SIMULATION OF INTERNATIONAL STANDARD PROBLEM NO.44 OPEN TESTS USING MELCOR COMPUTER CODE

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■ ABSTRACT

MELCOR 1.8.4 code has been employed to simulate the KAEVER test series of K123/K148/K186/K188 that were proposed as open 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 which calculates the aerosol distribution and settlement in a containment. For this, thermal hydraulic conditions are simulated first for the whole test period and then the behavior of hygroscopic CsOH/CsI and unsoluble Ag aerosols, which are predominant activity carriers in a release into the containment, is compared between the experimental results and the code predictions. The calculation results of vessel atmospheric concentration show a good simulation for dry aerosol but show large difference for wet aerosol due to a data mismatch in vessel humidity and the hygroscopicity.

■ INTRODUCTION

During an unmitigated severe accident in light water reactors (LWR) with core melting, aerosol-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 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. To get data on the aerosol behavior with well-defined thermo-hydraulic boundary conditions, the KAEVER (Core Melting Aerosol Experiments) experimental program has been performed in a medium-sized experimental plant (volume ≈ 10 m^3) in Germany. This program 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. Recently, the OECD-CSNI decided to propose containment aerosol behavior as the International Standard Problem No.44 (ISP44) [GRS-Cologne, 2000] via opening part of the KAEVER test data. This is for demonstrating the capability of current computer codes like MELCOR [SNL, 1990], CONTAIN [SNL, 1997] and FIPLOC [GRS, 2000] to model and calculate the aerosol distribution and settlement in a containment with sufficient accuracy.

In this paper, simulations for open four KAEVER tests like K123/K148/K188/K186, which used each or mixture of CsI, Ag, and CsOH aerosols as follows, have been done with MELCOR 1.8.4 code as a preliminary study of an ISP44 blind (K187) simulation:

K123: test with CsI aerosol
K148: test with Ag aerosol
K188: test with CsOH aerosol
K186: test with mixed aerosol of Ag and CsOH
K187: test with mixed aerosol of Ag, CsOH and CsI (blind calculation)

For the aerosol simulation, a good simulation of the thermal hydraulics is needed first though 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). The K188 is selected among several open ISP44 tests because it is recommended to test the computer code modeling of the KAEVER test vessel by comparing the calculated results to the K188 test for which measurement data are available for almost all of the aerosol test period. In the mean time, high relative humidity is expected 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.

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.

■ EXPERIMENTAL TASK

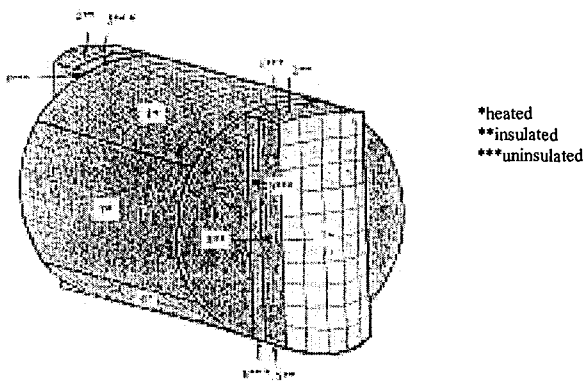


Figure.1 Perspective View of KAEVER Test Vessel

The test containment consisted of a cylinder with even front walls, rectangular door openings and sliding doors positioned outside (Figure 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. The inner free volume of the containment is 10.595 m^3. The cylinder and doors are heated and insulated. The front walls are insulated.
The walls of the test vessel are made of steel. Most parts of the outer surfaces, including the doorways and doors, carry an outer thermal insulation layer. The outer edge of the insulation layer carries an additional steel layer of 2mm in thickness.

Most of the insulated outer surfaces are also equipped with electric resistance heater mats between the steel wall and the insulating layer. On some parts of the doorways suitable insulation is not provided. In addition the structures of the door opening mechanism are attached there causing important heat transfer to the environment. Although it is not in direct contact with the containment atmosphere, an artificial wall part number 10 (=No.10) is proposed to simulate the cooling fin effect of the opening mechanism. The dimensions, layers and thermal characteristics of the different wall parts are given in Table 1.

