# Source Term Model Accuracy Evaluation in MELCOR Code Using International Standard Problem No.44

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MELCOR 1.8.5 code for an integrated severe accident analysis in nuclear power plants has been employed to simulate the KAEVER test series that were proposed as experiments of International Standard Problem No.44 by OECD-CSNI. The main purpose of this study is to evaluate the accuracy of the MELCOR aerosol model that calculates the aerosol distribution and settlement in a containment of the plant. For this, thermal hydraulic conditions are simulated first for the whole test period, and then the behavior of hygroscopic CsOH aerosols, which are predominant activity carriers in a release into the containment and then into environment, is compared between the experimental results and the code predictions. The calculation results of vessel atmospheric concentration show a good agreement for wet aerosol but show a large difference for dry aerosol. The difference in dry aerosol concentration is evaluated to be caused by the hygroscopicity model defects and modifying the solubility effect in hygroscopic aerosol particles enhances these results. Improved techniques on aerosol behavior evaluation will result in more accurate source term to the environment, which would contribute again to the accident management and mitigation in nuclear power plants.

KEY WORDS: Source term, MELCOR, KAEVER, aerosol, hygroscopic model, deposition, nuclear power plant

### I. Introduction

During an unmitigated severe accident in a light water reactor (LWR) with core melting, air-borne fission products are released into the containment while the containment building serves as a final barrier to the environment. Effects on long-term aerosol depletion in the LWR containment and also onto the radioactive source term are to be expected hereafter. The behavior of the aerosol after core melt and during the early phase of an accident is determined by the physico-chemical aerosol parameters and it depends on the aerosol component and the thermohydraulic boundary conditions. Recently, the OECD-CSNI decided to propose containment aerosol behavior as the International Standard Problem No.44 (ISP44)<sup>1)</sup> via the opening part of the KAEVER (Core Melting Aerosol Experiments) test data. The KAEVER test examines differences on the behavior of individual aerosol components and aerosol mixtures in an LWR containment in which the most important task was to determine the aerosol depletion rates under various thermohydraulic boundary conditions. ISP44 program is for demonstrating the capability of current computer codes like MELCOR<sup>2)</sup>, CONTAIN  $\frac{3}{3}$  and COCOSYS/ASTEC<sup>4)</sup> to model and calculate the aerosol distribution and settlement in a containment of the nuclear power plant with sufficient accuracy. In this study, simulations for a K188 KAEVER open test which used CsOH aerosols have been done with MELCOR 1.8.5 code. The K188 is selected among several open ISP44 tests due to the fact that measurement data are available for almost all of the aerosol test period.

### **II.** Experimental Task





The KAEVER experimental program has been performed in a medium-sized experimental plant (volume  $\approx 10 \text{ m}^3$ ) in Germany to get data on the aerosol behavior with welldefined thermal hydraulic boundary conditions. The test containment consists of a cylinder with even front walls, rectangular door openings and sliding doors positioned outside (Fig. 1). The cylindrical part is 2500 mm long and has an internal diameter of 2090 mm and a wall thickness of 25 mm. The door openings are 800 mm wide, 1900 mm high and have a wall thickness of 37 mm. During steam condensation, the condensate accumulates on the bottom of the cylindrical part and the contact area between the sump water and cylinder wall increases with increasing sump water mass. The inner free volume of the containment is 10.595 m<sup>3</sup>. The cylinder and doors are heated and insulated. The front

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walls are insulated. The test scheme of the K188 experiment is as follows:



#### **Phase-I: Preconditioning of the test vessel**

During this phase, the vessel is flushed with steam, and electric heating is applied to reach the set wall temperatures. The data acquisition system is not operated. Preconditioning continues until quasi-stationary conditions are obtained.

