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Sensitivity Analysis of the Phenomenological Parameters to the Airborne Concentration of Aerosol Particles in the Containment during a Severe Accident via I-COSTA

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1. Introduction

Aerosol particles are the most of common form of fission products released into the containment during a severe accident of nuclear power plant [1]. The aerosol particles show various kinds of behaviors e.g., coagulations of the two particles due to Brownian motion, gravitation, turbulent motion of a fluid, settling via diffusiophoresis, thermophoresis, gravitation, and etc. In order to analyze the behaviors of aerosol caused by the aforementioned phenomena, I-COSTA (In-Containment Source Term Analysis) has been developed by one of the authors [2]. The code is based on the two governing equations; multicomponent sectional equations, which describes the mechanisms of the coagulations and the depositions, and Mason equation which describe the mechanisms of hygroscopic growth. The coupling of the two aforementioned equations is done via a transition rate matrix which is formulated via interpolation of the solutions from Mason equations on the radius of the aerosol particles.

Recently, from the investigation on Fukushima accident and experimental study to support the result of the investigation [3], delayed release of fission products becomes highlighted issue [4]. It occurs from the deposited aerosol particles to produce chemical species other than aerosol particles. Therefore, it is necessary to couple aerosol dynamics code and iodine chemistry code for the analysis of delayed release. For the proper coupling of the two codes, it is necessary to figure out important parameters in the aerosol dynamics.

In this paper, we are going to perform sensitivity analysis on the phenomenological parameters in the aerosol dynamics with the KAEVER experiments which are included in the international standard problem Nº44 [5].

2. Summaries of the Numerical Methods in I-COSTA and Sensitivity Analysis Scheme

2.1 Numerical Methods in I-COSTA

In I-COSTA, the multicomponent sectional equation and Mason equations are coupled via transition rate matrix obtained by interpolation of the mass distribution within a section for each component in multicomponent sectional equations and the solutions of Mason equations. For the interpolation, we assume that the mass concentration within a section as the following form :

$$\frac{dM}{dv} = bv^s, \tag{1}$$

where v is particle mass and s is "slope" of the mass concentration function, defined as

$$s = \frac{\ln\left(\frac{\bar{Q}_{l+1} - \bar{Q}_l}{v_{l+1} - v_l}\right) - \ln\left(\frac{\bar{Q}_l - \bar{Q}_{l-1}}{v_l - v_{l-1}}\right)}{\ln\left(\sqrt{v_{l+1}\cdot v_l}\right) - \ln\left(\sqrt{v_l \cdot v_{l-1}}\right)}. \tag{2}$$

With the functions, the mass concentrations remaining in section l and those growing up to l+1 are expressed as the follows :

$$Q^*_{l,k}\left(t_0 + \Delta t\right) = fr \cdot Q_{l,k}\left(t_0\right), \tag{3}$$

$$Q^*_{l+1,k}\left(t_0 + \Delta t\right) = \left(1 - fr\right)\cdot Q_{l,k}\left(t_0\right), \tag{4}$$

where

$Q^*_{l,k}\left(t_0 + \Delta t\right)$, $Q^*_{l+1,k}\left(t_0 + \Delta t\right)$: mass concentration at $t_0+\Delta t$ in section l and l+1, respectively,

$$fr_{l,k} = \frac{v_{2,k}^{slop_{l,k}+1} - v_{1,k}^{slop_{l,k}+1}}{v_{l+1,k}^{slop_{l,k}+1} - v_{l,k}^{slop_{l,k}+1}} = \frac{Q_{l,2,k}}{Q_{l,k}}. \tag{5}$$

$$tr_{l,k} = 1 - fr_{l,k}. \tag{6}$$

If the hygroscopic growth is assumed in the form of linear and first order process, then the following equation is obtained with the aforementioned relationship :

$$\frac{d\vec{Q}^*_{l,k}}{dt} = A_{l,k}\cdot\vec{Q}^*_{l,k},\ \ \vec{Q}^*_{l,k}\left(t_0\right) = \vec{Q}_{l,k}\left(t_0\right), \tag{7}$$

where $A_{l,k}$ is an elemental transition rate matrix of hygroscopic growth for aerosol particles of component k in section l.

