELCOR by injecting cesium iodide as a radionuclide source. The radiation dose was set by user input for the iodine pool chemistry model, and the provided pH history was read from data table. The wall adsorption and desorption coefficients were set at values ( $9 \times 10^{-4}$  m/s,  $9 \times 10^{-7}$ /s) derived from a published results on RTF tests[3]. In the most of RTF tests, Initial pH was set to 10 considering CANDU condition.



Figure 2. RTF tests scheme

## 2.2. ISP-41 Experiment

ISP-41 (International Standard Problem no. 41) is an experiment suitable for demonstrating the ability of a code to model the pH behaviour of iodine volatility. In experiment, dose rate and temperature were constant, and pH was controlled. (Tab.1) Main concern of ISP-41 was 'partitioning', which is ratio of iodine concentration between pool, atmosphere and wall.

Table 1. ISP-41 test condition

Dose rate	1.36kGy/hr
Temperature	25℃
Initial I <sub>2</sub>	9 x 10 <sup>-6</sup> mol/L CsI
Aqueous Volume	25L
Gas Volume	315L
Aqueous Surface Area	5200cm <sup>2</sup>
Interfacial Surface Area	3700cm <sup>2</sup>
Gas Surface Area	$22000 \text{ cm}^2$
Pool pH	Controlled

# 2.3. P11T1 Experiment

The P11T1 experiment data was released to members of BIP (Behaviour of Iodine Project), the international cooperation research program of OECD/NEA. AECL, the operation agent (OA) of BIP, is performing some experiments about iodine behaviour including iodine adsorption to, and organic iodine formation from painted surface using RTF. And AECL released some former RTF experiment results (2 cases released, 3 cases on standby) to BIP members for analytic research as a part of BIP project. Actually, P11T1 is an organic iodine formation experiment, but  $I_2(gas)$  formation data is also available to our purpose. [4]

Table 2.	P11T1	test condition
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Dose rate	0.6kGy/hr
Temperature	25 ℃
Initial I <sub>2</sub>	9 x 10 <sup>-6</sup> mol/L CsI
Aqueous Volume	27.75L
Gas Volume	313.5L
Aqueous Surface Area	5200cm <sup>2</sup>
Interfacial Surface Area	3700cm <sup>2</sup>
Gas Surface Area	22000cm <sup>2</sup>
Pool pH	Controlled

# 3. Results of Calculation

The results of MELCOR analysis for these two experiments are summarized in the following.





- 1. Generally, overall trend of  $I_2(gas)$  concentration is similar to the experimental result in both calculation cases (fig3,4). In base phase (pH range 7~10), the more pH decrease, the more  $I_2(gas)$  concentration increases.
- 2. The MELCOR code extremely underestimates  $I_2(gas)$  concentration when pH is greater than 9.0. It may be insignificant result because maximum sump pH of PWR in accident condition is about 8.5. (For example, in case of Yonggwang 3,4 DBA analysis, pH range is 7.0~8.5 in 49~54°C considering operation of hydrazine and TSP.)
- 3. The MELCOR code estimates  $I_2(gas)$  concentration accurately when pH is about 8.0~9.0.
- 4. The MELCOR code underestimates  $I_2(gas)$  concentration when pH is lower than 8.0.  $I_2(gas)$  in calculation is about ten times lower than experiment results. In this range, it is necessary to improve the pool chemistry model of MELCOR.

## 4. Conclusions

We have simulated the iodine formation test ISP-41 and P11T1 using MELCOR1.8.5 for validation. The MELCOR code can properly simulate the molecular iodine gas formation against sump pH in accident condition. But calculation result shows some model development needs because there is a tendency to underestimate  $I_2(gas)$  concentration.

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