### **Phase-II: Execution of experiment**

The thermal-hydraulic conditions in the vessel are readjusted by controlled steam injection and electric heating ("heat injection"), in order to reach a quasi-stationary state that may differ from the final state of phase-I. Aerosols are then injected by turning on the inductive heating of the aerosol generators until the material in the crucibles is completely evaporated. The carrier gas feed then stops. Finally, the depletion of aerosols is observed without further change in the injection or boundary conditions. Nitrogen is injected into the test vessel as carrier gas for the aerosol and as cleaning gas for the tubes of the spectral photometer. At the filter sampling station, withdrawal of the test vessel atmosphere leads to a discharge of nitrogen which is measured. It is recommended to neglect the corresponding vapour mass withdrawal. The temperature of the environment (the room in which the vessel is located) is only measured once at the beginning of the experiment which was 18°C and is kept constant throughout the experiment. The aerosol generation and injection is established by inductive heating of crucibles with evaporating materials and by nitrogen carrier gas flow to transport the condensation aerosols into the test vessel. The carrier gas flow rate is monitored continuously. Filter samples from the aerosol injection line are taken several times and analysed for concentration and size distribution. From mass balance analyses, major differences between the initial aerosol material mass in the crucibles, the injection mass derived from the measurements

in the injection line, and the total mass deposited in the test vessel at the end of the experiment shows up, indicating the potential existence of large particles that are not properly detected by the measurement systems. Due to this observation and the discontinuous concentration data in the injection line, the time-dependent aerosol injection rate is reconstructed from the vessel photometer data, and adjusted by a constant factor to match the first filter sample concentration measurement in the test vessel.

## III. MELCOR Calculation 1. Thermal Hydraulics



Fig. 2 MELCOR Nodalization of Test Vessel

Figure 2 shows a MELCOR nodalization scheme with 5 control volumes and 24 heat structures, which are employed to simulate the test vessel. In the employment, the cylindrical part of the test vessel is nodalized with three control volumes (upper cylinder region, lower cylinder region, and sump region), the door part of the test vessel with two control volumes (left door region and right door region) and the environment with one time-independent control volume. The walls of the test vessel are shaped as a rectangular plate with horizontal or vertical surfaces and ten flow paths are defined to connect each control volume. For the simulation of an experiment, the KAEVER tests are calculated in two steps according to the test procedure. The first step is thermal hydraulic calculations for pre-conditioning phase-I whose initial and boundary conditions (for the rates of steam injection, heat injection, clearing N<sub>2</sub> gas injection, and air removal) are shown in Table 1 and Fig. 3, respectively.

Environment temp. [°C]	18
Test vessel pressure [bar]	1
Test vessel atmosphere temp. [°C]	18
Test vessel structure temp. [°C]	18
Sump water mass	0.0

Table 1 Initial Conditions for Phase-I



Fig. 3 Steam/Air/Heat Injection for Phase-I

The simulation results are compared with the measured final quasi-stationary conditions at the end of phase-I. Apart from the initial temperature difference in the heat structures, most of the calculated heat structure temperatures are very close to the measured values at the beginning of aerosol injection and depletion phase. The calculated trends of the vessel atmosphere temperature and pressure in **Fig. 4** show a very similar trend through the phase-II with slight differences which are less than 0.1 bar and 2.5°C respectively. The mass of sump water and N<sub>2</sub> gas also shows good simulation for the provided data. Exceptions are the humidity for which the MELCOR code can not predict over 100%.



Fig. 4 Vessel Atmosphere Pressure and Temperature

All thermal hydraulic results for K188 are found in ISP44 Comparison Draft Report<sup>5)</sup> and are verified in a competition between OECD nations where our thermal hydraulic simulation shows the most similar approach.

#### 2. Aerosol Injection and Deposition

The second step is aerosol injection and deposition calculations for main phase of the experiment whose boundary condition for the aerosol injection rate is shown in **Fig. 5**. The aerosol characteristic parameters are arranged in **Table 2** and the aerosol deposition area used in a MELCOR calculation is compared in **Table 3** with those values in the ISP44 report. Among the aerosol parameters, ISP44 recommends including the solubility effect (Van't Hoff factor) and Kelvin effect (surface tension) for soluble and unsoluble aerosols, respectively. In MELCOR, both effects are treated together by activation of the hygroscopic model. For solubility, original MELCOR model was found inappropriate in simulating the characteristic in Table 2 and changes are made which are described in the next paragraph. For Kelvin effect, MELCOR has no input to control the value of surface tension itself which makes it impossible to simulate the two effects separately. So, the hygroscopic model is activated in the simulation, considering supersaturated atmosphere conditions. Without the hygroscopic model, the aerosol (mainly wet aerosol) concentration in vessel atmosphere appears to keep high with little deposition, which is considered unrealistic.