Then the a global transition rate matrix can be obtained with Eq. (8):

$$\sum_{l=1}^{n_{bin}}\sum_{k=1}^{n_{comp}} A_{l,k} = A, \tag{8}$$

where n_{bin} in the number of sections of the aerosol particles considered in the multicomponent sectional equation.

With the global transition rate matrix and the system of multicomponent sectional equations, a system of equation can be written as

$$\frac{d\vec{Q}}{dt} = A \cdot \vec{Q} + P\left(\vec{Q}\right), \tag{9}$$

where $P\left(\vec{Q}\right)$ is vector form of the multicomponent sectional equations of the aerosol particles.

2.2 Summary of Sensitivity Analysis

In this work, the importance analyses are performed on the phenomenological parameters in the aerosol dynamics used in I-COSTA. The importance analyses scheme considered in this work is the same as the one in the previous study [6]. via Latin hypercube sampling on the parameters, sensitivity analyses via I-COSTA, and calculation of the correlation coefficients between the aforementioned parameters and figure of merits (airborne concentrations aerosol particles). The process is summarized on the following figure.

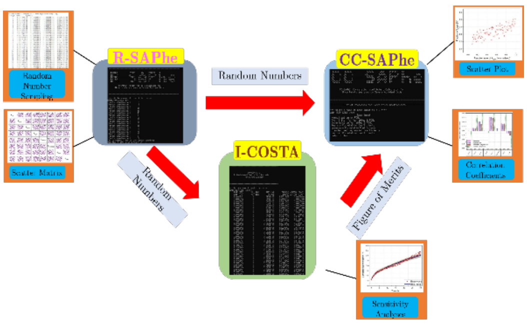

Fig. 2. Importance analysis scheme with I-COSTA

In the importance analyses, we considered 12 phenomenological parameters. The description on the parameters and its range of uncertainty considered in the importance analysis are shown in Table 1.

Table 1. Phenomenological parameters in the analysis

Parameters [Units]	Description	Mean	Min.	Max.
Satu_R	Humidity	Exp. cond	95%	105%
P_stick	Effect of Van der Walls force	1.0	0.1	1.0
Dy_shp	Drag of non-spherical particles	1.0	1.0	4.0
Agg_f	Spatial extent of non-spherical particle	1.0	1.0	4.0
Fslip	Deviation from continuum mechanics	1.37	1.1	1.3
Diffu_th [m]	Coagulation via Brownian diffusion	1.0e-05	1.0e-06	1.0e-04
Thrm_frc	Thermal conductivity on the particle	Exp. cond	93%	107%
Thrm_acco	Interaction between gas and particle in terms of temperature	1.0	0.5	1.5
ptl_den [kg/m^3]	Mixed particle density	1000.0	1000.0	5000.0
Turb_diss [m^2/sec^3]	Rate at which turbulent kinetic energy is converted into thermal energy	1.0e-03	5.0e-04	1.5e-03
Diffu_frc	Diffusion coefficient for vapor	Exp. Cond	95%	105%
R_to_g_to_P	Ratio of thermal conductivity of gas to that of particle	0.037	0.0002	0.055

3. Numerical Results

As discussed in the previous sections, we performed importance analysis via I-COSTA. In the analyses, we have considered three experiments in the KAEVER experiments; i) KAEVER-148 with Ag aerosols, ii) KAEVER-186 with a combination of Ag and CsOH aerosols, and iii) KAEVER-187 with a combination of Ag, CsI, and CsOH aerosols.

The number of samplings in the importance analysis are determined from the sensitivity analysis on the number of sampling. In the aforementioned sensitivity analysis, mean and standard deviation from the samplings are compared to ones obtained assuming the continuous distribution of the parameters. From the sensitivity analysis, we found that more than 2,000 sampling gives mean and standard deviations, the difference of which is less than 1.0E-05 in terms of relative error.

With the sampled parameters, the sensitivity on the change of airborne concentrations of the aerosols are shown in Figs. 2~4.

