Sensitivity Analysis on Aerosol Deposition Models in CINEMA code

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1. Introduction

Currently in Korea, a code for comprehensive severe accident analysis, CINEMA (Code for Integrated severe accident Evaluation and Management), is under development. The CINEMA code can simulate various phenomena related to the accident progression in large pressurized light water reactors, such as steady-state calculation for normal operation, and various phenomena during severe accident progression in nuclear power plants.

The CINEMA code consists of several individual modules capable of independently simulate individual phenomena that occur during a severe accident, enabling linkage analysis. The CINEMA code categorizes severe accident into in-vessel and ex-vessel phenomena for the analysis. To efficiently execute the code, the CINEMA is divided into four modules: CSPACE (Core meltdown progress simulation coupling with Safety and Performance Analysis CodE for nuclear power plant) for in-vessel phenomena, SACAP (Severe Accident Containment Analysis Package) for ex-vessel phenomena, SIRIUS (SImulation of Radioactive nuclide Interaction Under Severe accident) for analyzing FP behavior, and MASTER, a linkage analysis module that supports coordination between individual modules.

The SIRIUS module is designed to be divided into two main processes for the simulation on the behavior of FPs: the release and transport of FP from the core. The SIRIUS receives its own inputs as well as node and link information to calculate the initial inventory of FPs. The solid-phase FPs are converted into gas or aerosol phase based on the temperature profiles of fuel and disperse into adjacent nodes. The aerosol-phase FPs can be removed through the phenomena such as the evaporation and sedimentation. The gas and aerosol phase FPs transported to each node can be changed into each other's phase depending on the temperature of the node. The quantities of solids, gas, and aerosol phase FPs at a given time are determined through these series of processes. Conversely, it is assumed that the temperature of FPs at each node are equivalent to the fluid temperature at the node. Thus, the energy equation for the FPs is not considered.

Currently, a various model in the SIRIUS module is continuously being developed and improved. To further improve the models, additional research and verifications are needed. However, the CINEMA has not undergone continuous validation by users. Accordingly, the necessity of assessing the uncertainty stemming from the inherent uncertainties within the code has been magnified. For verification to be performed by various and multiple users in the future, the searching process for variables that can be effectively manipulated by users must precede the uncertainty analysis. Therefore, this study focused on conducting sensitivity analysis on manipulative variables within the SIRIUS as an initial stage of uncertainty analysis, and eventually validation of the SIRIUS and the CINEMA codes.

2. Methodology

In this section the OPR1000 simulation using CINEMA and techniques for producing SIRIUS output are described. CINEMA 2.0.2 was used, and the detailed version for each module is as follows.

MASTER: 2.0.2.108
SACAP:2.0.2.108
SPACE-SAM_O2p:2.0.2.311
COMPASS.DLL:2.0.2.311
SIRIUS:2.0.2.311

To conduct the SIRIUS simulation, a preliminary calculation was conducted on the LBLOCA case based on the OPR1000 CINEMA input. In this context, within CINEMA, all modules except SIRIUS are structured to provide comprehensive analysis by interconnecting thermal_hydraulic information at every moment. However, in the case of SIRIUS, it does not directly simulate processes such as nuclear fuel melting, or gas behavior. Instead, it receives necessary information for FP simulation from the linkage analysis module. A more detailed structure of CINEMA code is shown in Fig. 1[1].



Fig. 1 Structure of CINEMA code

Based on this coupling process, therefore, SISIUS can be calculated alone, and in this study, a linkage file for SIRIUS input was created for efficient sensitivity analysis and used to execute SIRIUS code.

2.1 preliminary calculation for SIRIUS analysis

The preliminary calculations were conducted for the OPR1000 LBLOCA scenario, and the input used for the preliminary calculations was based on the nodalization as shown in Fig.2 [2].



Fig. 2-1 OPR1000 NSSS model for CSPACE



Fig.2-2. OPR1000 Containment model for SACAP

The preliminary calculations were conducted after a steady-state calculation of 1000 seconds, followed by a break occurring at 0 second, and continued for 72 hours. In this scenario, no additional mitigation strategies were applied. Additionally, the research methodology involved the creation of a linkage file specifically tailored for SIRIUS through the manipulation of options in CSPACE module.