Wall part No.	Area inside (m^2)	Steel thickness (m)	Electric heater mat	Thermal insulation thickness (m)	Orientation
1	4.07	0.025	Yes	0.075	Ceiling
2	0.235	0.025	No	0.1	Ceiling
3	1.372	0.037	No	0.	Ceiling
4	4.07	0.025	Yes	0.075	Floor
5	0.235	0.025	No	0.1	Floor
6	1.372	0.037	No	0.	Floor
7	11.73	0.020	Yes	0.075	Side wall
8	4.685	0.025	No	0.25	Side wall
9	1.85	0.037	No	0.	Side wall
10	2.5	0.024	No	0.	Side wall

Table.1 Thermal Characteristics of the Vessel Walls

The thermal properties used for the vessel materials are given in Table 2.

	Thermal conductivity (W/m K)	Specific heat (J/kg K)	Density (kg/m^3)	Emissivity
Steel	45	480	7850	0.9
Insulation	0.091	840	110	0.25

Table.2 Thermal Properties of the Vessel Materials

The experiment scheme of the open KAEVER tests is as follows:

Phase-I: Preconditioning of the test vessel

During this phase, the vessel is flushed with steam, and electric heating is appropriately applied to reach the set wall temperatures. 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. 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 about 18~22°C and is kept constant throughout the experiment. 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.

■ MELCOR CALCULATION

Thermal Hydraulics

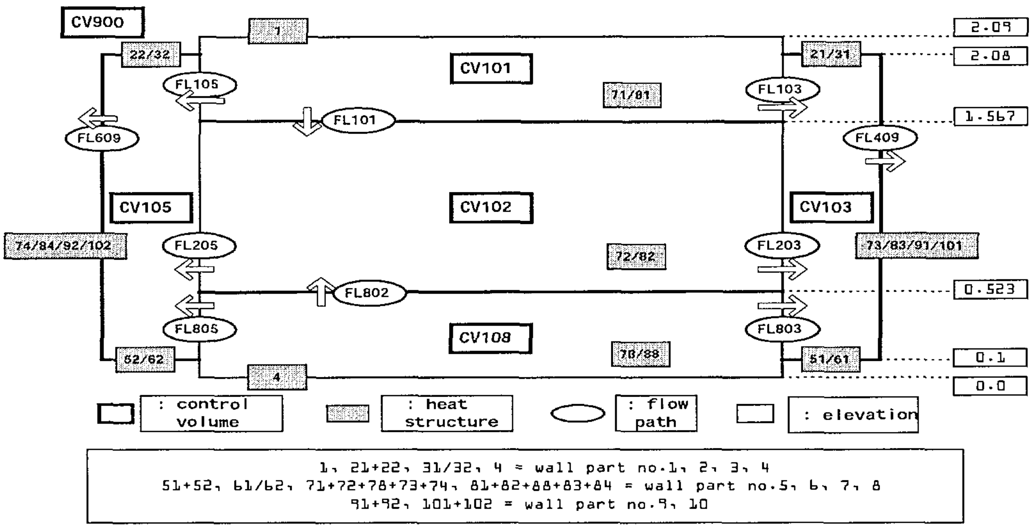
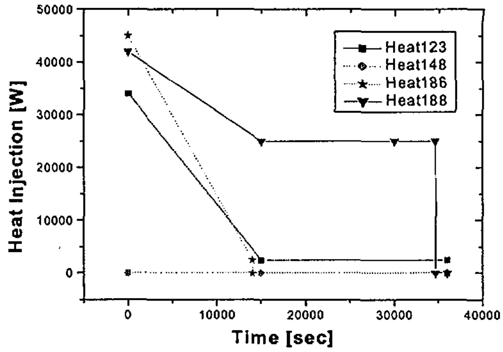


Figure.2 MELCOR Nodalization of Test Vessel

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 three steps according to the test procedure. The first step is thermal hydraulic calculations for preconditioning phase-I whose initial and boundary conditions (for the rates of steam (temperature =103~107°C) injection, heat injection, clearing N_2 gas injection, and air removal) are shown in Table 3 and Figure 3, respectively.

