Code Development on Aerosol Behavior under Severe Accident –Aerosol Coagulation

Kwang Soon Ha*, Sung Il Kim, Eun Hyun Ryu
Korea Atomic Energy Research Institute, 1045 Daedeok-daero, Yuseong-gu, Daejeon, Korea
**Corresponding author: tomo@kaeri.re.kr*

1. Introduction

Most of the radioactive material might escape in the form of aerosols from a nuclear power plant during a severe reactor accident [1], it is very important to predict the behavior of these radioactive aerosols in the reactor cooling system and also in containment building under the severe accident condition. Aerosols are designated as very small solid particles or liquid droplets suspended in a gas phase. The suspended solid or liquid particles typically have a range of sizes such as from 0.01 μm to 20 μm. Aerosol concentrations in reactor accident analyses are typically less than 100 g/m^3 and usually less than 1 g/m^3. At these concentrations, the aerosol particles little affect the gas hydrodynamics, but the gas dynamics profoundly affect the behavior of the suspended particles. The behaviors of the larger aerosol particles are described usually by continuum mechanics. The smallest particles have diameters less than the mean free path of gas phase molecules and the behavior of these particles can often be described well by free molecular physics. The vast majority of aerosol particles arising in reactor accident analyses have behaviors in the very complicated regime intermediate between the continuum mechanics and free molecular limit. In this regime, aerosol behavior must be described using some approximate solution of the Boltzmann equation [1].

When there are continuing sources of aerosol to the gas phase or when there are complicated processes involving engineered safety features much more complicated size distributions develop. It is not uncommon for aerosols in reactor containments to have bimodal size distributions at least for some significant periods of time early in an accident. Salient features of aerosol physics under reactor accident conditions that will affect the nature of the aerosols are: (1) formation of aerosol particles, (2) growth of aerosol particles, (3) shape of aerosol particles, (4) deposition of particles on surfaces, and (5) resuspension of aerosol particles [1].

In MAAP code [2], within a given compartment the transitions between the three states, vapor, aerosol, and deposited, are calculated using subroutine FPTRAN (subroutine FPTRNP in the primary system). This model predicts gravitational settling, diffusiophoresis (steam condensation), thermophoresis, impaction, vapor condensation, and vapor revolatilization for all fission products present in that compartment. The MAAP code calculation procedure for aerosols, with particles growing by coagulation, uses correlations for the solutions of the Smoluchowski equation not considering particle diameter distribution. This obviates the need to run a time-consuming computer subroutine involving aerosol coagulation and deposition.

In MELCOR code [3], the behavior of fission product aerosols and vapors are modeled in RadioNuclide (RN) package. The package includes initial inventories, release from fuel and debris, aerosol dynamics with vapor condensation and revaporization, deposition on structure surfaces, transport through flow paths, and removal by engineered safety features. Aerosol dynamic processes and the condensation and evaporation of fission product vapors after release from fuel are considered within each MELCOR control volume. The aerosol dynamics models are based on MAEROS [4], a multi-section, multicomponent aerosol dynamics code, but without calculation of condensation. Aerosols can deposit directly on surfaces such as heat structures and water pools, or can agglomerate and eventually fall out once they exceed the largest size specified by the user for the aerosol size distribution. Aerosols deposited on surfaces cannot currently be resuspended.

Domestic code has been developed to predict the behavior of fission product aerosols during the severe accident in a nuclear power plant. The aerosol dynamics models are adapted in the code based on a multi-sectional method similar to MAEROS code [4]. The aerosol coagulation models in the developed code are validated and verified with MAEROS results on the sample problems and ABCOVE experimental data [5].

