Formulation of Coupling Scheme for Multicomponent Sectional Equations and Hygroscopic Growth via Transition Matrix of Mason Equations

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1. Introduction

During a severe accident in a nuclear power plant, most of fission products released into the containment have forms of aerosols. Such aerosols show various behaviors in the containment, e.g., coagulations of two aerosol particles due to Brownian, gravitational motions, deposition on the surfaces in the containment via diffusiophoresis, thermophoresis, and gravitational settling, etc. In addition, the sizes of the aerosols change due to hygroscopic growth by steam condensation and evaporation on the aerosol surfaces [1]. Therefore, it is important to analyze such behaviors of the aerosols in the containment in order to evaluate off-site consequences due to release of fission products.

In the conventional calculations, such behaviors of the aerosols are described via two governing equations. One governing equations are multicomponent sectional equations which describe the mechanisms of the coagulations and the depositions. They are implemented in the well-known production codes, such as MAEROS [2], NAUA-Mod 5 [3], MELCOR [4] based on MAEROS, etc. The other governing equations are Mason equations which describe the mechanisms of hygroscopic growth. The equations are also implemented in NAUA-Mod 5, MELCOR, etc.

However, the two governing equations in the aforementioned production codes are not coupled rigorously. In other words, at each time step of calculation, solutions of the Mason equations are simply used as an initial condition of the multicomponent sectional equations.

In this paper, we explain a new formulation of coupling scheme for multicomponent sectional equations and Mason equations. The formulation is based on a transition matrix obtained from the solutions of Mason equations. It is implemented in the code named as I-COSTA (In-Containment Source Term Analysis), which is being developed to analyze behaviors of fission products in the containment during a severe accident.

2. Coupling Scheme of Multicomponent Sectional Equations & Mason Equations

2.1 Multicomponent Sectional Equations

On the mechanisms of coagulations and depositions, multicomponent sectional equations for aerosol particles of component k having mass of v_l and v_{l+1} is written as

$$\begin{aligned}\frac{dQ_{l,k}}{dt} &= \frac{1}{2}\cdot\sum_{i=1}^{l-1}\sum_{j=1}^{l-1}\left[{}^{1a}\bar{\beta}_{i,j,l}\cdot Q_{j,k}\cdot\bar{Q}_i + {}^{1b}\bar{\beta}_{i,j,l}\cdot Q_{i,k}\cdot\bar{Q}_j\right] \\ &\quad -\sum_{i=1}^{l-1}\left[{}^{2a}\bar{\beta}_{i,l}\cdot\bar{Q}_i\cdot Q_{l,k} - {}^{2b}\bar{\beta}_{i,l}\cdot\bar{Q}_l\cdot Q_{i,k}\right] \\ &\quad -\frac{1}{2}\cdot{}^{3}\bar{\beta}_{l,l}\cdot\bar{Q}_l\cdot Q_{l,k} - Q_{l,k}\cdot\sum_{i=l+1}^{m}{}^{4}\bar{\beta}_{i,l}\cdot\bar{Q}_i + \bar{S}_{l,k} \\ &\quad -\bar{R}_{l,k}\cdot Q_{l,k},\end{aligned} \tag{1}$$

where

$Q_{l,k}$: mass concentration of aerosol particles of component k in section l,

$\bar{Q}_l = \sum_{k=1}^{n_{comp}} Q_{l,k}$,

${}^{1a}\bar{\beta}_{i,j,l}$, ${}^{1b}\bar{\beta}_{i,j,l}$: coagulation rate of particles in sections lower than l forming a particle in section l,

${}^{2a}\bar{\beta}_{i,j,l}$: coagulation rate of particles in section l and sections lower than l forming a particle larger than those in section l,

${}^{2b}\bar{\beta}_{i,j,l}$: coagulation rate of particles in section l and sections lower than l forming a particle remaining in section l,

${}^{3}\bar{\beta}_{i,l}$: intra-sectional coagulation rate of particles in section l forming a particle larger than those in section l,

${}^{4}\bar{\beta}_{i,l}$: coagulation rate of particles in section l forming a particle larger than those in section l,

$\bar{S}_{l,k}$: source of particles in section l,

$\bar{R}_{l,k}$: removal rate of particles in section l via deposition.

The mathematical expressions of the aforementioned coefficients are written explicitly in Ref. [5].

