

ANALYSIS OF REACTING GAS JETS IN LIQUID POOLS USING THE SERAPHIM PROGRAM

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Abstract

When the water leaks from a failed heat transfer tube in a steam generator of sodium-cooled fast reactors, the high-temperature jet with sodium-water chemical reaction may cause wastage of the adjacent tubes. A computer program called SERAPHIM has been developed to calculate the multiphase flow involving the sodium-water reaction. In this study, the experiment on reacting gas jets in liquid pools was analyzed to validate the numerical models. The numerical results showed that the injected gas disappeared at a certain height. The calculated plume length showed good agreement with the experimental data. This analysis demonstrated validity of the proposed models.

Introduction

In a steam generator (SG) of sodium-cooled fast reactors, heat exchange takes place between the liquid sodium in the shell side and the water or vapor inside the heat transfer tubes. The liquid sodium has an excellent heat transfer characteristic. On the other hand, it has a chemical reactivity with the oxygen and the water. When the pressurized water or vapor leaks from a failed heat transfer tube, a high-velocity and high-temperature jet with sodium-water chemical reaction is formed in the shell side (see Fig. 1). It is known that the reacting jet may cause wear (wastage) on the adjacent tubes. The wastage phenomena are attributed to erosion, flow accelerated corrosion (FAC) or combination of them. Significant progress of the wastage will lead to a secondary failure (failure propagation). There is also a possibility that degradation of the mechanical strength of the tube by a rise in the temperature may cause over-heating rupture. Since minimization of the accident damage is important, prevention of the failure propagation is a major concern in design of the SG.

A mock-up test of the tube failure accident is one of the ways to evaluate possibility of the occurrence of the failure propagation, but the cost of the test is very high. Also, it is difficult to deal with the change of the design. Numerical analysis is a very useful way because it can compensate for the drawbacks of the mock-up test. For this reason, we have developed a computer program called SERAPHIM calculating the compressible multicomponent multiphase flow involving the sodium-water chemical reaction [1-3]. The SERAPHIM program is based on the mechanistic models. The multi-fluid model considering compressibility was adopted to calculate the multiphase flow with the water, the liquid sodium and the multicomponent gas. The mechanism of the sodium-water chemical reaction

was investigated and the new mechanistic model was constructed. The profiles of the velocities, temperatures and concentrations, which are necessary to evaluate possibility of the failure propagation, will be obtained by the SERAPHIM program.

The water vapor going out from an opening of the tube becomes a supersonic jet because the sodium-side pressure is lower than the critical pressure of the water vapor inside the tube. Validation of the above-mentioned numerical methods for supersonic gas jets into liquid pools with chemical reaction is an important issue in development of the SERAPHIM program. Avery and Faeth [4] carried out a pioneering study on the reacting gas jet in the liquid. In their experiment, the high-pressure chlorine gas was injected into the molten pool of the Na-NaCl mixture. The behavior of the jet was visualized by using the X-ray radiography technique. They observed that the jet disappeared at a certain height and proposed a correlation to predict the gas plume length. In this study, the experiment by Avery and Faeth was calculated to validate the chemical reaction model as well as the fluid dynamics model in the SERAPHIM program. About the three different experimental conditions, calculated behavior of the reacting jet was compared with the experimental results.

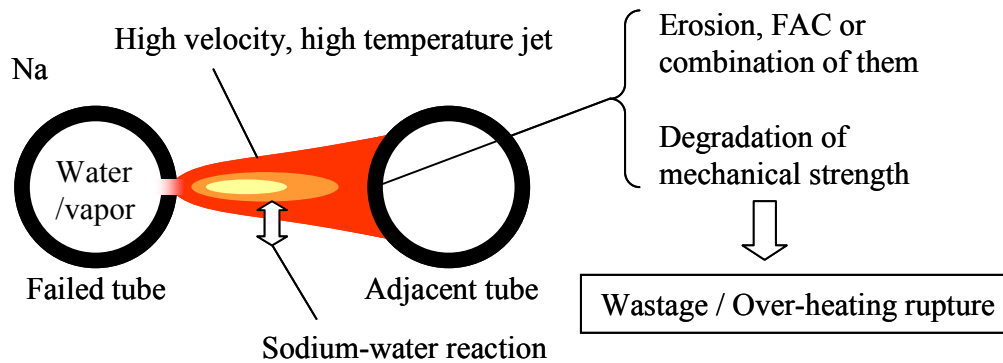


Figure 1 Reacting jet under tube failure accident.