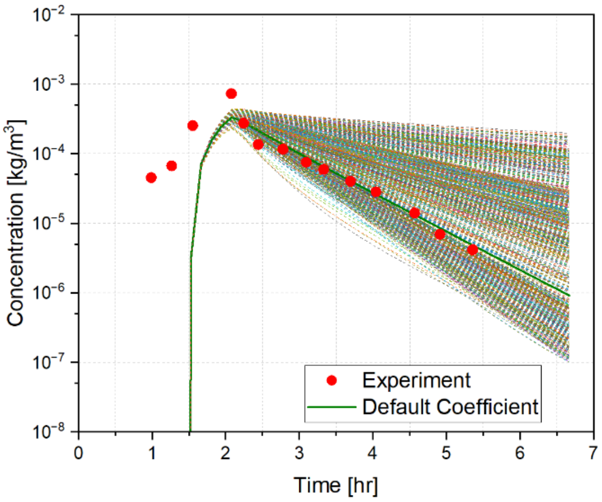

Fig. 2. Sensitivity analysis on the KAEVER-148 experiment.

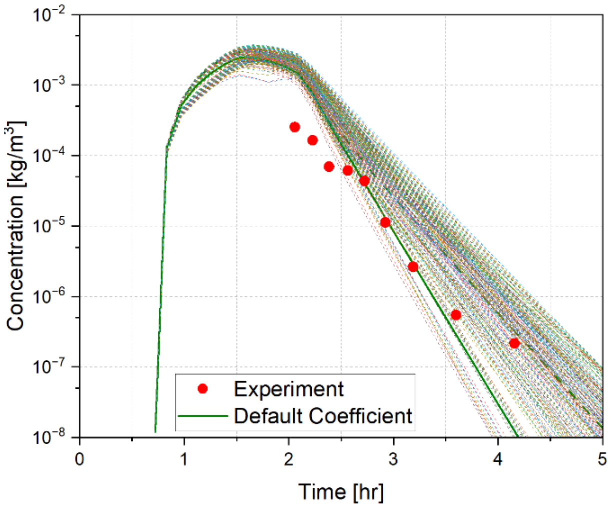

Fig. 3. Sensitivity analysis on the KAEVER-186 experiment.

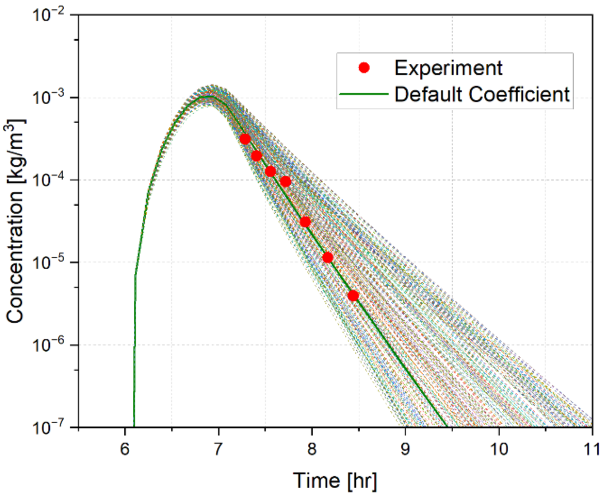

Fig. 4. Sensitivity analysis on the KAEVER-187 experiment.

As shown in the Figs 2~4, the airborne aerosol concentrations measured in the experiments lie within the range of sensitivity analyses via I-COSTA. In terms of maximum concentrations, the range of sensitivity in the analyses are ±50% of the reference value. According to the reports on the KAEVER experiments [3], the uncertainty in the measurement is ±7%. Since the analysis are performed based on the uncertainty range of the phenological parameters in the aerosol dynamics, the uncertainty ranges of the parameters lead to show the wider range of sensitivity in the numerical analyses than that in the experiment.

The correlation coefficient between the parameters and maximum airborne concentrations are shown in Figs. 5~7.