2. Aerosol Dynamic Equations

Gelbard and Seinfeld [6] had investigated a sectional method to estimate aerosol growth by the coagulation of multi-component. In the sectional method, the aerosol number density distribution is considered in the user-defined sectional ranges. Then, the aerosol mass in the *l*-th section is given by equation (1) for single component.

$$Q_l(t) = \int_{d_{l-1}}^{d_l} m(x)\, n(x,t)dx \quad (1)$$

Considering the temporal variation and the sectional transfer of the aerosol size distributions by the coagulation in the sectional method, five collision kernels are defined as equations (2) to (6) [6].

$$\beta^1{}_{l,ij} = \int_{d_{i-1}}^{d_i}\int_{d_{j-1}}^{d_j} \frac{\theta(m_{l-1} < m(x) + m(y) < m_l)[m(x) + m(y)]\beta(x,y)}{m(x)m(y)(d_j - d_{j-1})(d_i - d_{i-1})} dxdy \quad (2)$$

$$\beta^2{}_{l,i} = \int_{d_{i-1}}^{d_i}\int_{d_{l-1}}^{d_l} \frac{\theta(m(x)+m(y)<m_l)m(y)\beta(x,y)}{m(x)m(y)(d_l-d_{l-1})(d_i-d_{i-1})}dxdy \quad (3)$$

$$\beta^3{}_{l,i} = \int_{d_{i-1}}^{d_i}\int_{d_{l-1}}^{d_l} \frac{\theta(m(x)+m(y)>m_l)m(x)\beta(x,y)}{m(x)m(y)(d_l-d_{l-1})(d_i-d_{i-1})}dxdy \quad (4)$$

$$\beta^4{}_{l,l} = \int_{d_{l-1}}^{d_l}\int_{d_{l-1}}^{d_l} \frac{\theta(m(x)+m(y)>m_l)[m(x)+m(y)]\beta(x,y)}{m(x)m(y)(d_l-d_{l-1})(d_l-d_{l-1})}dxdy \quad (5)$$

$$\beta^5{}_{l,i} = \int_{d_{i-1}}^{d_i}\int_{d_{l-1}}^{d_l} \frac{m(x)\beta(x,y)}{m(x)m(y)(d_l-d_{l-1})(d_i-d_{i-1})}dxdy \quad (6)$$

Considering the aerosol coagulation mechanisms such as a gravitational, Brownian, turbulent shear and inertia, the coagulation coefficient in equations (2) to (6) can be calculated by equations (7) to (12) [7].

$$\beta(d_1,d_2) = \beta_G(d_1,d_2) + \beta_B(d_1,d_2) + \beta_T(d_1,d_2) \quad (7)$$

$$\beta_G(d_1,d_2) = \epsilon(d_1,d_2)\frac{\pi}{24}\gamma^2 g(\rho_p-\rho_g)|B(d_1)d_1^3 - B(d_2)d_2^3|(d_1+d_2)^2 \quad (8)$$

$$\beta_B(d_1,d_2) = 2\pi\kappa\, T_g\, \gamma[B(d_1)+B(d_2)](d_1+d_2) \quad (9)$$

$$\beta_T = \sqrt{\beta_{TB}^2 + \beta_{TI}^2} \quad (10)$$

$$\beta_{TS}(d_1,d_2) = \epsilon(d_1,d_2)\frac{1}{8}\gamma^3(d_1+d_2)^3\left(\frac{8\pi}{15}\frac{\epsilon_T\rho_g}{\mu_g}\right)^{1/2} \quad (11)$$

$$\beta_{TI}(u,v) = \epsilon(d_1,d_2)\frac{\gamma^2}{\chi}\frac{\rho_p}{18\mu_g}(d_1+d_2)^2 2\sqrt{2\pi}\left(\frac{8\pi}{15}\frac{\rho_g\epsilon_T^3}{\mu_g}\right)^{1/4}|d_1^2-d_2^2| \quad (12)$$

Some growth aerosols by the coagulation mechanisms might be deposited on the surfaces and finally removed. The aerosol removals by gravitational settling and diffusion can be evaluated by equations (13) and (14)

$$R_l = \int_{d_{i-1}}^{d_l}\frac{R(x,t)}{d_l-d_{l-1}}dx \quad (13)$$

$$R(d_p,t) = \frac{A_{set}}{V_c}U_{set}(d_p) + \frac{A_{dif}}{V_c}U_{dif}(d_p) \quad (14)$$

The gravitational settling velocity and diffusion adhesive velocity aerosol are expressed by equations (15) to (17).