	K123	K148	K186	K188
Environment temperature [°C]	20	18	22	18
Test vessel				



atmosphere	air	air	air	air
pressure [bar]	1	1	1	1
atmosphere temperature [°C]	20	18	20	18
structures [°C]	20	18	20	18
Sump				
water mass [kg]	0.0	100.0	0.0	0.0

Table.3 Initial Conditions for Phase-I

Figure.3a Phase-I Steam/Air Injection

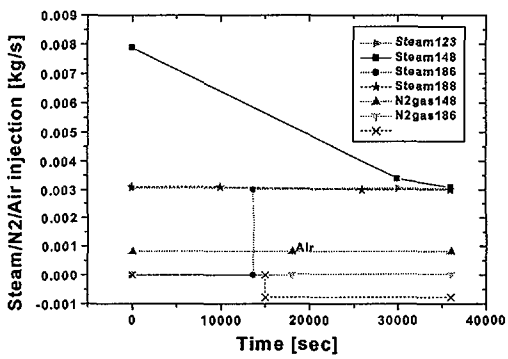


Figure.3b Phase-I Heat Injection

The simulation results are compared with the measured final quasi-stationary conditions at the end of phase-I in Table 4.

	K123		K148		K186		K188	
	Mea[1]	MEL[2]	Mea	MEL	Mea	MEL	Mea	MEL
Vessel Atmosphere								
pressure [bar]	1.1	1.05	1.04	1.05	0.99	0.99	1.09	1.19
temperature [°C]	104	104	92	92.0	97.8	97.8	109.5	109.5
humidity [%]	85	88	116	99.9	110	99.9	93	83
compound	Steam, N_2		Steam, N_2		Steam, N_2		Steam	
N_2* [kg]	0.057	0.23	2.72	2.855	0.533	0.585	0.0	0.2

Sump								
water mass* [kg]	0.0	0.0	290.0	290.0	67.3	67.3	4.6	4.6
temperature [°C]	101	104	80	80.0	94.1	94.1	101	101
Structure Temperature [°C]								
door sidewall (outside, uninsulated)	N/A	103.4	N/A	88.65	94.2	96.55	100	109.2
door side wall (inside)	N/A	103.4	N/A	88.65	96.9	96.55	101	109.2
cylinder wall (outside, uninsulated)	N/A	53.35	N/A	35.45	35.8	36.65	41	41.5
cylinder wall (inside)	N/A	103.9	N/A	91.25	97.4	97.55	112	109.4

[1]: Measure, [2]: MELCOR, *: calculated from injection data

Table.4 Thermal Hydraulic Conditions at the End of Phase-I

The temperature of the door side wall shows a slight difference because all control volumes inside the vessel boundary including the door side are fully open and well mixed. The main purpose of this first-step simulation is to establish a temperature profile inside the heat conducting structures that is close to steady-state conditions at the end of phase-I. In the subsequent phase of re-adjusting the thermal hydraulic conditions, the measured data are used to check if the calculated temperatures are in reasonable agreement with the measurements. Important factors to be adjusted are judged as an area of the uninsulated wall part No.10 and an effective vessel leak size into the environment. But the effective leak size of 10.2E-7 m^2 is recommended in the ISP44 specification report [GRS, 2000] which was determined from the post test calculation of the pressure curve. This leak size is simulated as an opening area to the environment with a loss coefficient of ζ = 2.7 without additional losses due to wall friction, etc. Therefore, in order to improve the agreement, the thermal losses from the uninsulated wall part No.10 are adjusted by modification of its surface area. The surface area is dependent upon the heat transfer correlation, which the MELCOR model applies on the outer side of the vessel. The measured and calculated vessel temperature transients are carefully compared from the beginning of phase-II until the start of aerosol injection, especially for the K188 test according to the ISP44 recommendation, and the wall part No.10 area of 2.5 m^2 is determined in order to provide suitable thermal hydraulic conditions for the aerosol phase.

