Numerical Investigation of Self-wastage Phenomenon using a Simulant Materials

Sunghyon JANG[1*], Takashi TAKATA[1], Akira YAMAGUCHI[1]

[1]Osaka University (Department of Energy and Environmental Engineering, Suita Osaka 565-0871, Japan)
jang_s@qe.see.eng.osaka-u.ac.jp

Keywords: Self-wastage Phenomenon, Sodium-water reaction, CFD, Thermal-hydraulic

Abstract: In a steam generator of sodium-cooled fast reactor, sodium-water reaction (SWR) would take place when a heat transfer tube fails and water vapor leaks into liquid sodium in the shell side. In some cases the leakage enlarges eventually by the self-wastage phenomenon (an erosion and corrosion) resulting in a transition to a larger leakage. In order to evaluate the effect of the self-wastage phenomenon, an experimental study using a simulant material has proposed. In the present study, a numerical investigation, which uses Computational Fluid Dynamics (CFD), of an exothermic reaction of acid and base solutions has been carried out to validate the simulant experiment and to determine conditions for the experiment. As a result of the numerical simulation, it has been found that the maximum temperature at the reaction zone increase to 326.5K. Through the numerical investigation, the condition for the experiment such as a concentration of the solution, injection velocity and shape of the nozzle, has been determined.

1. Introduction

Sodium-cooled fast reactor adopts sodium-heated steam generators in a secondary sodium circuit to raise the steam to drive the turbine. In most cases, these steam generators are of a shell-in tube type, with high pressure water and/or water vapor inside the tubes and low pressure sodium on the shell-side, with a single wall tube as a barrier between these fluids. Accordingly, the water and/or water vapor will leak into the sodium and a sodium-water reaction (SWR) will take place at the shell side of the steam generator when a heat transfer tube fails. When a leakage occurs through a tiny crack on the tube, there results an important phenomenon, so-called ‘self-wastage’, which takes place inside the leakage site itself. When a steam generator is operated for some time under this condition, the deterioration of mechanical strength occurs at the site of the initial leak hole, then eventually the leak hole get enlarged.

Twenty-nine micro leak tests had been carried out in three stagnant sodium pots of the SWAT-4 test rigs installed in PNC/OEC. Most outlines of the self-wasted nozzles are like a cone-shape which opens to the sodium side. All orifices after the complete self-enlargement are formed near the steam side. This indicates that as a result of the self-wastage phenomenon, the defect eventually get enlarged and the leak rate would increase to a level, which affects adjacent tube, brings about a secondary failure of the SG tube.

Thus a prediction and a prevention of the self-wastage phenomenon are important from the viewpoint of designing a steam generator and its leak detection systems. However, a measuring technique for the experiment, such as a phase temperature and void fraction is not sufficient to obtain data with high accuracy and spatial resolution.

To evaluate the sodium-water reaction, a numerical simulation methodology has been developed based on a multi-dimensional and multi-phase reacting flow analysis (SERAPHIM code). Thermal hydraulic properties in the reaction zone have been investigated quantitatively to evaluate the self-wastage rate in the reaction zone. Furthermore, an experiment, which uses simulant materials, has been designed to evaluate the effect of the reaction heat to the nozzle wall. In the experiment aqueous solution of acid and base has adopted to make neutralization reaction in the reaction zone.

In the present study, a numerical investigation of the experiment has been carried out to validate the experiment and determine experimental condition. In the analysis, governing equation of concentrations of the acid and base are implemented in to the commercial CFD tool, Fluent, and the reaction rate is calculated based on the Arrhenius law.

2. Experiment using a simulant material

2.1. Simulant material

When solutions of hydrochloric acid, $HCl_{(aq)}$, and the base sodium hydroxide, $NaOH_{(aq)}$, are mixed the following reaction occurs.

$$HCl_{(aq)} + NaOH_{(aq)} \rightarrow NaCl_{(aq)} + H_2 0 + \Delta H \qquad (1)$$

This reaction is exothermic, as a result of reaction, a reaction heat(ΔH), 57.7kJ/mol, is released. In the experiment, to simulate the effect of the reaction heat created by the neutralization reaction, this acid-base neutralization is adopted.

2.2. Schematic of experiment

In the experiment acid and base solutions and paraffin wax has chosen as a simulant material. A schematic of the experiment are shown in figure 1. In the experiment, *HCl* aqueous solution is injected to a reaction tank which filled with *NaOH* solution through the nozzle made by paraffin wax ($C_{25}H_{52}$) to make acid-base neutralization near the outlet of leak nozzle. Reaction heat due to the reaction would be released and may melt the wax nozzle in the reaction zone. The effect of the self-wastage phenomenon on the leak hole is evaluated by investigating the maximum diameter and the shape of the wax nozzle enlarged by the reaction heat.

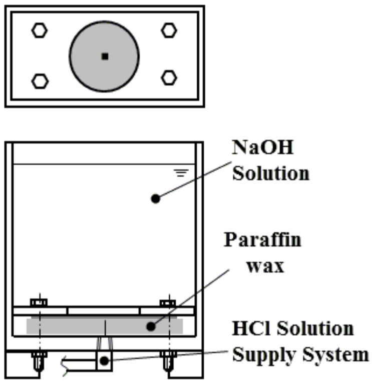

Figure 1. A schematic of the experiment

3. Numerical simulation methods and co nditions

3.1. Governing Equations.

The Fluent 6.3 CFD code, which can model mixing and transport of chemical species by solving conservation equation describing convection, diffusion and reaction sources for each component species, has been used for the numerical simulations performed in the present work.