1. Numerical methods

1.1 Governing equations

The multiphase flow is calculated by using the multi-fluid model considering compressibility. The governing equations for the gas and the liquid phase are as follows:

Equation of mass conservation

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g) = \Gamma^e - \Gamma^c + G^{sf} + G^{dif} \quad (1)$$

$$\frac{\partial}{\partial t}(\alpha_l \rho_l) + \nabla \cdot (\alpha_l \rho_l \mathbf{u}_l) = -\Gamma^e + \Gamma^c - G^{sf} \quad (2)$$

Equation of momentum conservation

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_g \rho_g \mathbf{u}_g) + \nabla \cdot (\alpha_g \rho_g \mathbf{u}_g \mathbf{u}_g) = & -\alpha_g \nabla p + \nabla \cdot (\alpha_g \boldsymbol{\tau}_g) + \alpha_g \rho_g \mathbf{g} + \mathbf{M}_g \\ & + \Gamma^e \mathbf{u}_l - \Gamma^c \mathbf{u}_g + G^{sf} \mathbf{u}_l + G^{dif} \mathbf{u}_g \end{aligned} \quad (3)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_l \rho_l \mathbf{u}_l) + \nabla \cdot (\alpha_l \rho_l \mathbf{u}_l \mathbf{u}_l) = & -\alpha_l \nabla p + \nabla \cdot (\alpha_l \boldsymbol{\tau}_l) + \alpha_l \rho_l \mathbf{g} + \mathbf{M}_l \\ & - \Gamma^e \mathbf{u}_l + \Gamma^c \mathbf{u}_g - G^{sf} \mathbf{u}_l \end{aligned} \quad (4)$$

Equation of energy conservation

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_g \rho_g h_g) + \nabla \cdot (\alpha_g \rho_g h_g \mathbf{u}_g) = & \alpha_g \frac{Dp}{Dt} + \alpha_g \Phi_g + \nabla \cdot (\alpha_g \lambda_g \nabla T_g) \\ & + \Gamma^e (h_l + i_l) - \Gamma^c h_{gv} + Q^{sf} + Q^{dif} - aH_{gl}(T_g - T_l) \end{aligned} \quad (5)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_l \rho_l h_l) + \nabla \cdot (\alpha_l \rho_l h_l \mathbf{u}_l) = & \alpha_l \frac{Dp}{Dt} + \alpha_l \Phi_l + \nabla \cdot (\alpha_l \lambda_l \nabla T_l) \\ & - \Gamma^e (h_l + i_l) + \Gamma^c h_{gv} - G^{sf} h_l - aH_{gl}(T_l - T_g) \end{aligned} \quad (6)$$

where α is the volume fraction, ρ the density, $\mathbf{u}$ the velocity vector, Γ^e the evaporation rate, Γ^c the condensation rate, G the mass generation rate, p the pressure, $\boldsymbol{\tau}$ the viscous stress tensor, $\mathbf{g}$ the gravity vector, $\mathbf{M}$ the interfacial drag force, h the enthalpy, Φ the dissipation function, λ the thermal conductivity, T the temperature, i the latent heat, h_{gv} the enthalpy of the species, Q the heat generation rate, a the interfacial area density and H the coefficient of heat transfer. Superscript *sf* stands for the surface reaction and *dif* the diffusion of the species. The surface reaction and its numerical model are described later. The transportation of the species j is calculated by the advection-diffusion equation:

$$\frac{\partial}{\partial t}(\alpha_g \rho_g Y_j) + \nabla \cdot (\alpha_g \rho_g Y_j \mathbf{u}_g) = \nabla \cdot (\alpha_g \rho_g D_{mj} \nabla Y_j) + \Gamma_j^e - \Gamma_j^c + \gamma^{sf} \quad (7)$$

where Y is the mass fraction, D_m the effective coefficient of diffusion and γ the source term due to the surface reaction. The physical properties appearing in the above equations are estimated from the equation of state, the theoretical estimation or the approximation formula.

