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Uncertainty Analysis of the SIRIUS Module in the CINEMA Code with a Focus on Aerosol Behavior and Correlation Factors Based on Linear Regression

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1. Introduction

In Korea, the development of CINEMA (Code for Integrated Severe Accident Evaluation and Management), a comprehensive code for severe accident analysis, is currently underway. CINEMA is designed to simulate a wide range of phenomena related to accident progression in pressurized light water reactors, encompassing steady-state calculations for normal operations as well as the various phenomena that occur during severe accidents in nuclear power plants.

CINEMA is composed of several independent modules, each capable of simulating specific phenomena associated with severe accidents, allowing for integrated analysis. The code categorizes severe accident phenomena into in-vessel and ex-vessel events. To conduct efficient execution, 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 fission product (FP) behavior, and MASTER, which is a linkage analysis module coordinating interactions between other individual modules[1-2].

Each module within CINEMA can perform standalone calculations using specific input files. SIRIUS is designed to simulate the behavior of fission products, focusing on the release of FP gases from the reactor core into the reactor coolant systems (RCS) and containment building. This includes FP transport, aerosol formation, and deposition within RCS pipes and steam generators, as well as within containment structures. The SIRIUS module is being developed in connection with the CINEMA module, and as it undergoes active development and enhancement, there is a critical need to quantify the uncertainties inherent within the code to accurately assess its improvements. Severe accident analysis codes like SIRIUS have inherent uncertainties due to factors such as limited knowledge of accident scenarios and phenomena, as well as user-determined code options. These uncertainties become particularly pronounced when simulating complex phenomena, such as the behavior of fission products.

SIRIUS specifically models the behavior of fission products, which are influenced by thermal-hydraulic phenomena and undergo transport and deposition in various forms—gaseous, aerosol, and solid. The physical behavior of aerosol is affected by several factors, notably the Collision Shape Factor (CSF) and the Particle Settling Shape Factor (SSF). To conduct an effective uncertainty analysis for modules like SIRIUS that simulate fission product behavior, it is essential to select uncertainty variables that accurately represent the physical behavior of aerosols. This study, therefore, focuses on identifying such uncertainty variables under engineering judgements, generating input sets through sampling, and executing multiple simulations to carry out a comprehensive uncertainty analysis of the SIRIUS module.

The objective of this study, which is the quantification of uncertainties in the SIRIUS module, primarily revolves around analyzing the correlations between uncertainty variables and the Figure of Merit (FOM). This framework involves analyzing the results from the generated output sets, performing linear regression analysis to derive correlation coefficients, and subsequently analyzing how uncertainty variables influence the code results. The quantification of uncertainties is thus achieved by determining the range of uncertainty present in the code outcomes.

2. Methodology

2.1 Computational Environments and Target System

The code used in this study consists of four submodules, all belonging to the version CINEMA2.0.2. The detailed versions of each submodule are as follows:

-MASTER2.0.2.118

-SACAP2.0.2.118

-SPACE-SAM_O2p2.0.2.327

-COMPASS.DLL2.0.2.327

-SIRIUS2.0.2.343

In this study, the hypothetical accident scenario for obtaining the generation of thermal-hydraulic data files is a large break loss of coolant accident (LBLOCA) in the optimized pressure reactor1000(OPR1000) without mitigation strategies. The nodalization of the code used in the simulation is shown in Figure1 [3].