Examining the thermal_hydraulic phenomena during the preliminary calculations, it was observed that the LBLOCA case's inherent characteristics led to a rapid progression of the accident sequence. Shortly after the accident initiation, an immediate reactor trip occurred, swiftly followed by depressurization reaching nearatmospheric pressure levels within 200 seconds. Around 3,590 s post-accident, a core material relocation to the lower plenum was predicted. Subsequently,

approximately 6,690 s into the accident, a consequential RPV failure occurred. The detailed pressure change of the primary and secondary systems is illustrated in Fig. 3.



Fig 4. Primary and secondary systems pressure change in LBLOCA scenario

2.2 Sensitivity parameter selection

The selection process of sensitivity variables pertaining to FP behavior within the SIRIUS module was primarily driven by a comparative analysis with MELCOR. Notably, the current version of SIRIUS provides users with adjustable parameters, predominantly focused behavior. on aerosol Consequently, the identification of sensitivity variables was grounded in a comparison between the variables utilized in MELCOR models that simulates aerosol behavior and the adjustable parameters accessible within the current SIRIUS framework. The sensitivity parameters examined in this study are specifically related to simulating aerosol removal through sedimentation in the context of FP aerosol behavior. A comprehensive list detailing these parameters are shown in Table. 1 below.

SIRIUS	MELCOR RN package
Gap	Gap release temperature
release temperature	(CLFAIL)
Collision shape factor	Agglomeration
(CSF)	shape factor (GAMMA)
Particle settling	Dynamic shape factor
shape factor (SSF)	(CHI)
Adjustable particle capture efficiency (PCE)	Gravitational collision efficiency (ε_g)
Density	
correction factor (DCF)	-

Table.1 Comparison of aerosol-related variables in SIRISU and MELCOR

While the PSS within SIRIUS and CHI in MELCOR, and the CSF in SIRIUS and GAMMA in MERCOR are described under distinct names, a closer examination in unveils that during the derivation of the aerosol correlation, these names refer to the same variable [3]. Delving deeper, some research expounds on the uncertainty analysis pertaining to MELCOR's Agglomeration shape factor and Dynamic shape factor [4]. Notably, this research embraces a distribution span ranging from 1.0 to 4.0. Accordingly, in our study, when executing sensitivity analysis on these two parameters, the range of values between 1.0 and 4.0 was employed for analysis.

For the gap release temperature, this study focused on the variable referred to as CLFAIL in MELCOR. The sensitivity analysis was conducted based on the default value of 1,137 K as specified in the MELCOR reference manual. As for PCE and DCF, the determination of sensitivity analysis ranges stemmed from the physical significance based on [3], enabling the selection of appropriate parameter ranges for our study. Additionally, regarding the simulation of aerosol behavior, sensitivity analysis was also conducted for three FP release models (CORSOR, CORSOR-M, CORSOR-O) within the SIRIUS framework. The equation of the emission rate applied to each model is shown below. Ki is the release rate, T is temperature, and R is gas constant. The release coefficients (Q_i , A_i , B_i , k_{0i} , R_{xi})are described on CINEMA manual [1].

CORSOR	$K_i = A_i \exp(B_i T)$
CORSOR-M	$K_{i} = k_{0i} \exp\left(-Q_{i}/RT\right)$
CORSOR-O	$K_{i} = R_{xi} k_{0i} \exp(-Q_{i}/RT)$

2.3 Sensitivity parameter classification

Based on the process of sensitivity parameter selection, these five parameters are categorized into two distinct types, assigning a Figure of Merit (FOM) to each category. FOM1 encompasses the total deposition of alkalic metal iodide across all nodes within SIRIUS, while FOM2 corresponds to the onset time of deposition for FPs. The correspondence between each FOM and its respective parameters is detailed in Table 2. Below.

FOMs	Parameters
FOM 1 (Total deposition of FP)	FP release model, CSF, SSF, PCE, DCF
FOM 2 (Deposition start time)	gap release time

 Table 2. FOMs and their corresponding sensitivity parameters

FOM1, serving as the ultimate representative of aerosol deposition, led to the selection of sensitivity parameters associated with aerosol removal models-CSF, SSF, PCE, and DCF. Additionally, considering the of FP release model, wherein the determination of release rates takes precedence over the release timing, this aspect harmonizes seamlessly within FOM1's scope of sensitivity analysis. In the case of FOM2, it related in the initiation of deposition rather than the magnitude of aerosol deposition, the gap release temperature was selected as a target variable of FOM2.