For geometric constraint of $v_{i+1} \geq 2v_i$, and with some algebra, Eq. (1) is rewritten as

$$\begin{aligned}\frac{dQ_{l,k}}{dt} &= \sum_{i=1}^{l-2}\left[{}^{1a}\bar{\beta}_{i,l-1,l}\cdot Q_{l-1,k}\cdot\bar{Q}_i + {}^{1b}\bar{\beta}_{i,l-1,l}\cdot Q_{i,k}\cdot\bar{Q}_{l-1}\right] \\ &\quad +\frac{1}{2}\cdot\left[{}^{1a}\bar{\beta}_{l-1,l-1,l} + {}^{1b}\bar{\beta}_{l-1,l-1,l}\right]\cdot Q_{l-1,k}\cdot\bar{Q}_{l-1} \\ &\quad -\sum_{i=1}^{l-1}\left[{}^{2a}\bar{\beta}_{i,l}\cdot\bar{Q}_i\cdot Q_{l,k} - {}^{2b}\bar{\beta}_{i,l}\cdot\bar{Q}_l\cdot Q_{i,k}\right] \\ &\quad -\frac{1}{2}\cdot{}^{3}\bar{\beta}_{l,l}\cdot\bar{Q}_l\cdot Q_{l,k} - Q_{l,k}\cdot\sum_{i=l+1}^{m}{}^{4}\bar{\beta}_{i,l}\cdot\bar{Q}_i + \bar{S}_{l,k} \\ &\quad -\bar{R}_{l,k}\cdot Q_{l,k}.\end{aligned} \tag{2}$$

2.2 Mason Equation for Hygroscopic Growth

In terms of change of mean radius of aerosol particles, Mason equation for condensation & evaporation process is expressed as

$$\frac{dr}{dt}=\frac{1}{r}\cdot\frac{\left(S-S_r\right)}{a+b}, \tag{3}$$

where

S : saturation ratio,

S_r : effective saturation ratio at the surface of the aerosol particle, expressed as

$$S_r = A_r\cdot\exp\left(\frac{2\cdot M_w\cdot\sigma}{R\cdot T_\infty\cdot\rho_w\cdot r}\right), \tag{4}$$

$$a=\left(\frac{\Delta h_f^2\cdot M_w\cdot\rho_w}{R\cdot T_\infty\cdot T_\infty\cdot k_a^*}\right), \tag{5}$$

$$b=\left(\frac{R\cdot T_\infty\cdot\rho_w}{D_v^*\cdot M_w\cdot p_{sat}\left(T_\infty\right)}\right), \tag{6}$$

D_v^* : effective vapor diffusion coefficient expressed as

$$D_v^*=\frac{D_v}{\left(\dfrac{r}{r+\Delta_V}\right)+\left(\dfrac{D_v}{r\cdot\alpha_c}\cdot\left(\dfrac{2\cdot\pi\cdot M_w}{R\cdot T_a}\right)^{1/2}\right)}, \tag{7}$$

k_a^* : effective thermal conductivity of atmosphere expressed as

$$k_a^*=\frac{k_a}{\left(\dfrac{r}{r+\Delta_T}\right)+\left(\dfrac{k_a}{r\cdot\alpha_T\cdot\rho_a\cdot c_{p,a}}\cdot\left(\dfrac{2\cdot\pi\cdot M_a}{R\cdot T_a}\right)^{1/2}\right)}, \tag{8}$$

and other terms explained in MELCOR reference manual [4].

2.3 Coupling of Multicomponent Sectional Equations & Mason Equations via Transition Matrix

Since the solutions of Mason equations are mean radii of the aerosol particles, they should be converted in terms of mass concentrations of aerosol particles in order to couple them with the solutions of multicomponent sectional equations. Assume that the mass concentration within a section is expressed as [4]

$$\frac{dM}{dv}=bv^s, \tag{9}$$

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

$$s=\frac{\ln\left(\dfrac{\bar{Q}_{l+1}-\bar{Q}_l}{v_{l+1}-v_l}\right)-\ln\left(\dfrac{\bar{Q}_l-\bar{Q}_{l-1}}{v_l-v_{l-1}}\right)}{\ln\left(\sqrt{v_{l+1}\cdot v_l}\right)-\ln\left(\sqrt{v_l\cdot v_{l-1}}\right)}. \tag{10}$$

