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Assessment of the Hygroscopic Aerosol Model of the SIRIUS Module in the Severe Accident Analysis Code

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1. Introduction

Hygroscopic aerosols such as CsI and CsOH can grow in size by absorbing moisture under atmospheric environmental conditions where humidity is less than 100%. The grown particles are affected by gravitational sedimentation and thus affect the overall aerosol behavior of the nuclear power plant in the severe accident. Therefore, it is intended to verify the hygroscopic aerosol model of the SIRIUS module of the CINEMA code, which is the severe accident analysis code.

For the SIRIUS module of the CINEMA code, the process of calculating the radius through which the absorbed aerosol mixture can grow to an equilibrium state was reviewed. To this end, variable parameter values calculated through debugging in the relevant subroutine of the CINEMA code were compared with mathematical calculation results.

The AHMED test, an aerosol deposition experiment, was simulated through the SIRIUS module of the newly revised CINEMA code. For the three typical humidity conditions, the experimental data of the concentration change according to the growth and gravitational sedimentation of hygroscopic NaOH aerosol particles were compared with the code calculation results for the code validation.

2. Research Background

The SIRIUS (Simulation of Radioactive Nuclear Interaction Under Severe Accidents) module [1] provides a comprehensive analysis of the behavior of fission products in the CINEMA code. The SIRIUS module is intended to predict the amount of fission products attached to or released into the containment building while the fission products in the gas phase and aerosol are driven into the RCS by the steam-non-condensing mixture and analyze the behavior in the containment building.

Hygroscopic aerosols such as CsI and CsOH can grow in size by absorbing moisture under atmospheric environmental conditions where humidity is less than 100%. As the influence of gravitational sedimentation increases, the grown particles affect the overall aerosol behavior of the power plant in the critical event. The SIRIUS module provides user options to apply the hygroscopic model for CsOH and CsI. Aerosol particles with hygroscopic characteristics can absorb moisture in the atmosphere due to the difference between the relative humidity of the atmosphere and the condensation ratio on the surface of the aerosol particles, and absorb moisture until the aerosol reaches an equilibrium radius.

The Finnish Technical Research Center of Film (VTT) conducted an experiment using NaOH aerosol in an AHMED (Aerosol and Heat Transfer Measurement) experimental apparatus to observe the characteristics of the Hygroscopic aerosol [2]. The AHMED experimental apparatus is a cylindrical Vessel with a height of about 1.425 m and a diameter of about 1.27 m. In this experiment, an initial mass concentration condition was established by injecting NaOH aerosol of about 2.4 μm under various humidity conditions, and then aerosol sedimentation caused by Hygroscopic phenomenon was measured for about 13,000 seconds.

For this experiment, verification calculation [3] was performed with the SIRIUS module, but it was predicted that all aerosols settled much faster than the experiment. In other words, unlike the experiment, it was calculated that all NaOH aerosols in the air settled within about 250 seconds. As the analysis results of the experiment differ greatly, it was judged that verification was necessary rather than the uncertainty of the code prediction model.

3. Verification of Hygroscopic Aerosol Model

3.1 Hygroscopic aerosol model of the SIRIUS module

The aerosol particles having hygroscopic characteristics may absorb moisture in the atmosphere due to the difference between the relative humidity of the atmosphere and the condensation ratio on the surface of the aerosol particles, and absorb moisture until the aerosol reaches an equilibrium radius.

Condensation growth of hygroscopic nuclei in low-saturated or saturated vapor environments is an important factor in the analysis of aerosol behavior in containment buildings. The relationship [4] between the relative humidity, Φ, and equilibrium radius r of aqueous solution droplets formed by pure water-soluble seed particles of effective radius R_{eq} may be expressed as the following equation (1).

$$(\Phi - 1)\, r^4 - \frac{2\,\sigma}{\rho_w\, R_w\, T\, R_0} r^3 + \left(1 - \Phi + \frac{M_w\, \rho_a}{M_a\, \rho_w}\right) r + \frac{2\,\sigma}{\rho_w\, R_w\, T\, R_0} = 0 \quad (1)$$

$$r = \frac{R_{eq}}{R_0}, \qquad \Phi = \frac{P_{st}}{P_{sat}}$$

P_{sat} : saturated steam pressure P_{st} : steam pressure
R_0 : aerosol minimum radius

Here, equation (1) can be used to calculate the radius ratio (r) of the particles reflecting the hygroscopic model. At this time, it is assumed that the density and surface tension of the water are always constant. If the radius ratio is much greater than 1, it can be reasonably assumed because the properties of water dominate. In equation (1), the minimum radius of the aerosol is assumed to be 10^{-6} m.