During the ISP44 tests, steam is injected to obtain supersaturated atmosphere conditions in the aerosol phase-II. This condition means a humidity of 100% and weak fog formation. In the K188 test, however, 93% humidity and atmospheric pressure and temperature of 1.09 bar and 382.65 K were observed at the end of phase-I. But, the steam partial pressure at the observed atmospheric temperature and humidity is calculated to be larger than the observed total volume pressure (=atmospheric pressure). Considering this data mismatch and technical error bounds of the measuring transducer systems, measured volume pressure and humidity are converted to values of 1.19 bar and 83%, respectively, in the calculation. The final thermal hydraulic conditions are then used as initial thermal hydraulic conditions in MELCOR calculation for phase-II simulation.

The second step is thermal hydraulic calculations for phase-II whose boundary conditions (for the rate and temperature of steam/heat/carrier gas/clearing gas injections and N_2 removal) are measured in the experiments. In phase-II, the thermal hydraulic behavior is determined by operation of the electric heater elements, the injections, the heat losses and the leakage. Steam is injected through a 2.5m long pipe near the vessel bottom into control volume 108. The carrier gas for aerosol injection and clearing gas for the photometer tubes is nitrogen and the injections are into control volume 101. Controlled sampling from the atmosphere in control volume 101 is carried out as steam/gas/aerosol mixture over an aerosol filter and a cooling device, where the steam is condensed; the non-condensable gas (almost composed of nitrogen) flow is then determined. No electric heat is injected through phase-II except for the K123 test.

The simulated results are compared with the measured conditions at the beginning of aerosol injection in Table 5.

	K123		K148		K186		K188	
	Mea[1]	MEL[2]	Mea	MEL	Mea	MEL	Mea	MEL
Vessel Atmosphere								
pressure [bar]	1.49	1.56	1.64	1.58	0.99	0.98	0.99	1.05
temperature [°C]	102.4	101.2	92.5	88.8	97.7	97.1	97.7	99.5
humidity [%]	90	100	116	100	110	100	110	100
compound	Steam, N_2		Steam, N_2		Steam, N_2		Steam, N_2	
N_2* [kg]	3.917	4.03	8.314	8.398	0.533	0.614	0.9	0.98
Sump								
water mass* [kg]	42.7	40.0	301.1	300.5	69.1	68.8	65.3	67.5
temperature [°C]	98.6	101.5	79.7	89.9	94.0	97.2	94.8	98.4
Structure Temperature [°C]								
door sidewall (outside, uninsulated)	N/A	99.28	N/A	82.15	93.9	96.11	96	96.9
door side wall (inside)	N/A	98.62	N/A	82.63	96.8	96.77	96.7	97.5
cylinder wall (outside, uninsulated)	N/A	47.44	N/A	33.20	35.5	36.40	33.3	32.7
cylinder wall (inside)	N/A	100.5	N/A	88.10	97.3	96.99	97.1	99.3

[1]: Measure, [2]: MELCOR, * : calculated from injection data

Table.5 Thermal Hydraulic Conditions at Beginning of Aerosol Injection

Except 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 vessel atmosphere temperature and pressure are shown in Figure 4 (see the last page) with the measured values. The calculated and measured values show 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_2 gas also shows good simulation for the provided data. Exceptions are the humidity for which MELCOR code can not predict over 100% and sump water temperature in the K148 test which shows larger difference from the vessel atmosphere temperature compared with the other tests and is judged to be an erroneous data.