3. Results and Discussion

3.1 Result of Sensitivity Analysis on FOM1

Grounded in the previously determined sensitivity parameters and their corresponding FOMs, a comprehensive sensitivity analysis was executed. The initial attention was directed towards the variable aligned with FOM1. The examination unveiled the aerosol wall deposition, showcasing the differences across these sensitivity parameters. The interplay of data is portrayed through Figs. 5-9.



Fig. 5 Analysis result of FOM1 according to PCE



Fig. 6 Analysis result of FOM1 according to DCF

In Fig. 5, the impact of a selected sensitivity parameter, PCE, on FOM1 is presented. Notably, the exhibited trend unveils a proportional relationship, wherein a decrease in PCE corresponds to a reduction in FOM1. This correlation can be attributed to prevalence of particle capture event, prompting acceleration particle growth. Consequently, this phenomenon accelerates gravitational sedimentation, thereby influencing the observed decrease in FOM1. In contrast, Fig. 6 depicts a distinct narrative. The sensitivity parameter DCF elicits minimal variations in FOM1. This phenomenon can be attributed to the mathematical formulations inherent to the applied modeling. A detailed discussion regarding these observations is expounded upon conclusion section.



Fig. 7 Analysis result of FOM1 according to SSF



Fig. 8 Analysis result of FOM1 according to CSF

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Fig. 7 and 8 provide a comprehensive insight into the impact of aerosol particle morphology and the sensitivity parameters SSF and CSF, respectively, in relation to the variation in FOM1. Fig. 7 offers an analysis of the impact of SSF variation on the observed discrepancies in FOM1. Remarkably, as SSF increases by a factor of four, FOM1 exhibits 0.47 times the size of the CSF_(1.0) case. Contrarily, Fig. 8 showcases the impact of a four-fold increase in CSF, resulting in FOM1 expanding by 2.5 times. This dichotomy can be attributed to the effects stemming from particle morphology, where the manifestation of such trends becomes more pronounced as particle size becomes increasingly irregular.



Lastly, a sensitivity analysis concerning the FP release model was conducted. The employed models encompass three variants accessible within the realm of SIRIUS: CORSOR, CORSOR-M, and CORSOR-O. Upon scrutinizing the results, an intriguing trend emerges: FOM1 magnitude decreases in the order of CORSO-M, CORSOR, and CORSOR-O. Notably, CORSOR-O, being the smallest, is approximately 0.71 times the size of the CORSOR-M model, signifying a notable reduction. The outcomes of the sensitivity analysis for the five cases are consolidated in Table. 3 below

Para	ameters	FOM1
PCE	1.09(default)	4.19
	0.5	3.58
	0.7	3.58
DCF	1.0(default)	4.19
	0.5	4.28
	0.7	4.23
SSF	1.0(default)	4.19
	3.0	2.17
	4.0	1.84
CSF	1.0(default)	4.19
	3.0	8.67
	4.0	10.22
FP release model	CORSOR	4.10
	(default)	4.19
	CORSOR-M	4.75
	CORSOR-O	3.41

Table. 3 Results of sensitivity analysis for FOM1

3.2 Result of FOM2

The results of the sensitivity analysis regarding FOM2, which pertains to the gap release temperature were also conducted. The investigation unveiled variations in FOM2, indicating differences in the onset of FP deposition. As per physical intuition, a decrease in gap release temperature is associated with an accelerated release onset. Nonetheless, the observed disparities,

Para	ameter	FOM2
	1,000 K	1,754 s
Gap release	1,173 K	1,908 s
temperature	(default)	
	1,264 K	1,974 s

spanning a few hundred seconds, appear to wield a negligible impact on the overall accident dynamics.

Table. 4 Result of sensitivity analysis for FOM2

3.3 Discussion on the presented results

To facilitate user-driven validation of the SIRIUS code, this study conducted sensitivity analysis on key variables. A total of six parameters were considered, and the sensitivity was assessed based on two distinct FOMs.