Fig. 5 Aerosol Injection for Aerosol Phase

Parameter	CsOH
Volume median particle diameter [µm]	0.37
Number median particle diameter [µm]	0.26
Particle size distribution	Log-normal
Geometric standard deviation	1.45
Dry aerosol density [kg/m3]	3675
Molecular weight [kg/kmol]	150
Surface tension (Kelvin effect)	none
Solubility (Van't Hoff factor)	none
Dynamic shape factor	1.0
Agglomeration shape factor	1.0

Table 2 Aerosol Characteristic Parameters

	ISP-44	MELCOR
Floor	$7 \text{ m}^2$	$5.67 \mathrm{m}^2$
Ceiling	$7 \text{ m}^2$	$5.67 \mathrm{m}^2$
Wall	$17.6 \text{ m}^2$	$20.51 \text{ m}^2$
Total	31.6 m <sup>2</sup>	$31.8 \text{ m}^2$

Table 3 Aerosol Deposition Area

The K-188 test is simulated using MELCOR1.8.5 to compare with the results using MELCOR1.8.4 with old and new hygroscopic models. As shown in **Fig. 6**, the calculation results of vessel atmospheric concentration in version 1.8.5 show a large difference for dry aerosol, and show a good simulation for wet aerosol. Good simulation in wet aerosol concentration is judged to be caused by the enhanced volume condensation model in version 1.8.5. The difference in dry aerosol concentration is evaluated to be caused by the hygroscopicity model defects in both versions of 1.8.4 and 1.8.5. The figure shows that dry aerosol concentration shows a better simulation via modifying the solubility effect in hygroscopic aerosol particles in a new hygroscopic model. In a old model, all elements are treated to have the same solubility and ionization factors as those of soluble elements, which results in the unsoluble elements having soluble characteristics. So, changes are made in which only CsI and CsOH, instead of all elements, are considered to be soluble.



Fig. 6 Aerosol Concentration in Vessel Atmosphere

The dry aerosol mass distribution on the floor (mainly sump), ceiling/wall, and atmosphere is shown in Fig. 7.



Fig.7 Aerosol Deposition on Heat Structure Surfaces

The results show that most of injected aerosol mass, which was 11.8 g in the K188 test, goes to the floor as time goes on. Part of the injected aerosol mass goes to the floor even during the aerosol injection period and the peak aerosol concentration in vessel atmosphere appears before the end of aerosol injection which was about 30%. As calculated, the aerosol deposited fraction at the end of aerosol injection is proportional to the aerosol injection, about 10% of total injected mass exists in vessel atmosphere and about 50% ( $\pm 10\%$ ) of aerosol in vessel atmosphere deposite during this 1000 seconds after the end of injection. The results reflect the

hygroscopic aerosol transport and deposition under supersaturated (humidity of 100% and weak fog formation) atmosphere conditions.

### **IV. CONCLUSIONS AND DISCUSSIONS**

The ISP44 tests are simulated using MELCOR 1.8.5 code with detailed nodalization scheme of control volume and heat structure. The code predictions for the wet aerosol concentration in the vessel atmosphere show a strong relationship with the test results. For dry aerosols, the calculated concentration using modified hygroscopic model shows almost the same trend throughout the experiment period. The peak aerosol concentration in vessel atmosphere appears during the aerosol injection and then starts to decrease, resulting in about a half of atmospheric aerosol mass deposits during the next 1000-second period.

For the aerosol simulation, a good simulation of the thermal hydraulics is needed first. However, an emphasis is put on the time dependency and distribution of fission products and aerosols, which are most important to mitigate the accident (e.g. by venting) in this paper. Furthermore, the results reflect the hygroscopic aerosol transport and deposition under supersaturated (humidity of 100% and weak fog formation) atmosphere conditions. High relative humidity is expected under severe accidents during an early phase of a release into the containment because of the water quantities present in the containment or the considerable water quantities expected to be injected during accident management measures in nuclear power plants. Through this study, an analytical prediction capability of MELCOR thermal hydraulic and aerosol models is evaluated. Experimental results and code predictions would be used to quantify the safety margins existing in the safety systems of operating reactors, and to explore the possibilities of mitigating severe accident consequences.

#### Acknowledgement

This project has been carried out under the Nuclear R&D Program by Ministry of Science and Technology (MOST) in Korea.

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