1.2 Interfacial drag force

The interfacial drag force model used in the present work is based on the high mixing volume flow regime map [5]. As with the map, the two-phase flow pattern was assumed as follows:

a bubbly flow for $\alpha < 0.5$ and a droplet flow for $\alpha > 0.95$. There is a transition region between them. The interfacial drag force term in the equation of momentum conservation is given by

$$\mathbf{M}_l = -\mathbf{M}_g = \frac{3}{4} \frac{1}{d} \alpha \rho_c C_D |\mathbf{u}_g - \mathbf{u}_l| (\mathbf{u}_g - \mathbf{u}_l) \quad (8)$$

where d is the diameter of the bubble or the droplet and C_D the drag coefficient. Subscript c stands for the continuous phase. We estimated the drag coefficient C_D from the existing experimental data and the correlation. The correlation of the drag coefficient for the bubbly flow was determined from the experiment on the bubbly jet by Neto et al. [6]. It has a form which depends on the bubble Reynolds number. On the other hand, the drag coefficient for the moving particles in the supersonic gaseous flow [7] was applied to the droplet flow. The interfacial drag force for the transition region was calculated by the void-fraction-weighted average of them.

1.3 Chemical reaction model

In our previous studies, we developed the numerical model for the chemical reaction at the interface between the water vapor and the liquid sodium. The model is called the surface reaction model. The analysis of the chlorine jet into the Na-NaCl mixture was performed by applying the surface reaction model. The surface reaction model is outlined below.

The surface reaction model is based on the assumption of the infinite reaction rate. In other words, the progress of the chemical reaction at the gas-liquid interface is limited by the mass flow rate of the reactant gas toward the liquid surface. The mass flow rate of the reactant gas j is written as

$$\gamma_j^{sf} = Sh \frac{D_{mj}}{l} \rho_g Y_j a \quad (9)$$

where Sh is the Sherwood number, l the characteristic length and Y the mass fraction. Equation (9) includes some unknown parameters. By using the analogy between the heat and mass transfer, Eq. (9) is rewritten as

$$\gamma_j^{sf} = -Le^{b-1} \frac{H_{gl}}{C_{pg}} Y_j a \quad (10)$$

where Le is the Lewis number, b the empirical constant and C_p the specific heat. Tanabe et al. [8] conducted the experiment on the water vapor leakage into the sodium and reported that the coefficient of heat transfer on the surface of the heat transfer tube in the reacting zone was approximately 10000 W/m²/K. Heat transfer on the gas-liquid interface seems to be similar to that on the tubes because the liquid-phase velocity is much smaller than the gas-phase velocity. For this reason, we applied the coefficient of heat transfer measured on the tube to that in Eq. (10). The Lewis number is determined from the heat diffusivity and the

coefficient of diffusion. The experimental heat transfer correlations for the turbulent flow indicate that the empirical constant b becomes less than unity. There is the knowledge that b is not so effective on the reacting zone [9]. Hence b was set to 0 in the present analysis. The interfacial area density a is given by the Nigmatulin model [10]. The reaction heat is calculated from the standard enthalpy of formation of the reaction products.

1.4 Evaporation/condensation rate

The evaporation/condensation rate is given by

$$\Gamma^e = \begin{cases} \lambda_e a \rho_l \alpha_g (R_g / M_w)^{1/2} (1 - \alpha_g) (T_l - T_s) / \sqrt{T_s} & T_l \geq T_s \\ 0 & T_l < T_s \end{cases} \quad (11)$$

$$\Gamma^c = \begin{cases} 0 & T_g > T_s \\ \lambda_c a \rho_g (1 - \alpha_g) (R_g / M_w)^{1/2} \alpha_g (T_g - T_s) / \sqrt{T_s} & T_g \leq T_s \end{cases} \quad (12)$$

where λ is the empirical constant, R_g the universal gas constant, M_w the molecular weight and T_s the saturation temperature. Based on some researches [10, 11], the empirical constant λ was determined to be 0.1. Takata and Yamaguchi [1] analyzed the Edwards pipe blowdown problem by using the SERAPHIM program and demonstrated applicability of the above model. As described later, the liquid phase is the Na-NaCl mixture in the present analysis. The saturation temperature of the Na-NaCl mixture was determined from the data by Smirnov et al. [12]. They reported the saturation temperature of the Na-NaCl mixture as a function of the mol % of Na.

1.5 HSMAC method for compressible multiphase flow

The set of the governing equations is solved by the HSMAC (Highly Simplified Marker And Cell) method modified for compressible multiphase flows. The HSMAC method for incompressible single-phase flows was developed by Hirt and Cook [13]. In this method, the pressure and the velocity are corrected so as to satisfy the continuity by using the Newton-Raphson method. The HSMAC method is very useful for parallel computation because there is no need to solve a simultaneous linear equation. Extension of the HSMAC method to compressible multiphase flows is described here.

