Validation of a Bulk Condensation Model for a Steam Jet Simulation

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1. Introduction

In case of a severe accident in a nuclear power plant, containment integrity should be maintained under high pressure elevated by released hot steam and hydrogen concentration also needs to be restrained from flammable or explosion limit. Key facility to mitigate consequences from severe accident is spray injection system installed beneath the containment dome. Spray can decrease peak pressure inside the containment with mechanism of bulk and wall condensation but also may cause increase hydrogen concentration due to decreased steam volume. Thus, condensation phenomena should be understood thoroughly to devise an optimal strategy for spray injection.

Bulk condensation includes nucleation from vapor and condensational growth from the nucleated seed or a droplet. In this study, a bulk condensation model is reviewed and validated by utilizing simple steam injection experimental data. For the analysis of water aerosols from condensed steam, 'aerosolEulerFoam' solver developed on the OpenFOAM framework[1] was utilized.

2. Methods and Results

'aerosolEulerFoam' is an Eulerian aerosol solver[2] which can simulate nucleation, aerosol coalescence, condensation/evaporation and deposition. In this work, we focus on the model of nucleation and condensation/ evaporation. In this section, governing equations of 'aerosolEulerFoam' and aerosol models are described.

2.1 Governing equations

Generally, continuity, momentum and energy equations need to be solved for fluid flow. For aerosol transport simulation, equations for aerosol number density, mass fraction of vapor and particle are additionally solved[2].

Continuity equation

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u}) + \nabla \cdot [\boldsymbol{f}(1-\gamma)] = 0, \qquad (1)$$

where, $\boldsymbol{u}, \rho, \boldsymbol{f}, \gamma$ are velocity vector, mixture density, total flux of liquid concentration drifting away from the mixture motion, and ratio between local vapor density and local particle density, respectively.

Momentum equations

$$\partial_t(\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u} \boldsymbol{u}) = -\nabla p - \nabla \cdot \boldsymbol{\tau}, \qquad (2)$$

where, *p* is static pressure and $\boldsymbol{\tau}$ is defined as $\boldsymbol{\tau} = -\mu [\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T] + \frac{2}{2}\mu (\nabla \cdot \boldsymbol{u})\boldsymbol{I}$. μ is viscosity.

Energy equation

$$c_p[\partial_t(\rho T) + \nabla \cdot (\rho u T)] = \nabla \cdot (k \nabla T) - (\tau : \nabla u) + D_t p,$$
(3)

where, k, c_p are thermal conductivity and specific heat, respectively.

Number density equation

$$\partial_t(\rho M_i) + \nabla \cdot (\rho \boldsymbol{u} M_i) + \nabla \cdot (\rho \boldsymbol{u}_i^p M_i) = \nabla \cdot (\boldsymbol{p}_i^p \nabla \rho M_i) + J_{M_i},$$
(4)

where, M_i , u_i^p , D_i^p , J_{M_i} are aerosol number density divided by density, particle velocity, particle diffusion coefficient, source term related with nucleation and condensation, respectively. The subscript *i* is used to denote a section index for an aerosol size group.

Mass fraction equations

$$\partial_t (\rho Y_j) + \nabla \cdot (\rho \boldsymbol{u} Y_j) - \nabla \cdot (Y^{-1} \boldsymbol{h} Y_j) = R_j, \qquad (5)$$

$$\partial_t (\rho Z_j) + \nabla \cdot (\rho \boldsymbol{u} Z_j) - \nabla \cdot (Z^{-1} \boldsymbol{f} Z_j) = S_j, \qquad (6)$$

where, Y_j , Z_j , h, R_j , S_j are vapor mass fraction, particle mass fraction, vapor mass concentration drift flux($h = \gamma f$), vapor and particle mass concentration source terms, respectively.

2.2 Nucleation model

A generalization of classical multi-component theory for homogeneous nucleation was presented in [3]. Nucleation mass flow S_j^{nuc} is obtained using nucleation rate, J_N , number of molecules of component j in a critical cluster, N_j , molecular mass of species j, m_j as

$$S_i^{nuc} = 2J_N N_i m_i. aga{7}$$

The nucleation rate J_N is calculated by multiplying average growth rate, Zeldovich factor characterizing the contribution of Brownian motion to the formation of the critical cluster, and equilibrium concentration. Average growth rate is obtained using condensation rate of component *j* and mole fraction of species *j*.