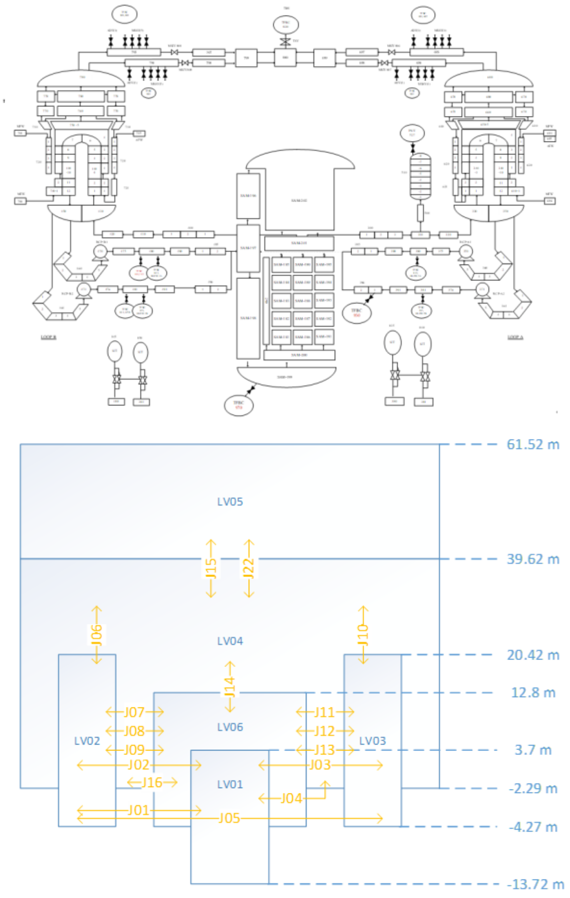

Fig 1. OPR 1000 nodalization model

In performing the uncertainty analysis, the thermal-hydraulic information required for SIRIUS was pre-calculated using other modules, and the resulting thermal-hydraulic data files were generated. These pre-generated thermal-hydraulic data files were then applied to the SIRIUS module to reduce the computational resource associated with multiple code executions necessary for the uncertainty analysis. In other words, the thermal-hydraulic information needed for the SIRIUS calculations was sourced from these data files, while the uncertainty variables were directly input into the SIRIUS module.

The calculation for the generation of thermal-hydraulic data files took 1,000 seconds steady state calculation to establish the appropriate uncertainty analysis, followed by a 72hours simulation. The steady-state calculation of 1000 seconds was selected as a steady-state calculation option generally taken when conducting a study of the severe accident analysis code.

2.2 Uncertainty variables and pre-processing

The uncertainty variables selected in this study are based on variables and their corresponding probability density functions used in previous uncertainty analysis studies conducted with other widely used severe accident analysis codes, such as MELCOR and MAAP5. These variables and their associated probability density functions are detailed in the table below [4]. According to the paper, the uncertainty analysis of aerosol behavior using MELCOR and MAAP was based on variables representing the shape and physical properties of aerosols. Key variables expected to have a dominant influence were selected from those used in MELCOR's aerosol behavior simulation model.

Variables	range
CSF(Collision Shape Factor)	1.0-4.0
SSF(particle Settling Shape Factor)	1.0-4.0
PCE(Particle Capture Efficiency)	0.5-1.0
DCF(Density Correction Factor)	0.5-1.0
RHO(Aerosol Density)	1000-5000
Hy_sol(Hygroscopic Solubility)	1-2
Hy_min(Hygroscopic minimum size)	1.E-07-2.E-06
GAPT(Gap Release Temperature)	1033-1366

Table 1. Considered Uncertainty Variables

The probability density functions applied to the uncertainty variables in this study were all determined to follow a uniform distribution. The size of the generated input set was calculated using Wilks' formula to ensure that it meets a 95/95 confidence level, requiring a total of 153 input files [5]. The FOMs adopted to evaluate the results of the uncertainty analysis was determined to be the mass of aerosols suspended within the Reactor Coolant System (RCS) and the containment building. The considered aerosol group is Alkali metal iodide whose representative nuclei is Cesium Iodide (CsI). The reason for setting the FOM to airborne aerosols is that, during a severe accident, radionuclides suspended in the containment can be released into the atmosphere, leading to human exposure. Therefore, a focused analysis was conducted, considering the factors affecting the behavior of airborne aerosols.

2.3. Pre-processing

Uncertainty analysis requires the generation of multiple input files, which involves sampling each uncertainty variable according to its respective probability density function. While commercial codes like MELCOR are equipped with uncertainty analysis tools such as DAKOTA, similar tools are not yet available for SIRIUS and CINEMA. Therefore, in this study, an in-house code was developed using Python to efficiently conduct the uncertainty analysis. This in-house code was used to perform pre-processing for the SIRIUS module.

The Python in-house code developed for this study is structured using Python classes, allowing for the application of different ranges and probability density functions to each uncertainty variable. The code supports various sampling methodologies, including Monte Carlo sampling and Latin Hypercube Sampling (LHS). Given that the size of the input set in this study is relatively small, the LHS method was chosen for its efficiency in generating sufficient samples with a smaller number of input file.

3. Results

The "horse tail" pattern observed in the code calculation results is illustrated in the figure below. The airborne aerosol, characteristic of the LBLOCA (Large Break Loss of Coolant Accident) scenario, were released rapidly during the initial stages of the accident and showed a significant decline within the first 5,000 seconds.