With the functions, mass concentrations remaining in section l and growing up to section l+1 due to hygroscopic growth are expressed as Eqs. (11) and (12), respectively :

$$Q_{l,k}^*\left(t_0+\Delta t\right)=fr\cdot Q_{l,k}\left(t_0\right), \tag{11}$$

$$Q_{l+1,k}^*\left(t_0+\Delta t\right)=\left(1-fr\right)\cdot Q_{l,k}\left(t_0\right), \tag{12}$$

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,

$$fr=\frac{v_2^{s+1}-v_1^{s+1}}{v_{l+1}^{s+1}-v_l^{s+1}}=\frac{\bar{M}_{1,2}}{\bar{M}_l}, \tag{13}$$

and the relationship among the coefficients used in Eq. (13) is shown in Fig. 1.

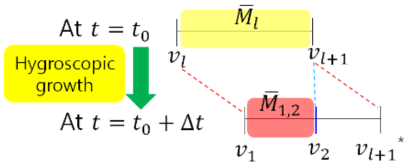

Fig. 1. Concept of fraction of mass remaining in section l

Using the frs of the sections, a transition matrix of Mason equation can be constructed. Then, we have the following relationship between mass concentration vectors and the transition matrix as

$$\vec{Q}^*\left(t_0+\Delta t\right)=B\vec{Q}\left(t_0\right), \tag{14}$$

where B is transition matrix of Mason equation.

In order to convert the solutions of Mason equations to those of ordinary differential equations on the mass concentrations, the hygroscopic growth can be expressed as

$$\frac{d\vec{Q}^*}{dt}=A\cdot\vec{Q}^*,\ \vec{Q}^*\left(t_0\right)=\vec{Q}\left(t_0\right). \tag{15}$$

By an implicit scheme, Eq. (15) is discretized over the time as

$$\vec{Q}^*\left(t_0+\Delta t\right)=\left(I-A\cdot\Delta t\right)^{-1}\cdot\vec{Q}^*\left(t_0\right). \tag{16}$$

From the Eq. (14), we have the following relationship :

$$\left(I-A\cdot\Delta t\right)^{-1}=B. \tag{17}$$

With Eqs. (15) and (2), we can write a coupled system of Mason equations and multicomponent sectional equations as a system of non-homogeneous ordinary differential equations. The system is expressed as

$$\frac{d\vec{Q}}{dt}=A\cdot\vec{Q}+P\left(\vec{Q}\right), \tag{18}$$

where

$P\left(\vec{Q}\right)$: multicomponent sectional equations expressed as a vector form.

After some algebra, mass concentrations of the aerosol particles at $t_0+\Delta t$ can be expressed as

$$\vec{Q}\left(t_0+\Delta t\right)=B\cdot\left\{\Delta t\cdot P\left(\vec{Q}\left(t_0+\Delta t\right)\right)+\vec{Q}\left(t_0\right)\right\}. \tag{19}$$

Note that Eq. (19) is the explicitly coupled solution of the system of Mason equations and multicomponent sectional equations through the transition matrix, B. Configuration of transition matrix becomes similar with that of identity matrix as saturation ratio becomes close to the effective saturation ratio on the aerosol particles.

However, as the saturation ratio differs from the effective saturation ratio, the configuration of the transition matrix becomes different from that of identity matrix, which will make the results of the calculations distinguished from those of conventional calculations.

2.4 Comparison with the Algorithm in MELCOR

A calculation procedure of I-COSTA, in which the aforementioned formulation is implemented, is compared to that of MELCOR in Fig. 2. The key difference between the two procedures is usage of the transition matrix.

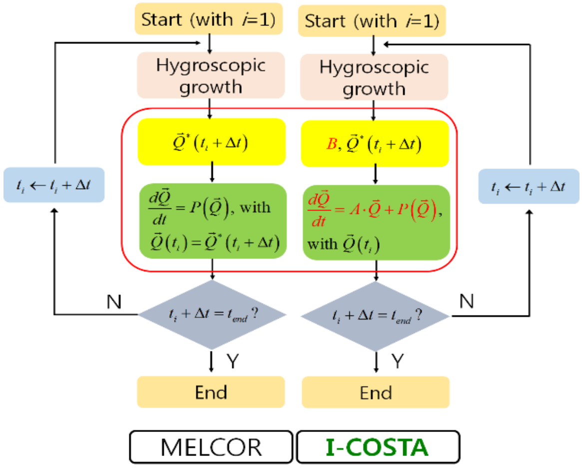

Fig. 2. Comparison of the algorithms in MELCOR and I-COSTA used in aerosol dynamics