- ✓ PCE, representing the efficiency of capturing smaller particles along the path of larger particles settling under gravity, indicates the effectiveness of capturing smaller particles as they get entrapped during the process. For the sensitivity parameters PCE, there is a discernible trend of reduced overall aerosol floor deposition (FOM1) as its value decreases. Specifically, when PCE is maintained as its original value of 70%, FOM1 is diminished to approximately 0.909 times, and when PCE drops to 50%, FOM1 further decreases to around 0.845 times. This behavior can be attributed to the diminished efficiency of particle capture with decreasing PCE, leading to a decrease in the overall aerosol deposition on the walls.
- ✓ DCF is used to correct the decreasing density value due to the porosity of aerosol assuming a spherical shape. In this case, since aerosols are assumed to be spherical, the values of CSF and SSF are fixed at 1. For the sensitivity variable DCF, there is minimal change observed in the values of FOM1 with respect to variations in the variable. This can be attributed to the fact that the aerosol's shape, being spherical, has the smallest surface area, which has a negligible impact on the aerosol growth and removal processes even if DCF changes. This physical characteristic is supported by the CINEMA manual's aerosol removal modeling equation, where the absolute value of the exponent of DCF is confirmed to be 0.128 or lower [5].
- ✓ CSF and SSF are variables that apply corrections to aerosol particle growth and removal processes based on the shape of the particles. SSF reflects the physical phenomenon that hinders aerosol removal as the particle shape becomes more irregular, while CSF reflects the phenomenon where aerosol particles collide and grow more actively as their shape becomes more irregular. Therefore, an increase in the value of SSF leads to a decrease in the value of FOM1, and an increase in the value of CSF leads to an increase in the value of FOM1. Specifically, when the value of SSF becomes four

times the original value, FOM1 decreases to approximately 0.431 times the original level. On the other hand, when the value of CSF becomes four times the original value, FOM1 increases to approximately 2.44 times the original level. This indicates that these two parameters exhibit greater sensitivity compared to the previous PCE and DCF variables, signifying that their influence on FOM1 is relatively significant. These two parameters are variables related to the shape of aerosol particles, and these results suggest that the floating amount and floating time of the aerosol particles in SA situation are predominantly affected by the shape of the particles, not by variables related to the size or density of the aerosol particles.

- ✓ Furthermore, a sensitivity analysis of the aerosol removal model for FOM1 was conducted. The primary model used in this study was the CORSOR model, with comparisons made to the CORSOR-M and CORSOR-O models. The results revealed that the CORSOR-O model exhibited the smallest FOM1 value, while the CORSOR-M model showed the largest FOM1 value. The difference between them was approximately 0.71 times, which is a significant variation that cannot be overlooked.
- ✓ Finally, a sensitivity analysis of the gap release temperature on the aerosol deposition initiation time (FOM2) was conducted. Gap release temperatures of 1000K, 1137K, and 1246K were considered, and the resulting differences in FOM2 were on the order of several hundred seconds. These variations are quite small in comparison to the overall timescales of the accident scenario.

4. Conclusion and future study

The comprehensive sensitivity analysis revealed that PCE and DCF had a relatively minor impact on aerosol deposition, whereas CSF, SSF, and the aerosol removal model exhibited more substantial influences on aerosol deposition. This means that the aerosol particles having an irregular shape have a great influence on the floating amount and time of the aerosol particles. However, considering that CSF and SSF are both related to aerosol particle shape, they may not be entirely independent variables. Further investigations are warranted in this regard.

Notably, the aerosol removal model's variability, allowing for up to a 70% change based on user selection, underscores the significant role it plays in overall accident analysis when utilizing SIRIUS. Although the expectation was that gap release temperature would have a notable impact on FOM2, the observed effect was relatively limited.

While this study focused solely on sensitivity analysis regarding parameters associated with aerosol deposition within SIRIUS, it is crucial to extend this analysis to other adjustable parameters. Additionally, a comparative analysis with other major accident analysis codes is essential for a comprehensive understanding. Ultimately, this sensitivity analysis serves as a foundation for conducting uncertainty analysis of SIRIUS and CINEMA, an imperative step toward enhancing safety assessment.

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