2.3 Condensation and evaporation

Condensation and evaporation are reverse processes of one mechanism. Condensed mass is added to the particle mass and at the same time same mass is subtracted from the vapor mass, and vice versa for evaporated mass.

Mass flow rate due to condensation and evaporation is expressed as

$$S_{j}^{evap/cond} = 2\pi D_{j} \bar{d} \rho Y_{j}^{s} f(\bar{d}, \lambda) \left(E_{j} - \frac{s_{j}}{W_{j}} \right) N, \quad (8)$$

where, \bar{d} , Y_i^s , f, E_i , S_j , W_i , N are count mean diameter, saturation mass fraction of component j, Fuchs factor, equilibrium saturation of component j, saturation of species *j*, mole fraction in the droplet's phase, number concentration of particle(= ρM), respectively. If E_i – $S_i/W_i > 0$, Eq.(8) denotes evaporation and if E_i – $S_i/W_i < 0$, Eq.(8) means condensation.

2.4 Geometry of steam jet injection



Fig. 1. Layout of a steam jet experiment[4]

Condensation characteristics of water droplets in a turbulent steam jet was investigated in [4]. They measured particle size distribution, temperature, velocity, total number concentration utilizing phase Doppler particle analyzer (PDPA) system. Key characteristics for steam jet flow are temperature decay rate along the axial center line, temperature half width, and particle size distribution.

Inner diameter of the pipe nozzle is 10 mm and distance between the pipe nozzle tip and the floor is more than 2 m. Temperature of the steam at the nozzle exit is 105 °C and mass flow rate is 50 kg/h. For this condition, Reynolds number is 140,700. Ambient temperature is 19 °C.

2.5 Simulation of steam jet injection

Number of cells composed of hexahedra is 298,080 as shown in Fig. 2. Wall boundary condition was set to the bottom of the computational domain and 'inletOutlet' boundary condition was set for the side and top of the computational domain. $k - \omega$ SST turbulent model was applied.



Fig. 2. Grid system

Mass of condensed droplets was calculated and data were achieved when the flow field has come to a steady state condition. Fig. 3 shows total mass of species in the computational domain. It is shown that the flow field has come to a steady state about 2 seconds.



Fig. 3. Species total mass in computational domain



Fig. 4. Temperature distribution

Fig. 4 shows temperature distribution and the hot steam cools down rapidly.



Fig. 5. Particle concentration (#/kg, 11th section)



Fig. 6. Particle concentration (#/kg, 12th section)



Fig. 7. Particle concentration (#/kg, 13th section)



Fig. 8. Particle concentration (#/kg, 14th section)



Fig. 9. Particle concentration (#/kg, 15th section)



15 sections of which representative mass range from 5E-24 to 5E-10 kg were fixed to track the aerosol evolution from nucleation to condensational growth. Fig. $5 \sim$ Fig. 9 show particle concentrations for each section. For the 11th section, particle mass is 5E-14 kg, for 15th section 5E-10 kg. Droplets has formed along the

centerline of the steam jet. As the steam goes down, droplets grow.

Number concentration according to particle diameters are displayed in Fig. 10. The data was extracted at z/d=10 which means that vertical distance from the nozzle tip is 10 times of the nozzle inner diameter. 'r' is radial distance from the centerline and 'r_{10.5}' denotes a location at which temperature difference between steam and ambient air becomes half of temperature difference between steam at the centerline and ambient air. Number concentration data using 'aerosolEulerFoam' solver are in good agreement with experimental data. This means that nucleation and condensational growth models are adequate for this steam jet case.

It was found out that the inlet boundary condition of the steam jet test may strongly affect the numerical simulation results. Additional study will be carried out to evaluate solution dependency on the inlet boundary conditions, especially, injection of larger aerosols formed on the injection pipe wall which is caused by low temperature of the pipe wall of the experimental facility.

3. Conclusions

Nucleation and condensational models implemented in the 'aerosolEulerFoam' solver has been validated by comparing with a steam jet experimental data. Droplet formation was well simulated and number concentration was compared with experiment. From this approach, adequacy of the nucleation and condensational model addressed for steam jet was proven.

This research work will contribute to integration of the models for bulk condensation and aerosol behaviors and containmentFoam which is a solver for hydrogen safety evaluation [5] in a NPP containment.

ACKNOWLEDGEMENT

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science, ICT) (No. 2017M2A8A4015277)

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