3. Numerical Results

Geometric and thermophysical conditions of the problem are shown in Table 1. In the problem, behaviors of the aerosols are analyzed for 200 sec. The saturation ratio and the effective saturation ratio on the aerosol particles are assumed to be 1.00005 and 1. Temperature-dependent chemical and thermophysical properties used in the calculations are taken from MELCOR 1.8.6 [4]. The two codes use 1.0E-02 s as a time step (Δt). Distribution of mass concentrations of the aerosols is shown in Fig. 3. Distributions of mass concentrations at t=0.1, 10, 100, and 200 s are also shown in Figs. 4~7.

Table 1. Geometric and thermophysical conditions for the test problem

Parameters	Data
Volume of chamber [m^3]	2.86
Temperature [K]	298
Pressure [Pa]	1.01E+05
Density of aerosol particle [kg/m^3]	1,000
Number of sections (n_{section})	20
Minimum and maximum diameter of the particles [m] (min, max)	1.0E-08, 2.0E-05
Simulation time [s]	200

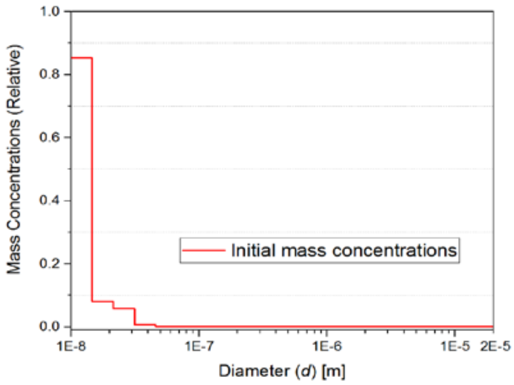

Fig. 3. Distribution of mass concentrations at t=0

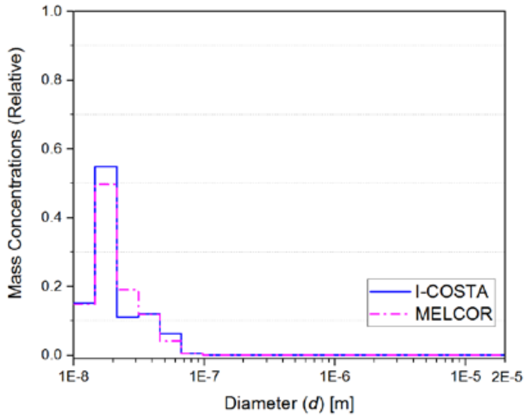

Fig. 4. Distribution of mass concentrations at t=0.1 s

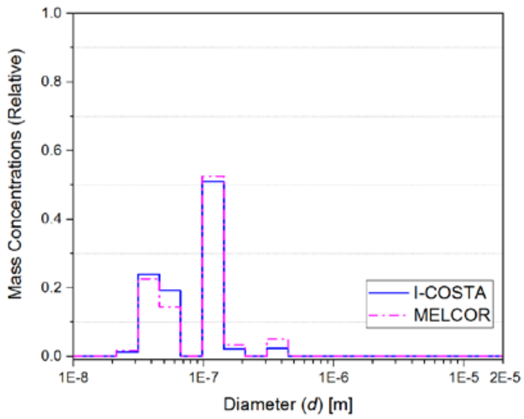

Fig. 5. Distribution of mass concentrations at t=10 s

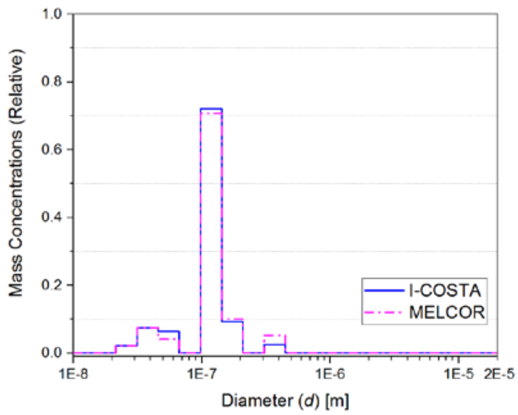

Fig. 6. Distribution of mass concentrations at t=100 s

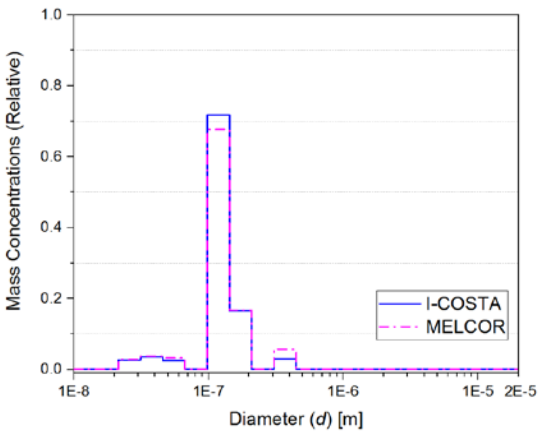

Fig. 7. Distribution of mass concentrations at t=200 s

As shown in Figs. 4~7, aerosol particles grow slower in I-COSTA than those in MELCOR i.e., at t=200 s, relative mass concentration in sections higher than 10 (d≥3.05E-07m) is 0.23 in MELCOR and that in I-COSTA is 0.19. The causes of the results are that, as shown in Fig. 2, solutions of the Mason equations at each time step are used as an initial condition of multicomponent sectional equations in MELCOR, which is unrealistic since aerosol particles grow by simultaneous processes of hygroscopic growth and coagulations. However, in I-COSTA, the two equations are coupled explicitly and solved simultaneously. Computing time of the two codes is compared in Table 2.

Table 2. Computing time of MELCOR and I-COSTA

	I-COSTA	MELCOR
Computing time [s]	516.7	510.5

Computing time of I-COSTA is comparable to that of MELCOR. Even though, multiplications of the transition matrix are additionally required in I-COSTA, computation burden of such multiplications seems to be insufficient.

4. Conclusions