Finally, starting with a minimum radius of 10^{-6} m (R_0) as shown in Fig. 1, the radius (R_{eq}) of the mixture of aerosols and droplets absorbed in equilibrium is calculated from the r value calculated through equation (1).

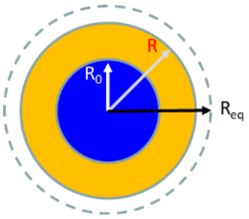


Fig. 1. Growth of moisturized aerosol mixture to equilibrium radius.

3.2 Verification by mathematical calculations

The process of calculating the radius (R_{eq}) in which the aerosol mixture absorbed in Equation (1) can grow to an equilibrium state was verified. Variable parameter values calculated through debugging in the subroutine of the related CINEMA code were compared with those calculated through mathematical calculation.

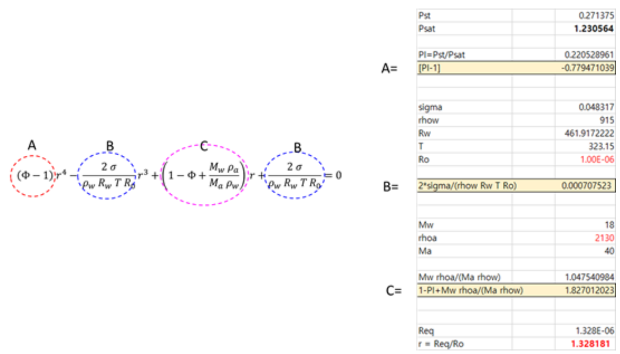


Fig. 2. Mathematical verification process.

At this time, the variable parameter values of the comparison target are calculated under the actual AHMED experimental conditions. Figure 2 shows the calculation results of the main variable parameters in the equation (1) obtained in this mathematical verification process.

The parameters and equilibrium radius in the equation (1) are obtained by debugging the relevant subroutine of the SIRIUS module and summarized in Table 1.

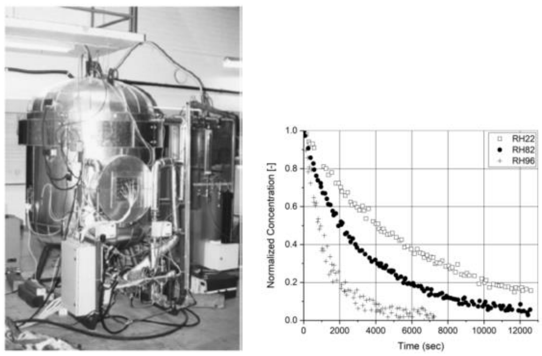
Table 1: Problem Description

Mathematical calculation		Debugging results (before modification)		Debugging results (after modification)	
A	-0.77947	C[4]	-0.77947	C[4]	-0.77947
B	0.0007075	-C[3] C[0]	0.0007075 0.0007075	-C[3] C[0]	0.0007075 0.0007075
C	1.827	C[1]	1.827	C[1]	1.827
$r = \frac{R_{eq}}{R_0}$	1.328	r_new	5.0	r_new	1.328

As shown in Table 1 above, the related SIRIUS model subroutine calculation error of the CINEMA code was confirmed and corrected. The part that differs before and after correction is the calculation of the radius of equilibrium state (1.328 ≠ 5.0). This is due to the fact that the bisection method, which was used as a numerical analysis solver of the equation before correction, was not normally applied (coding problem or calculation error). As described above, in the modified SIRIUS version, it can be seen that the result of calculating by changing to the Newton-Raphson method as a numerical analysis solver of the equation is the same as the mathematical calculation.

The SIRIUS model modified in this process was used to simulate the actual AHMED experimental results in the next section. Through this, the prediction result of the concentration reduction change according to the growth and adsorption of aerosol particles in a hygroscopic state is compared and verified with the experimental results.

3.3 AHMED test



(a) Test facility (b) test results

Fig. 3. AHMED test facility (a) and main test results (b).