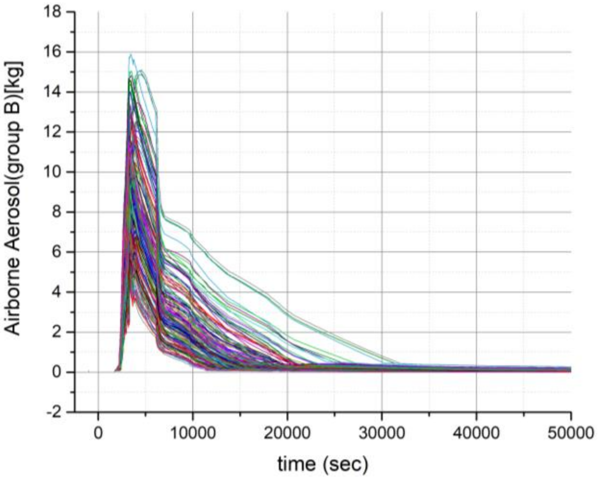

Fig 2. The horse tail of Airborne Alkali metal Iodide Aerosol

The Figure of Merit (FOM) was analyzed by conducting linear regression for each predetermined uncertainty variable at every time step, and the Pearson correlation coefficients were computed at every time step. The results indicated that, except for the Collision Shape Factor (CSF), Particle Settling Shape Factor (SSF), and Gap Release Temperature, the absolute values of the correlation coefficients for other variables were very low, below 0.1, demonstrating minimal correlation. In contrast, CSF, SSF, and Gap Release Temperature exhibited significant correlations during the early phases of the accident. The Pearson correlation coefficients are illustrated in the figure below.

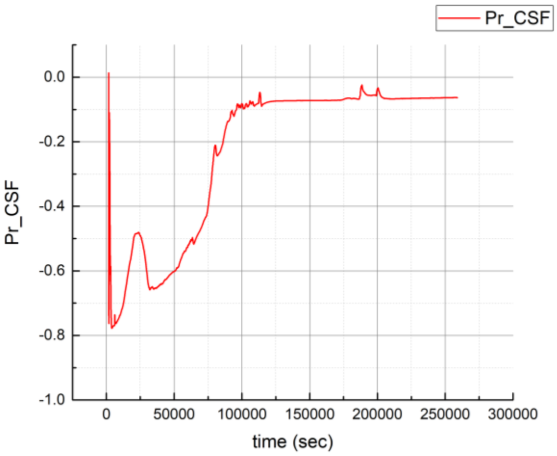

Fig 3. Time-series Pearson Correlation Coefficient data of CSF

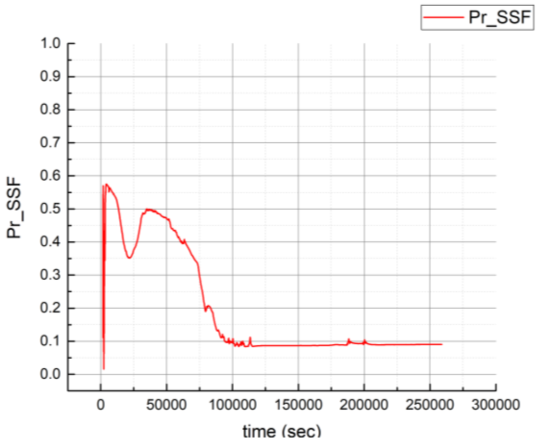

Fig 4. Time-series Pearson Correlation Coefficient data of SSF

For the Collision Shape Factor (CSF), the correlation coefficient during the early phases of the accident was negative, indicating that as the CSF increased, the amount of suspended aerosol decreased. The CSF represents the likelihood of aerosol particles colliding with other particles due to irregularities in their shapes. Therefore, an increase in CSF implies that aerosol particles become more irregularly shaped, leading to faster growth of the particles. Consequently, in environments with a high CSF during the early phases of the accident, the removal of aerosols occurs more quickly.

In contrast, for the Particle Settling Shape Factor (SSF), the correlation coefficient during the early phases was positive, indicating that as the SSF increased, the amount of airborne aerosol also increased. The SSF represents the physical phenomenon where the irregularity of aerosol shapes affects their ability to remain suspended in the flow within the system. Thus, a higher SSF suggests that aerosols can stay suspended in the system's flow for a longer period. Therefore, in environments with a high SSF during the early phases of the accident, aerosol particles settle more slowly, leading to a delay in their removal [6].

Based on the time-series correlation coefficient data presented in the figure above, a comparison of the correlation coefficients at the point where their absolute values are largest reveals that the influence of the shape factors is significantly more dominant compared to other uncertainty variables.

	Pearson Correlation Coefficient	R^2
CSF	-0.7746	0.6
SSF	0.5661	0.3204
DCF	0.0234	0.00549
PCE	-0.0350	0.00123
GAPT	-0.0402	0.00162
Hy_min	-0.1614	0.0261
Hy_sol	0.1234	0.0152
Density	0.0644	0.00415

Table 2. Correlation Coefficient of Uncertainty Variables (at 13750sec)

For the Gap Release Temperature, a high positive correlation was observed at the 2,500-second mark during the early stages of the accident. This indicates that a higher Gap Release Temperature results in a delayed release compared to lower temperatures, leading to a situation where suspended aerosols remain in the systemat later phase of the accident. This effect is reflected in the prolonged presence of aerosols as time progresses.