In this paper, we proposed coupling scheme of multicomponent sectional equations and Mason equations for hygroscopic growth to analyze the aerosol behaviors in the containment. The coupling of the two governing equations is done via construction of the transition matrix obtained from the solutions of Mason equations in which changes of mean radius of aerosol particles in each section are calculated.

The coupling scheme was implemented in I-COSTA and compared to MELCOR. The results obtained from I-COSTA showed that the aerosol particles grow slower than those in MELCOR. The causes of the results were that the Mason equations for hygroscopic growth and the multicomponent sectional equations were coupled explicitly and solved simultaneously. However, in MELCOR, solutions of the Mason equations are used as an initial condition of the multicomponent sectional equations at each time step, which is unrealistic since the aerosol particles grow by the simultaneous processes of hygroscopic growth and coagulations.

Meanwhile, even though multiplications of the transition matrix are additionally required in I-COSTA, computing time is comparable to that of MELCOR. Computation burden of such multiplications seems to be insufficient.

With the formulation for coupling of Mason equations and multicomponent sectional equations, we expect that I-COSTA will analyze the aerosol behaviors more explicitly for the conditions that the hygroscopic growth or evaporations on the aerosol particles are significant. However, in such conditions, the conventional codes cannot analyze aerosol behaviors explicitly. As future work, we will perform analyses on such cases in order to study on the influence of the formulations on the aerosol behaviors. Then, I-COSTA will be coupled with a severe accident analysis code.

ACKNOWLEDGEMENTS

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REFERENCES

[1] B. R. Segal et al., Nuclear Safety in Light Water Reactor, Elsevier Inc, 2012.

[2] F. Gelbard, MAEROS User Manual, MUREG/CR-1391, SAND80-0822, Sandia National Laboratories, Albuquerque, NM, 1982.

[3] H. Bunz et al., NAUA Mod 4 – A Code for Calculating Aerosol Behavior in LWR Core Melt Accidents, KfK 3554, Kernforschungszentrum Karlsruhe, 1983.

[4] R, O. Gaunnt et al., MELCOR Computer Code Manuals Vol. 2 : Reference Manual , Version 1.8.6 Sandia National Laboratories, Albuquerque, NM, 2005.

[5] F. Gelbard and J. H. Seinfeld, “Simulation of Multicomponent Aerosol Dynamics,” *J. Colloid Interface Sci*, **78**, No. 2, pp. 485-501, 1980.