$$U_{set}(d_p) = \frac{\rho_p C(d_p) g d_p^2}{18\mu_g\chi} \quad (15)$$

$$U_{dif}(d_p) = \frac{D_p}{\delta_D} \quad (16)$$

$$D_p = \frac{\kappa\, T_g}{3\pi\mu_g d_p\chi}C(d_p) \quad (17)$$

If the aerosols are supplied into the control volume at specific time, the aerosol source term is designated as equation (18).

$$S_l = \int_{d_{i-1}}^{d_l} m(x)S(x,t)dx \quad (18)$$

Using the equations (1) to (18), the final aerosol dynamic equation by the sectional method can be driven in equation (19) for the number of sections of N.

$$\frac{dQ_l}{dt} = \frac{1}{2}\sum_{i=1}^{l-1}\sum_{j=1}^{l-1}\frac{\beta_{l,ij}^1}{V_c}Q_iQ_j + Q_l\sum_{i=1}^{l-1}\frac{\beta_{l,i}^2}{V_c}Q_i - Q_l\sum_{i=1}^{l-1}\frac{\beta_{l,i}^3}{V_c}Q_i - \frac{1}{2}\frac{\beta_{l,l}^4}{V_c}Q_lQ_l - Q_l\sum_{i=l+1}^{N}\frac{\beta_{l,i}^5}{V_c}Q_i - R_lQ_l + S_l \quad (19)$$

Based on the aerosol dynamic equation as shown in equation (19), a code has been prepared by using C++ language and Runge-Kutta-Fehlberg (RK45) solving method to evaluate the aerosol behaviors by coagulations and removals.

3. Results and Discussion

The aerosol coagulation and removal models in the developed code were validated and verified by comparing with MAEROS results on the sample problems and ABCOVE experimental data.

3.1 Sample Problems

Sample problems were set and solved by the developed code, and the results were compared with MEAROS results. The sample problems were assumed that NaCl aerosol particles with the density of 2,160kg/m^3 were initially injected in a nitrogen gas tank with the volume of 1 m^3, room temperature, and atmospheric pressure, and that the initial NaCl aerosol particles were distributed in the log-normal number density with a specific geometric mass mean diameter (GMMD) and a geometric standard deviation (GSD). It was also assumed that there were no aerosol removals. The initial conditions of the sample problems are listed in Table I.

Table I: Initial conditions of the sample problems

Case	Case-S1	Case-S2
GMMD (μm)	0.4	2.0
GSD	1.10	1.05
Mass concentration(kg/m^3)	7.566 x 10^{-6}	9.336 x 10^{-6}

Using the sample condition as shown in Table I, the variations of the aerosol particle size distributions by the aerosol coagulations until 10,800 seconds were calculated by the developed code. Figure 1 shows that the comparison of the results in variations of the number of sections. As shown in Fig.1, the smaller particles are coagulated with each other, and finally the larger particles are generated as time increases. If the number of sections increases, the section width in each section decreases, and finer sectional aerosol distribution can be estimated, and finally the aerosol distribution function is smoothen. As shown in Fig. 1, the peak value in high section number (the number of sections: 40) is smaller than in smaller section number (the number of sections: 20).

Figures 2 and 3 show the comparisons of the results with MAEROS ones. The variations of aerosol mass distributions are similar to the MAEROS. The small discrepancy between the results occurs due to the differences of some factors such as collision efficiency, collision shape factor, dynamic shape factor, *etc*.

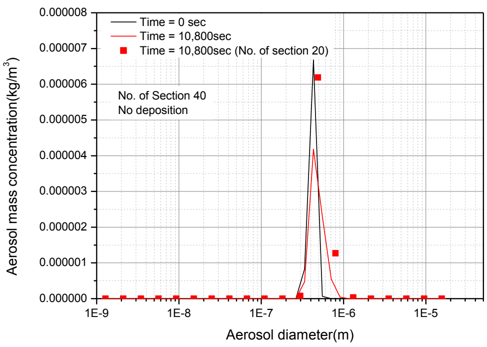

Fig.1. Variations of aerosol particle distributions with respect to the number of sections (Case-S1)