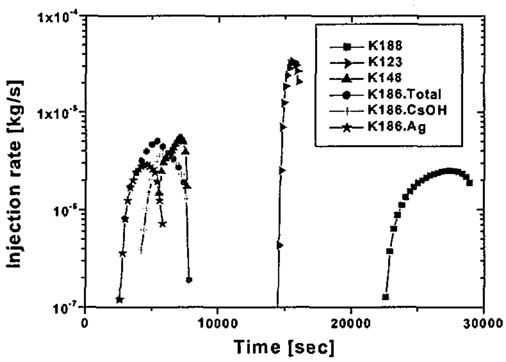
Aerosol Injection and Deposition

The third step is aerosol injection and deposition calculations for main phase of the experiment whose boundary condition for the aerosol injection rate is shown in Figure 5. The aerosol characteristic parameters are arranged in Table 6. The aerosol deposition area used in a MELCOR calculation is compared in Table 7 with those values in the ISP44 report. Among aerosol parameters, ISP44 recommends to include solubility effect (Van't Hoff factor) and Kelvin effect (surface tension) for soluble and unsoluble aerosols, respectively. In MELCOR1.8.4, both effects are treated together by activation of the hygroscopic model. For solubility, original MELCOR model has found inappropriate in simulating the characteristic in Table.6

and changes are made which are described in the next section of hygroscopic model change. 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 hygroscopic model, the aerosol (mainly wet aerosol) concentration in vessel atmosphere appears to keep high with little deposition, which is considered unrealistic.

Parameter	K123(CsI)	K148(Ag)	K186(Ag + CsOH)	K188(CsOH)
Volume median particle diameter [μm]	1.634	0.996	0.567	0.37
Number median particle diameter [μm]	0.691	0.516	0.402	0.26
Particle size distribution	log-normal	log-normal	log-normal	log-normal
Geometric standard deviation	1.80	1.40	1.2	1.45
Dry aerosol density [kg/m^3]	4510	10510	(10510+3675)/2	3675
Molecular weight [kg/kmol]	260	108	108 / 150	150
Surface tension (Kelvin effect) [N/m]	none	0.0512	0.0512 / none	none
Solubility (Van't Hoff factor)	1.7	None	None / 2.0	2.0
Dynamic shape factor	1.0	1.0	1.0	1.0
Agglomeration shape factor	1.0	1.0	1.0	1.0

Table.6 Aerosol Characteristic Parameters



	ISP-44	MELCOR
Floor	7 m^2	5.67 m^2
Ceiling	7 m^2	5.67 m^2
Wall	17.6 m^2	20.51 m^2
Total	31.6 m^2	31.8 m^2

Table.7 Aerosol Deposition Area

Figure.5 Aerosol Injection

In the aerosol injection phase the carrier gas causes an increase of pressure as shown in Figure 4. Also, the atmosphere temperature rises slightly, mainly caused by the injected steam and condensation heat transfer coefficient which decreases with increasing nitrogen in the atmosphere. In the aerosol depletion phase the nitrogen loss by leakage and aerosol sampling causes a slight pressure and temperature decrease.

The measured concentration transients for dry (CsOH/CsI/Ag) aerosols and wet (CsOH/CsI/Ag + H_2O) aerosols given after the start of aerosol injection are compared in Figure 6 (see the last page) with the calculational results for vessel atmosphere. For dry aerosol, in the K148 and K186 tests, the calculated concentration is very close to the experimental data through the whole measured period. In the K188 test, the calculated concentration is very close to the experimental data during the first half an hour after the end of aerosol injection and then the calculated starts to overestimate the measured. As time goes the gap grows between them, representing a slower decrease in the calculated concentration. On the contrary, In the K123 test, the calculated concentration is very close to the experimental data during the first two hours after the end of aerosol injection and then the calculated starts to underestimate the measured, representing a faster decrease in the calculated concentration. For wet aerosols, in all open tests, the calculated concentration shows almost the same trend throughout the experiment time but with two-order difference. The unit of measured data was m^3/m^3, which is inappropriate considering general unit of a concentration is mass/volume like the unit of calculated data, and water density is applied in the unit conversion. Anyhow the unit conversion is uncertain from which the difference is considered to result. In the mean time the calculated concentration of wet aerosols using the old hygroscopic model shows a much faster decrease. The reason for the different shapes results from the bug in the original hygroscopic model which is described in the next section.