The recurrence equation for the pressure correction is written as

$$p^{m+1} = p^m + \delta p = p^m - D^m / \left(\frac{\partial D}{\partial p} \right)^m \quad (13)$$

where superscript m stands for the iteration step. The divergence D approaches to 0 by the iterative calculation. In the case of multiphase flows, similarly to the method proposed by Matsumoto and Murai [14], we define D by

$$D = -\sum_k \frac{\partial \alpha_k}{\partial t} \quad (14)$$

Substituting Eqs. (1) and (2) into Eq. (14), D is rewritten as

$$D = \sum_k \left\{ \frac{\alpha_k}{\rho_k} \frac{\partial \rho_k}{\partial t} + \frac{1}{\rho_k} \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) \right\} \quad (15)$$

From Eqs. (3), (4), (13) and the equation of state, we can derive a final form of the pressure correction:

$$\delta p = -\omega \frac{D^m + \sum_k \left\{ \frac{\alpha_k^n}{\rho_k^n} \left(\frac{\partial \rho_k}{\partial T_k} \frac{\delta T_k}{\Delta t} + \frac{\partial \rho_k}{\partial M} \frac{\delta M}{\Delta t} \right) \right\}}{\sum_k \left[\frac{\alpha_k^n}{\rho_k^n} \left\{ \frac{\partial \rho_k}{\partial p} \frac{1}{\Delta t} + 2 \Delta t \left(\frac{1}{\Delta x^2 + \Delta y^2 + \Delta z^2} \right) \right\} \right]} \quad (16)$$

where ω is the relaxation factor. The $m+1$ -th pressure is calculated by Eqs. (13) and (16). The velocity is updated after the pressure correction.

2. Results and discussion

The computational domain is shown in Fig. 2. The region is 0.4 m in width and 1 m in height. There is an inlet boundary (nozzle exit) at the center of the bottom surface. The analysis mesh cannot reproduce the round shape of the nozzle exit because of the use of the structured mesh. Hence the area of the inlet boundary was set to be equal to the cross-section area of the tube whose diameter is 2 mm. The vessel was initially filled with the Na-NaCl mixture at the temperature of 1130 K (50 K of the degree of subcooling) and at the hydrostatic pressure. The chlorine gas goes into the pool vertically and reacts with the sodium. The flow of the chlorine gas becomes a critical state at the nozzle exit. From the assumption of an isentropic flow, the physical quantities at the critical state are given by

$$u^* = \sqrt{\frac{2\gamma}{\gamma+1} \frac{p_0}{\rho_0}} \quad (17)$$

$$p^* = p_0 \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma}{\gamma-1}} \quad (18)$$

$$T^* = T_0 \frac{2}{\gamma + 1} \quad (19)$$

$$\rho^* = \rho_0 \left(\frac{2}{\gamma + 1} \right)^{\frac{1}{\gamma - 1}} \quad (20)$$

where γ is the specific heat ratio. Superscript * stands for the critical state and subscript 0 the stagnation point. The boundary conditions at the inlet boundary were determined from Eqs. (17) to (20). The velocity at the inlet boundary became approximately 205 m/s (sound speed). The void fraction was 1. The pressure at the top surface was assumed to be constant at the atmospheric pressure. The gas phase can go out from the top surface. The analysis mesh was constructed with the 45472 unequally-spaced cells. The reaction formula of the chlorine and the sodium is



Similarly with the analysis of the sodium-water reaction, we assumed that the reaction product NaCl exists as an aerosol in the gas phase. Three different experimental conditions were chosen for validation. The stagnation pressure of the chlorine and the concentration of the sodium were taken as parameters. The analysis conditions are summarized in Table 1.