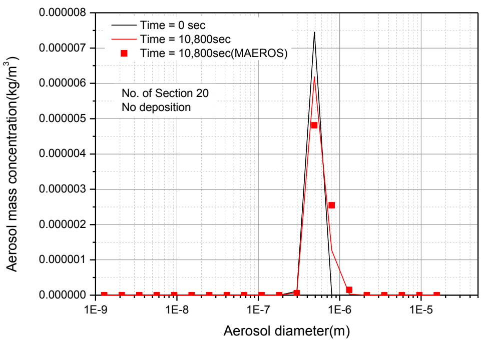

Fig.2. Variations of aerosol particle distributions compared with MAEROS results (Case-S1)

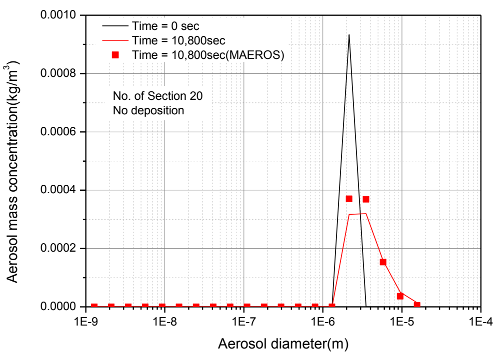

Fig.3. Variations of aerosol particle distributions compared with MAEROS results (Case-S2)

3.2 ABCOVE-5 Experiment

ABCOVE-5 experiment [5] was one of the International Standard Problems to examine the computer code capability to predict aerosol behavior in the containment. In AB-5, sodium aerosol with mass mean diameter of 1.5μm and standard deviation of 1.8 was used to simulate aerosol behavior under high concentration conditions. The sodium aerosol was injected with injection rate of 0.455kg/sec during 13 to 885 seconds into a large vessel with a volume of 12m^3, and the airborne aerosol concentration was measured until sections.

Figure 4 shows the calculation results on the AB-5 experimental conditions. The airborne aerosol concentration was highly affected by gas temperature in injection period. The dynamic shape factor is an important factor on aerosol removal process as shown in Fig. 4.

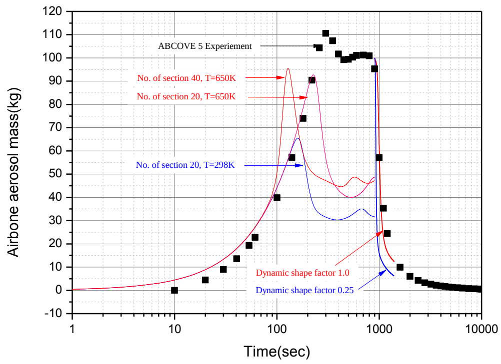

Fig.4. Temporal variation of airborne aerosol mass compared with ABCOVE-5 experimental results

3. Conclusions

A code has been developed to predict the behavior of fission product aerosols during the severe accident in a nuclear power plant. The aerosol dynamics models were adapted in the code based on a multi-sectional method similar to MAEROS code. The aerosol coagulation models in the developed code were validated and verified with MAEROS results on the sample problems and ABCOVE experimental data.

In addition to the gravitational settling, diffusiophoresis (steam condensation), thermophoresis, impaction, vapor condensation, and vapor revolatilization for the radioactive aerosols will be modeled in the code and the code will be validated by comparing with experimental data and results from similar codes.

NOMENCLATURE

A_{dif} deposition surface area by diffusion

A_{sct} deposition surface area by gravitational settling
$B(d_p)$ particle mobility of diameter d_p
$C(d_p)$ Cunningham slip correction factor of diameter d_p
d_l aerosol particle diameter at *l*-th section
g gravity constant
m(x) aerosol mass of particle diameter x
n(x,t) aerosol particle number distribution of diameter x at time t
n(x,t)dx aerosol particle number of diameter x at time t
Q_l aerosol mass in *l*-th section
T_g gas temperature
U_{dif} deposition velocity by diffusion
U_{sct} deposition velocity by gravitational settling
V_c volume of aerosol control

Greek symbols
γ collision shape factor
δ_D Diffusion boundary layer thickness (0.001cm)
$\epsilon(d_1, d_2)$ collision efficiency
ϵ_T turbulent energy dissipation rate
μ_g gas viscosity
ρ_g gas density
χ dynamic shape factor
κ Boltzmann constant

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