The calculated dry aerosol mass distribution on the floor (mainly sump), ceiling/wall, and atmosphere is shown in Figure 7, especially for the K188 test, which shows typical trend for all open tests. 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 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. As shown in Table.8, the aerosol deposited fraction at the end of aerosol injection is proportional to the aerosol injection period. At 1000 seconds after the end of aerosol injection, about 10% to 33% of total injected mass exists in vessel atmosphere for all open tests and about 50% (±10%) of aerosol in vessel atmosphere deposits during this 1000 seconds after the end of aerosol injection. The results reflect the hygroscopic aerosol transport and deposition under supersaturated (humidity of 100% and weak fog formation) atmosphere conditions.

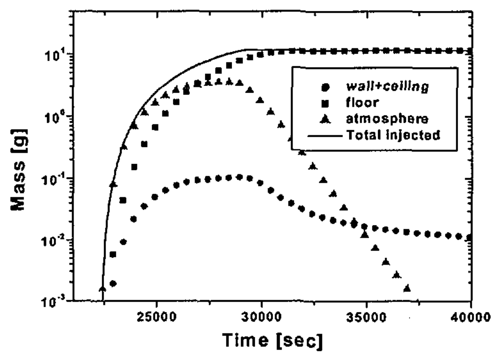


Figure.7 Aerosol Distribution in K188

Aerosol injection period [sec]	2120	4200	7200	7680
Fraction of aerosol in atmosphere				
At end of aerosol injection	70.0	49.6	25.7	22.4
At end of aerosol injection + 1000sec	33.0	26.2	10.4	9.9
Deposition fraction during 1000 sec	0.53	0.47	0.60	0.56

Table.8 Aerosol Injection and Deposition

Hygroscopic Model Change

Hygroscopic phenomena enhance aerosol growth rate as water vapor condenses or evaporates on the aerosol surface. As condensation or evaporation occurs, atmosphere vapor pressure and temperature are affected, and may have a significant impact on those variables. In particular, the condensation of water vapor on an aerosol surface is the most important reason to cause the aerosol to grow; this growth increase the aerosol agglomeration rate because the larger aerosol surface has a higher probability of interacting with other aerosols. In MELCOR, the hygroscopic model is based on the Mason equation and includes the Kelvin and solubility effects. The Mason equation states that the rate of condensation or evaporation of water on an aerosol particle is expressed by the equation below:

$$\frac{dr}{dt}=\frac{1}{r}\frac{(S-S_r)}{(a+b)}$$

where

$$S_r = A\exp(\frac{2M_w\sigma}{RT_\infty\rho_w r}),\qquad A = \text{chemical activity}$$

$$b=\frac{RT_\infty\rho_w}{D_v M_v P_{sat}(T_\infty)} \text{ and } b=\frac{\Delta h_f^2 M_w \rho_w}{RT_\infty K_a}$$

in which,
r = aerosol particle radius,
t = time, and
S = saturation ratio $[P_v/P_{sat}(T)]$.

The chemical activity is modelled as

$$A=1/(1+\sum_i l_i n_i / n_w)$$

where
l_i = the Van't Hoff ionization factor for solute 1 (= 2) for all solutes
n_i = moles of solute i within the droplet, and
n_w = moles of water within the droplet.

In the above Mason equation, the Kelvin effect (the exponential term) and the solubility effect (the A term) are treated in one equation and activated by a hygroscopic model flag. The Van't Hoff ionization factors are used in modelling hygroscopic effects that promote steam condensation on hygroscopic aerosol particles. In MELCOR1.8.4 model, all elements are treated to have the same solubility and ionization factors as those of soluble elements, which results in unsoluble elements to have soluble characteristics. So, changes are made in which only CsI and CsOH, instead of all elements, are considered to be soluble. Figure 6 shows that wet aerosol concentration decays at a much faster rate with old hygroscopic model, which is totally different from the measured data.