In 1991, the aerosol technical group [5] of the Technical Research Center of Finland (VTT) injected NaOH in the form of an aerosol into the humidity controlled atmosphere and conducted a series of hygroscopic aerosol experiments in the AHMED

(Aerosol and Heat Transfer Measurement) Test Facility [2], as shown in Fig. 3. This experiment provided a lot of data on hygroscopic and non-hygroscopic aerosol behavior under controlled temperature and humidity conditions.

3.4 Code modelling of the AHMED test

The cylindrical container with a radius of 0.635 m, a sedimentation area of 1.27 m^2, and a volume of 1.81 m^3 used in the AHMED experiment may consist of a single control volume (CV1) with no inflow or outflow flow path when modeled with a lumped parameter code such as the CINEMA code or the MELCOR code (Fig. 4). The main points for code modeling are as follows.

1) The aerosol sedimentation area given from the experiment is applied to the sedimentation surface (or corresponding heat structure wall) modeling of the bottom of the container.
- The temperature of the wall surface is equal to the temperature of the initial atmospheric gas.

2) The atmosphere in the experimental vessel is defined to consist of 79% nitrogen and 21% oxygen.
3) The initial pressure in the control volume is 1.013×10^5 Pa (atmospheric pressure).
4) As summarized in Table 2, the initial gas temperature and relative humidity measured in each experiment are assigned to a single control volume (initial boundary conditions for the atmosphere in the vessel).
- When the initially measured NaOH concentration is set as the aerosol source, the initial concentration is set by injecting NaOH aerosol at a constant rate between 0.0 and 0.1 seconds.

5) Code users define the distribution of aerosol source size by entering AMMD and GSD obtained from the experiment (AMMD = 2.4×10^{-6} m, GSD = l.64).
- AMMD: Aerodynamic mass center diameter, GSD: Geometric standard deviation

6) Aerosol class 2 (basic Cs class) is used for NaOH. The molecular weight is 40 (= M_{NaOH}) and the atomic weight is 23 (= M_{Na}).
7) Calculations are essentially performed using 10 size sections with 16 aerosol classes.
- Each class has one aerosol component.
- NaOH aerosol is class number 2, and water aerosol is class number 14.
- The minimum aerosol diameter is 1.0×10^{-8} m (maximum aerosol diameter is 30.0×10^{-6} m).

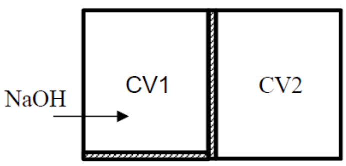


Fig. 4. Nodalization of the AHMED test.

Table 2: Summary of test conditions for simulation

Run	Relative Humidity (%)	Temperature (K)	Initial Mass Concentration (mg/m^3)
RH22	22	323.15	112
RH82	82	300.15	208
RH96	96	296.15	218

3.5 Validation against the AHMED test results

MELCOR and CINEMA code calculations were performed on three AHMED experiments to evaluate the ability to predict the deposition of absorbed aerosols according to humidity conditions.

First, the effect of error correction of the CINEMA code on the aerosol growth model with an equilibrium diameter shown in equation (1) was evaluated. To this end, the calculation results before and after error correction were compared for the RH22 experimental condition (22% humidity condition) in Fig. 5.

Prior to the modification of the aerosol particle growth prediction model, the aerosol concentration rapidly decreased from the beginning (red line in Fig. 5), decreasing below 10% (0.1) of the initial concentration after 200 seconds, and decreasing below 1% (0.01) of the initial concentration after 224 seconds, but the error-corrected version of calculation reached 10% (0.1) of the initial concentration after 12,000 seconds (blue line in Fig. 5). Although the aerosol concentration is predicted to be lower than the experimental results, it can be seen that the overall trend of gravity sedimentation effect is predicted better than before. In addition, even in the absence of the moisture absorption model, the prediction is underestimated compared to the measured aerosol concentration (green line in Fig. 5). Therefore, from the validation results in this case, it is judged that the CINEMA code not only excessively predicts aerosol growth but also overestimates the phenomenon of aerosol deposition caused by other factors.