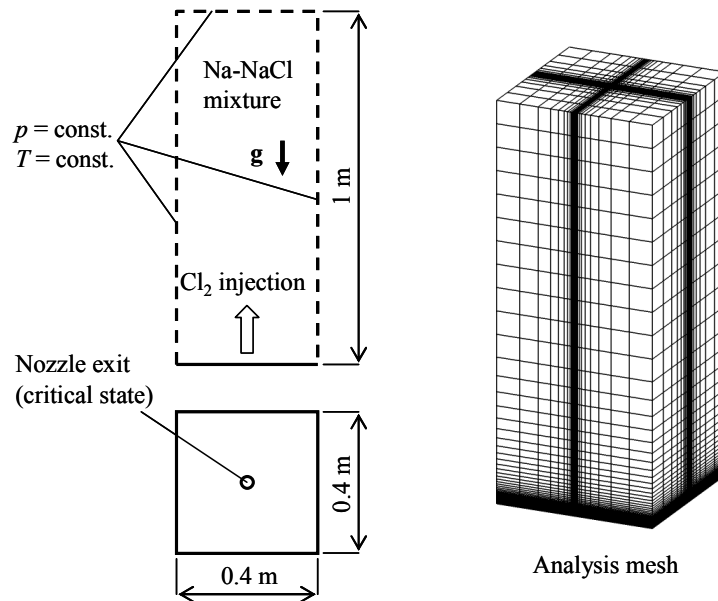


Figure 2 Computational domain and analysis mesh.

Table 1 Analysis conditions.

	Mol fraction of Na	Stagnation Pressure [MPa]	Ambient pressure [MPa]	Ambient temperature [K]
Case 1	2.65	0.337	0.101325	1130
Case 2	1.95	0.331		
Case 3	1.66	0.234		

Figure 3 shows the distributions of the time-averaged void fraction, gas-phase temperature, volume fraction of the chlorine and volume fraction of the NaCl gas on the vertical plane in the case 1. It can be seen that the void fraction disappears at a certain height. This is the same as the observation by Avery and Faeth. The plume length (disappearance height of the jet) measured by Avery and Faeth are shown in Fig. 3 for comparison ($L/D = 82.4$). The numerical result shows good agreement with their experimental data. The gas-phase temperature went up to about 2000 °C by the chemical reaction. At the center of the jet, the gas-phase temperature is relatively low. This is because of the existence of the unreacted chlorine gas. The NaCl gas appeared around the chlorine gas.

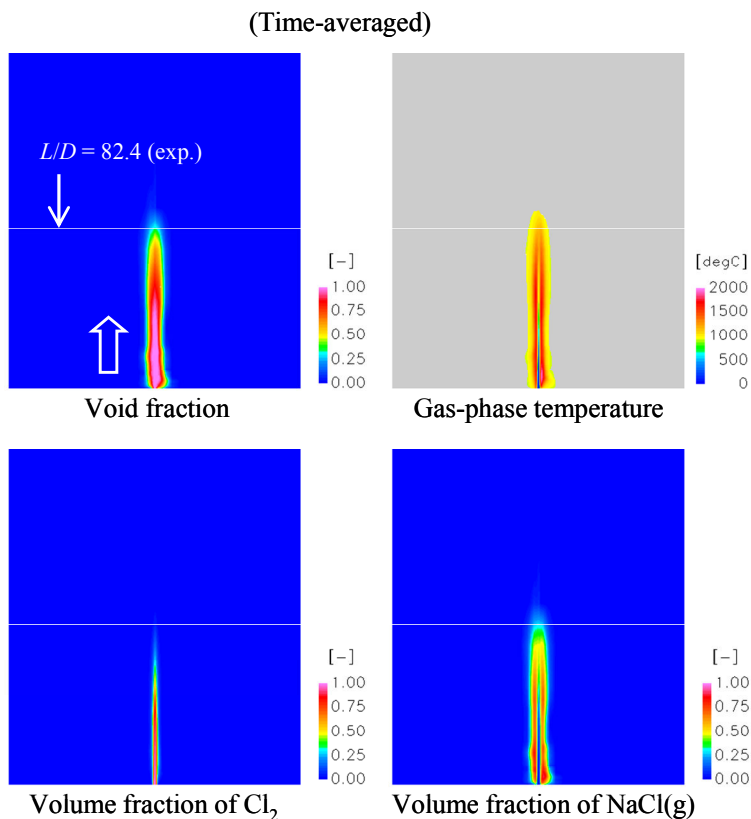


Figure 3 Numerical results (case 1).