■ CONCLUSIONS AND DISCUSSIONS

The ISP44 open tests are simulated using MELCOR 1.8.4 code with detailed nodalization scheme of control volume and heat structure. The characteristics found during the three-step simulation for the preconditioning phase, stationary thermal hydraulic conditioning phase and the aerosol injection and depletion phase are:

1) The code predictions for the thermal hydraulic conditions at the end of phase-I show a good agreement with the measured values except the uninsulated door side wall temperature. The temperature of the door side wall shows a slight temperature difference because all control volumes inside the vessel boundary including the door side are fully open and well mixed in the code calculation. In this simulation process, an area of an artificial wall part (No.10) and an effective vessel leak size into the environment are critical. In our simulation, the area of wall part No.10 is only adjusted without tuning the effective vessel leak size to simulate the unexpected heat loss to the environment.
2) Data mismatch is found between the atmospheric pressure, temperature and humidity at the end of phase-I in the K188 test. The steam partial pressure at the observed volume temperature and humidity is calculated to be larger than the observed total volume pressure. Considering the data mismatch and technical error bounds of the measuring transducer systems, corrected volume

pressure and humidity are used.

3) The code predictions for the thermal hydraulic conditions including heat structure temperatures and the mass of N_2 gas and sump water at the beginning of aerosol injection are in a good agreement with the measured conditions. Especially, the vessel atmosphere temperature and pressure are predicted well throughout the phase-II during which the differences are less than 0.1 bar and 2.5°C respectively. Exceptions are the humidity for which MELCOR code can not predict over 100% and sump water temperature in the K148 test which is considered to be an erroneous data compared with the other tests.
4) The code predictions for the dry aerosol concentration in vessel atmosphere show a good agreement with the test results. For wet aerosols, the calculated concentration using modified hygroscopic model shows almost the same trend throughout the experiment period but with two-order difference. The reason for two-order difference is expected to be from obscure measuring unit but is not certain for the time being. In the mean time, the calculated wet aerosol concentration using the old hygroscopic model shows a totally different shape representing a much faster decrease which results from the bug in the original hygroscopic model.
5) The peak aerosol concentration in vessel atmosphere appears during the aerosol injection and then starts to decrease. At 1000 seconds after the end of aerosol injection, less than 35% of total injected mass exists in vessel atmosphere in all open tests where about a half of atmospheric aerosol mass deposits during this 1000-second period. Most of injected aerosol mass is appeared to deposit on the floor.

Based on the analyses made in this paper for KAEVER open test series of K123/K148/K186/K188, the analytical prediction capability of MELCOR1.8.4 thermal hydraulic and aerosol models is evaluated to be accurate except the hygroscopic model which needs modification for the solubility related defects.

