Modeling of Aerosol Washout by Spray Operation for Fission Product Removal in a NPP Containment

Jongtae Kim^{a*}, Keun Sang Choi^a, Jaehoon Jung^a ^a KAERI, Daeduk-daero 989-111, Daejeon, Korea ^{*}Corresponding author: ex-kjt@kaeri.re.kr

1. Introduction

During a severe accident with a core degradation in a nuclear power plant (NPP), fission products (FP) in the form of various species are released from the reactor core into the containment building.

Fission products such as Xe are released in gaseous form, whereas iodine and Cesium are very active and can exist mostly in the form of aerosols in the containment. Spraying water is a representative method of reducing FP concentration by removing FPs in the form of aerosols.

The spray system installed in a large dry containment of a pressurized water reactor is used as a pressure control measure and also used to remove aerosols distributed in the containment atmosphere. Therefore, aerosol removal by water droplets from the spray system can be used as a very important means for reducing fission products.

A validated analytical model is required to quantitatively evaluate aerosol removal by the containment spray during the accident. This paper describes the development and verification of an analysis module to simulate aerosol removal by spray droplets.

2. Modeling

The aerosol removal or washout model has been implemented in the Lagrangian spray model of the OpenFOAM CFD platfoam [1].

A gas field in a compartment is modeled by the Eulerian approach with the ideal gas assumption, where gas is considered as a multicomponent species mixture.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}) = S_{\rho} \tag{1}$$

$$\frac{\partial t}{\partial t}(\rho \boldsymbol{U}) + \nabla \cdot (\rho \boldsymbol{U} \boldsymbol{U}) - \nabla \cdot \boldsymbol{R} = -\nabla \mathbf{p} + \rho \boldsymbol{g} + \boldsymbol{S}_m \quad (2)$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho Y_i U) - \nabla \cdot J_i = S_{Y_i}$$
(3)

$$\frac{\partial}{\partial t}(\rho h_s) + \nabla \cdot (\rho h_s \boldsymbol{U}) - \nabla \cdot \boldsymbol{q}$$
$$= \frac{\partial p}{\partial t} - \left[\frac{\partial}{\partial t}(\rho K) + \nabla \cdot (\rho K \boldsymbol{U})\right] + S_h \tag{4}$$

Equations (1) through (4) represent the governing equations for the gas phase.

Aerosols floating in the gas field is modeled as passive scalars with discrete size distributions on the assumption of thermo-mechanical equilibrium between the gas and aerosol fields.

$$\frac{\partial \rho C_i}{\partial t} + \nabla \cdot (\rho U C_i) - \nabla \cdot (D_i \nabla C_i) = S_{C_i}$$
(5)

, where C_i is the mass concentration [kg/m³] of an aerosol with i-th size. Currently, the mass source S_{C_i} in Eq. (5) considers only a mass loss by the spray washout.

A spray droplet field in modeled by the Lagrangian approach, where each parcel of spray droplets is tracked by solving the Newton's equation. OpenFOAM has a hierarchy of parcel models, which includes KinematicParcel, ThermoParcel, ReactingParcel, and ReactionMultiphaseParcel. The characteristics of each parcel type is summarized in ref [2]. SprayParcel derived from ReactingParcel has atomization and breakup models additional to the interfacial transport models such as momentum, energy, mass. For the modeling of the aerosol washout, SprayParcel has been modified to include aerosol removal mechanisms. Among them, the dominant three mechanisms such as inertial impaction, interception, and Brownian diffusion shown in Fig. 1 were implemented in the spray parcel model.



Fig. 1. Aerosol washout mechanisms of (A) inertial impaction, (b) interception, and (c) Brownian diffusion, [3, 4]

The aerosol washout efficiencies of a single droplet by the inertial impaction, interception and Brownian diffusion can be defined as Eq. (6), (7) and (8).

$$\eta_{imp} = \begin{cases} 0, & St \le 0.0833\\ 8.57 \left(\frac{St}{St+0.5}\right)^2 (St - 0.08336), 0.0833 < St < 0.2 \end{cases}$$
(6)

$$\left[\left(\frac{st}{st+0.5} \right)^2, \qquad St \ge 0.2 \\ n_{1,\ldots} = \frac{1-\alpha_l}{\alpha_l} \left[\left(\frac{R}{s} \right) + 0.5 \left(\frac{R}{s} \right)^2 \left(3\sigma + 4 \right) \right]$$
(7)

$$\eta_{int} = \frac{1}{J + \sigma K} \left[\left(\frac{1}{1 + R} \right) + 0.5 \left(\frac{1}{1 + R} \right)^{-1} \left(\frac{50}{1 + R} \right)^{-1} \right]$$
(7)
$$\eta_{diff} = (2Ped_d)^{-0.5}$$
(8)

The total washout efficiency by a single droplet is calculated as shown in Eq. (9)

$$\eta_{tot} = 1 - (1 - \eta_{imp})(1 - \eta_{int})(1 - \eta_{diff})$$
(9)

Finally, the i-th size aerosol's mass removed by washout of a single drop during dt time can be obtained by Eq. (10)

$$dm_i = \eta_{tot} \left(\frac{\pi}{4} d_d^2 U_d dt\right) C_i \tag{10}$$

3. Code Verification

A code module to simulate aerosol washout by spray droplets is developed based on the analytical models described above and implemented in the OpenFOAM library. Before applying the module to fission aerosol scavenging by spray operation in a nuclear reactor containment, it is necessary to verify and validate feasibility and accuracy of the code module.

The code module consists of two parts, one of which is the aerosol transport modeling and the other is aerosol washout modeling. They need to be validated consistently.

3.1 Aerosol Mixing by a Convection

The aerosol transport part of the module was verified by simulating aerosol mixing in a cavity with a moving lid. Initially, the three aerosol components are accumulated near the center of the cavity as shown in Fig. 2. When the top lid is moving with a constant velocity, a recirculating convective flow is developed by a gas viscosity. The aerosols are passively driven by the gas flow. The distributions of the aerosol concentrations change over time and they are mixed each other as shown in Fig. 2. This lid-driven cavity flow with three aerosol groups depicts that the aerosol transport part of the developed code module well simulate aerosol mixing by a convective flow.



Fig. 2. Lid-driven cavity flow with three groups of aerosols.

3.2 Aerosol Washout by Spray

The aerosol removal tests, UTARTS, has been conducted by the Univ. of Tokyo [4]. The main component used for the tests is a cylindrical vessel with a height of 2.5 m, internal diameter of 1.5 m. ZrO_2 particles with mass mean diameter of 0.15 µm were used

as aerosols. For water droplet flow, full-cone spray nozzle was used, which has performance of 2 l/m with 27° or 66° spray angle.

To verify the developed aerosol washout module, one of the aerosol removal tests UTARTS was simulated. The test of Case-1 with a spray angle of 27° was simulated using the developed module.



Fig. 3. A mesh of the UTARTS vessel for simulation of the aerosol washout test Case-1.

Fig. 3 shows the mesh used for simulation of the aerosol washout test Case-1. Initially, the aerosol particles are distributed uniformly in the test vessel. As the spray nozzle starts injecting water droplets, the aerosol particles slowly removed. Fig. 4 shows change of aerosol distribution with a size of 0.583 µm over time.



Fig. 4. Aerosol distributions over time from the simulation.

4. Conclusions

A code module for simulation of aerosol washout by spray droplets has been developed. It is shown that the analysis module predicts well the aerosol washout qualitatively. It is underway to quantitatively evaluate the rate of the aerosol washout by the spray droplets.

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