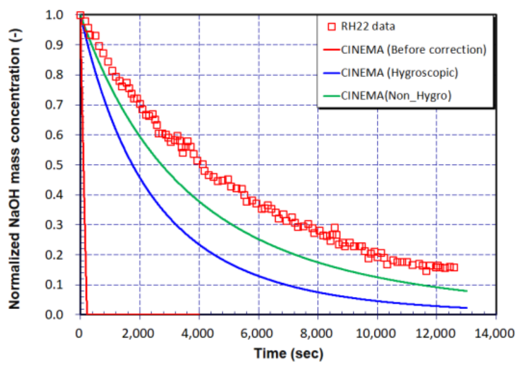


Fig. 5. Comparison of calculation results before and after CINEMA code error correction (RH22 experiment).

In Fig. 6 the code calculation results were compared for RH82 experimental conditions (82% humidity condition). In the case of the previous calculation, it can be seen that the growth and sedimentation rate of aerosol particles increase as the humidity increases compared to the case (22% humidity condition). However, the CINEMA code prediction is still overestimated for the concentration decrease due to aerosol sedimentation (under-predicting aerosol concentration). On the other hand, the prediction of the MELCOR code generally agreed well with the results of this experimental condition.

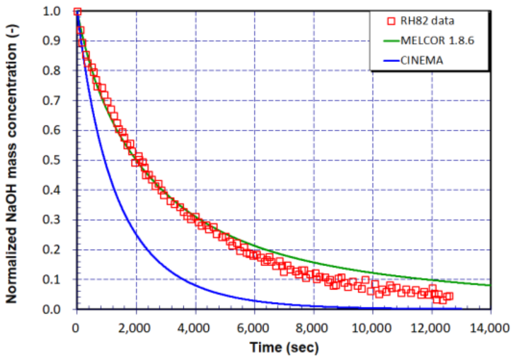


Fig. 6. Comparison of code predictions with test results of RH82.

In Fig. 7 the code calculation results were compared for RH96 experimental conditions (96% humidity conditions). Compared to the previous calculations (22% and 82% humidity conditions), it can be seen that the aerosol particle growth and sedimentation rate further increase as the humidity increases.

The CINEMA code prediction was similar for this 96% humidity condition. This is because the aerosol concentration was predicted to be low under the previous 82% humidity condition, but the aerosol concentration measurement result was lower in this 96% experiment result, while the code prediction result was similar to this experiment result while maintaining almost the previous low prediction result.

On the other hand, for RH96 experiments with the highest humidity conditions, the prediction of the MELCOR code did not agree with the experimental results, unlike the previous prediction of the results of lower humidity conditions.

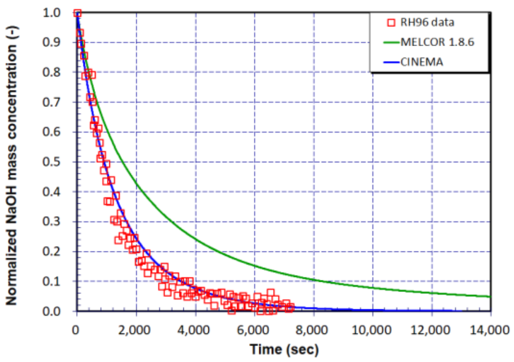


Fig. 7. Comparison of code predictions with test results of RH96.

3. Conclusions

The existing SIRIUS module of the CINEMA code has a numerical error in the process of calculating the equilibrium aerosol particle size when the hygroscopic aerosol model is applied, causing all aerosols to be deposited at once. Therefore, it is confirmed that the tendency of the experimental results simulating the growth and deposition of hygroscopic aerosol particles after the numerical error correction process is well reflected.

In addition, as a result of performing a validation analysis of AHMED, an aerosol deposition experiment, the evaluation of the hygroscopic aerosol model of the SIRIUS module of the CINEMA code is as follows.

- The tendency for the growth and deposition of wet aerosol particles to increase with increasing humidity is predicted in the limited humidity region.
- The aerosol deposition is largely overestimated, except for the highest humidity conditions of 96%.
- Even when aerosol growth according to the hygroscopic model is not applied, it is found that the deposition is overestimated, indicating that model evaluation for gravitational sedimentation, etc. should also be made.

For the future works, we will examine closely whether Eq. (1) is valid for modeling of the hygroscopic growth in the present SIRIUS module of the CINEMA code.

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