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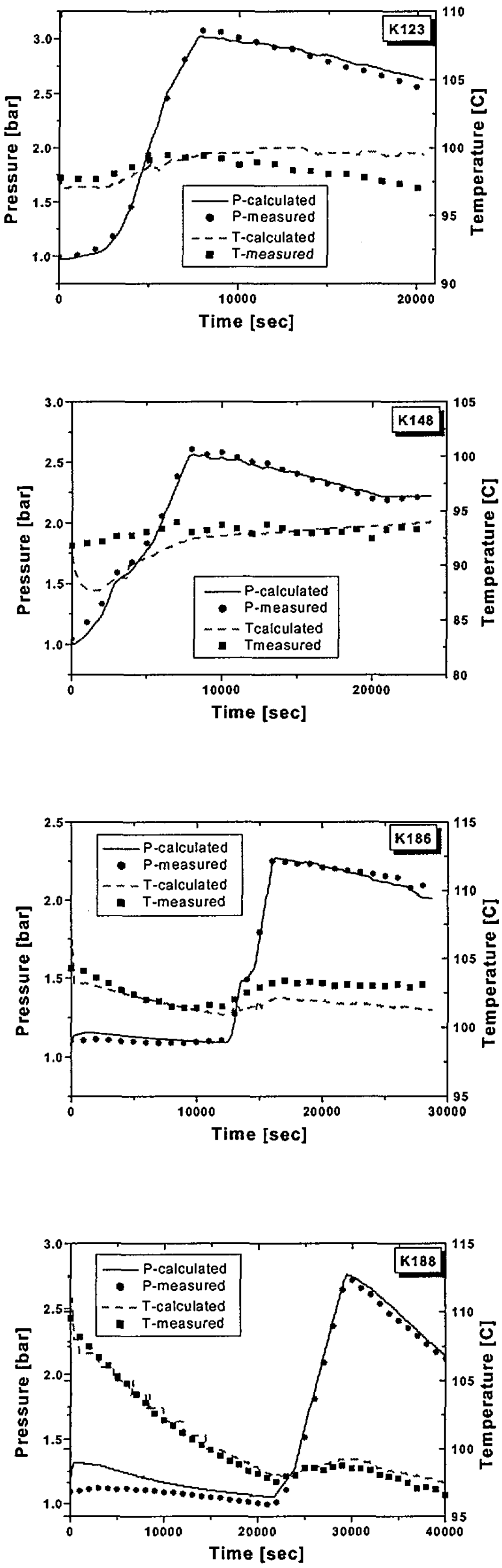

Figure.4 Vessel Atmosphere Pressure and Temperature

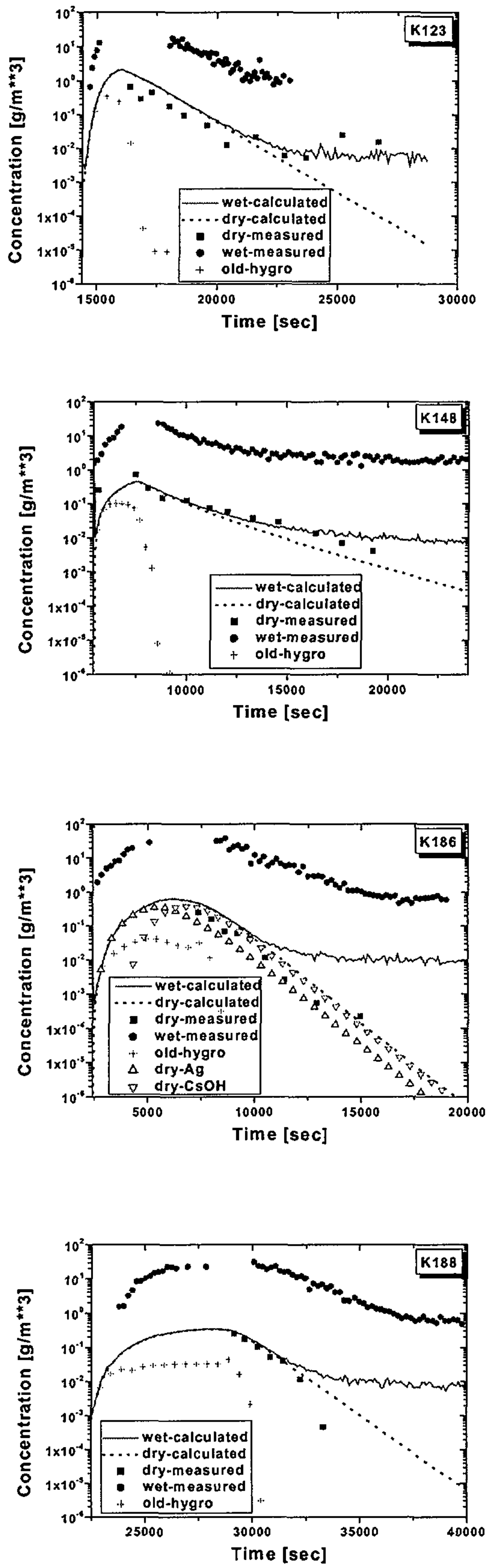

Figure.6 Aerosol Concentration in Vessel Atmosphere