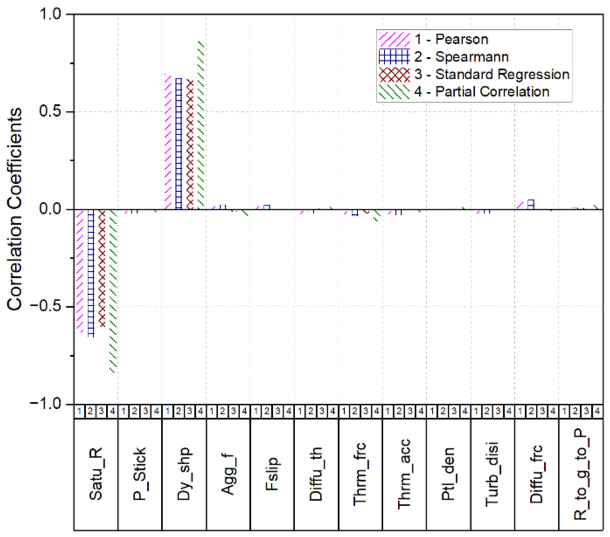

Fig. 5. Correlation coefficients for the KAEVER-148 experiments

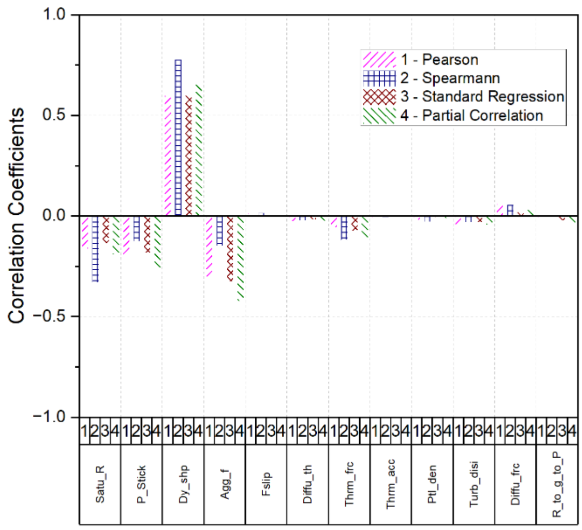

Fig. 6. Correlation coefficients for the KAEVER-186 experiment

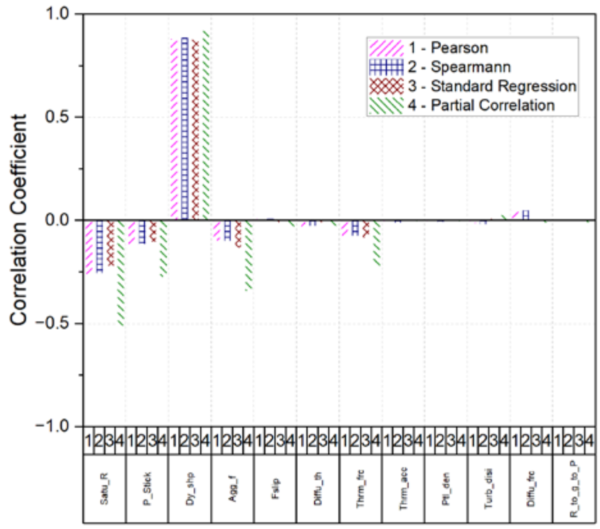

Fig. 7. Correlation coefficients for the KAEVER-187 experiment

As shown in Figs. 5~7, the dynamic shape factor shows strong positive linear relationship with the maximum airborne concentrations. In the case of saturation ratio, it shows strong negative linear relationship with the maximum airborne concentrations. Therefore, among the various phenomenological parameters, detailed analyses on the dynamic shape factor and saturation ratio are required to couple the I-COSTA with iodine chemistry codes especially when the formation of aerosol particles from iodine chemicals is considered.

4. Conclusions

In this paper, we performed the importance analyses on the phenomenological parameters in the aerosol dynamics. This was done with sampling of the reaction coefficients via Latin hypercube sampling, sensitivity analyses on the airborne concentrations of the aerosol particles, and correlation coefficients between the aforementioned parameters and figure of merits (maximum airborne concentrations).

From the above importance analyses, the dynamics shape factor and the saturation ratio can be considered important parameters regarding to the maximum airborne concentrations of the aerosol particles. Therefore, detailed analyses on the dynamic shape factor and saturation ratio are required to couple the I-COSTA with iodine chemistry codes especially when the formation of aerosol particles from iodine chemicals is considered.

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