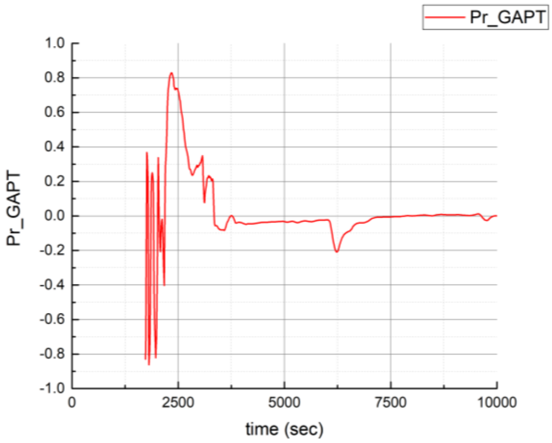

Fig 5. Time-series Correlation Coefficient data of GAPT

4. Conclusions

This study provides a detailed uncertainty analysis of the SIRIUS module within the CINEMA framework, focusing on its role in simulating fission product behavior during severe accidents in pressurized light water reactor. Various uncertainty variables, including Collision Shape Factor (CSF), Particle Settling Shape Factor (SSF), and Gap Release Temperature, were selected for analysis. Latin Hypercube Sampling (LHS) was employed to generate the input sets. The Figure of Merit (FOM) used for evaluating the results was the mass of airborne aerosols within the Reactor Coolant System (RCS) and containment building. To ensure a manageable number of samples while maintaining a 95/95 confidence level, the sampling was done through certain range and probability distribution function for each uncertainty variable. This pre-processing was conducted by an in-house Python code developed for SIRIUS. The findings contribute to a deeper understanding of how different uncertainty variables affect fission product behavior and underscore the importance of accurately characterizing these factors to enhance the reliability of severe accident simulations and improve safety assessments in nuclear power plants.

- ✓ The analysis of the FOM, specifically the mass of airborne aerosols, revealed significant findings in relation to the uncertainty variables during the LBLOCA scenario. The Pearson correlation coefficients demonstrated that, apart from the Collision Shape Factor (CSF), Particle Settling Shape Factor (SSF), and Gap Release Temperature, other variables showed very low correlation with the airborne aerosol mass, indicating minimal impact.
- ✓ CSF had a negative correlation in the early phases, suggesting that higher CSF values lead to reduced aerosol amount due to accelerated particle growth and removal, because the high CSF value means that the high irregularity of the particle of aerosol enhances the growth of aerosol particle.
- ✓ SSF exhibited a positive correlation, indicating that higher SSF values result in increased aerosol suspension times within the system, resulting in reduced amount of aerosol removal.
- ✓ The Gap Release Temperature also showed a significant positive correlation at the 2,500-second point, indicating that higher temperatures delay aerosol release, thereby extending their presence in the system. The analysis underscores the dominant influence of shape factors on aerosol behavior compared to other uncertainty variables, highlighting their critical role in modeling and predicting aerosol dynamics in severe accident scenarios.

Future research will address the uncertainties associated with variables other than the Collision Shape Factor (CSF), Particle Settling Shape Factor (SSF), and Gap Release Temperature, which were not fully explored in this study. Also, other FOMs, for example, gap release fraction will be adopted as a future research object. Additional analyses will be conducted to investigate potential correlations beyond linear regression for these variables. Furthermore, partial correlation analysis will be employed to isolate and quantify the effects of individual uncertainty variables, controlling for the influence of other variables. This approach aims to achieve a more accurate quantification of uncertainties within the SIRIUS module.

ACKNOWLEDGEMENT

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REFERENCES

[1] Korea Hydro & Nuclear Power Co., Ltd., User Manual for CINEMA 2.0, 2022
[2] Korea Hydro & Nuclear Power Co., Ltd., Theory Manual for CINEMA 2.0, 2022.
[3] JinHo Song, DonGun Son, JunHo Bae, SungWon Bae, Kwang-Soon Ha, Comparative Simulation of Severe Accident Progression by CINEMA and MAAP5, October 2022 Nuclear Engineering and Design, Volume 404, 2023, 112181, ISSN 0029-5493,
[4] Mateusz Malicki, Terttaliisa Lind, Parametric MELCOR 2.2 sensitivity and Uncertainty Study with a Focus on Aerosols based on Phebus test FPT1, Progerss in Nuclear Energy, Volume 158, 2023, 104609
[5] Attila Guba, Mihaly Makai, Lenard Pal, Statistical Aspects of Best Estimate Method – 1, Reliability Engineering and System Safety, Volume 80, 2023, 217232
[6] Michael Epstein, Phillip G. Ellison, Robert E. Henry, Correlation of Aerosol Sedimentation, Journal of Colloid and Interface Science, Volume 113, No.2, 1986