Figure 4 shows the distributions of the time-averaged void fraction for the three analysis cases. The plume length in the case 2 is shorter than that in the case 1. This seems to be due to the difference of the saturation temperature between the two cases. The saturation temperature of the Na-NaCl mixture decreases with increasing the mol fraction of the sodium. In the case 3, both of the sodium mol fraction and the stagnation pressure are lower than that in the case 1. The flow rate of the chlorine gas is lower than that in the case 1 or the case 2. Therefore, the plume length became shortest in the three cases. Figure 5 shows the profiles of the gas-phase velocity and the void fraction along the centerline of the jet. It can be seen that the gas phase velocity exceeds the sound speed (205 m/s). This is due to the appearance of the underexpansion. The void fraction gradually decreases with increasing the distance from the inlet. We regarded the position at which the void fraction is 0.5 as the plume length. The relative error between the calculated plume length and the experimental result is 7 % in case1, 18 % in case 2 and 11 % in case3. We can say that the chemical reaction and the condensation determine the plume length of the reacting jet. The numerical analysis could reproduce the change of the plume length. The calculated plume length showed good agreement with the measurement. This indicates that the proposed numerical methods represent the mechanisms of the reacting gas jets in the liquid pools.

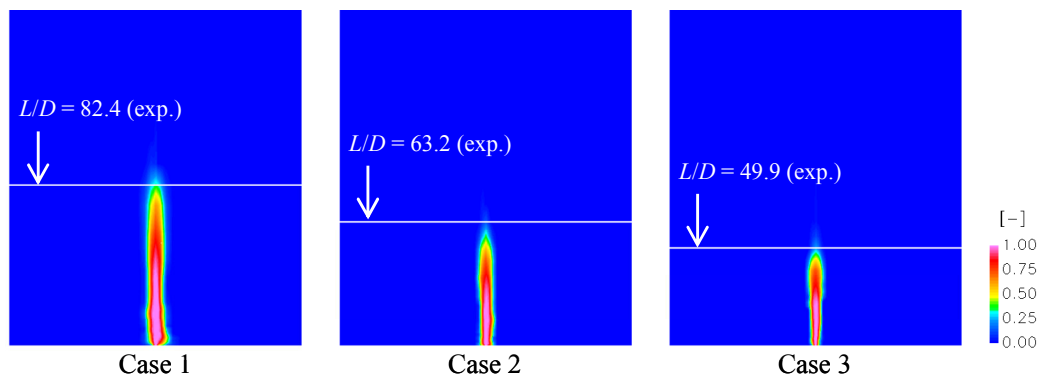


Figure 4 Change of plume length.

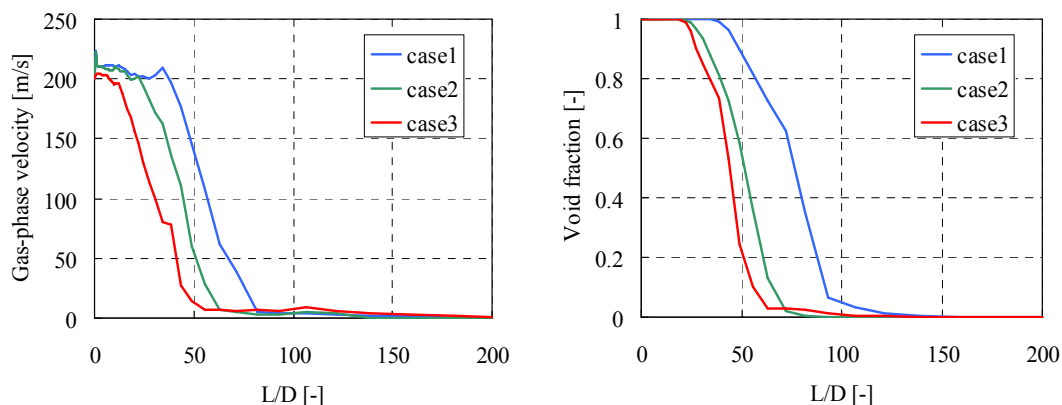


Figure 5 Void fraction and gas-phase velocity along centerline of jet.

3. Conclusion

Numerical analysis of the supersonic gas jets into liquid pools with chemical reaction was performed by using the SERAPHIM program. The program uses a multi-fluid model considering compressibility. The high mixing volume flow regime map was applied to the calculation of the interfacial drag force. The drag coefficient was estimated from the existing experimental data and the correlation. The mass generation rate by the chemical reaction between the gas and liquid phase was calculated by the surface reaction model which is derived from the assumption of the infinite reaction rate.

The experiment on the vertical supersonic chlorine jet into the Na-NaCl mixture was chosen as a validation problem. Numerical results showed that the gas phase disappears at a certain height. The estimated plume length showed good agreement with the experimental data in the all analysis cases. It was demonstrated that the proposed numerical method is applicable to the compressible multicomponent multiphase flow involving the chemical reaction between the gas and liquid phase.

4. References

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