Following conservation equations for chemical species has been solved.

$$\frac{\partial}{\partial t}\left(\rho Y_i\right)+\nabla\cdot\left(\rho v Y_i\right)=-\nabla\cdot\vec{J}_i+R_i+S_i \qquad (2)$$

where R_i is the net rate of production of species *i* by chemical reaction and S_i is the rate of creation by addition form the dispersed phase plus any user define sources. $\vec{J}_i$ is the diffusion flux of species *i*, which arises due to concentration gradient. In this study, the dilute approximation, under which the diffusion flux can be written as

$$\vec{J}_i=-\rho D_{i,m}\nabla Y_i \qquad (3)$$

Here $D_{i,m}$ is the diffusion coefficient for species in the mixture.

Laminar finite-rate model, which the effect of turbulent fluctuations is ignored and reaction rates are determined by Arrhenius expressions, has been adopted in this study.

The net source of chemical species *i* due to reaction is computed as the sum of the Arrhenius reaction sources over the N_R reaction that the species participate in

$$R_i=M_{w,i}\sum_{r=1}^{N_R}\hat{R}_{i,r} \qquad (4)$$

Where $M_{w,i}$ is the molecular weight of species *i* and $\hat{R}_{i,r}$ is the Arrhenius molar rate of creation/destruction of species *i* in reaction *r*.

The molar rate of creation/destruction of species i in reaction r is given by

$$R_{i,r}=k_r\left[C_{j,r}\right]^{\left(\eta'_{j,r}+\eta''_{j,r}\right)} \qquad (5)$$

Where

k_r = rate constant for reaction
$C_{j,r}$ = molar concentration of species *j* in reaction *r*
$\eta'_{j,r}$ = rate exponent for reactant species *j* in reaction *r*
$\eta''_{j,r}$ =rate exponent for product species *j* in reaction *r*

For the reaction of *HCl* and *NaOH,* the rate exponents are 1 respectively. The rate expression, equation (5) can be written as

$$R_{i,r}=k_r\left[HCl\right]\left[NaOH\right] \qquad (6)$$

The overall order of the reaction is second.

The rate constant is independent of the concentrations but depends on the temperature. It is computed using the Arrhenius equation.

$$k_r=A_r e^{-E_a/RT} \qquad (7)$$

where

A_r = pre-exponential factor
E_a = activation energy for the reaction
R = universal gas constant

To discretize of the continuity equation, Pressure-based solver has adopted and SIMPLE algorithm has chosen to enforce mass conservation and to obtain the pressure field. First-order-upwind algorithm has applied to get discretization equation for the momentum, species and energy.

3.2 Modeling and Boundary Conditions

Numerically simulated region of the nozzle is shown in figure 1 and the boundary condition is described in figure 2.

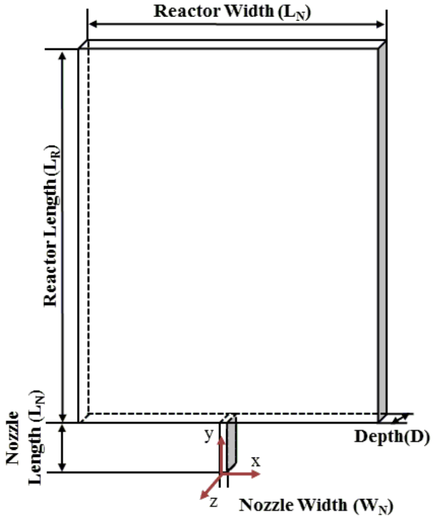

Figure 2. A schematic of the computational domain

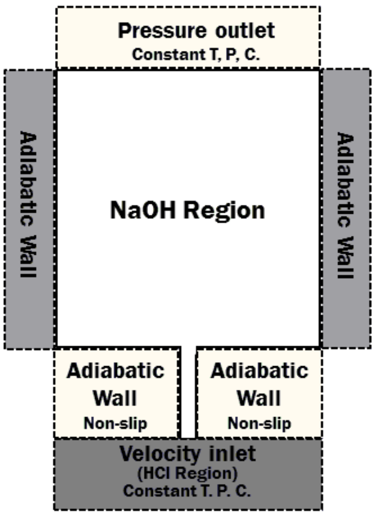

Figure 3. Boundary conditions for the domain

The characteristics of the computational grid have been determined to simulate the flow of SWAT4 Experiment. According to the experimental data for the SWAT4, initial leak rate of the water vapor was from 7.3E-9m^3 (7.3E-3ml) to 8.1E-8m^3 and Reynolds number of the flow is about 10 at the inlet of nozzle. The characteristics of the grids and total number of meshes are given in Table 1 and Table 2 respectively.

Table 1. Characteristics of the computational grid

	Width(m)	Length(m)	Depth(m)
Nozzle	2.0E-3	1.0E-2	2.0E-3
Reactor	8.0E-2	1.0E-1	1.0E-3

Table 2. The total number of meshes of the grid

	Nozzle	Reactor	Total
Number	5600	340	5940

The system consists of a velocity, pressure outlet, adiabatic wall and the fluid region. *HCl* aqueous solution is injected to *NaOH* region, through inlet with a constant velocity, temperature and pressure. The geometry is assumed to be invariant along the *z* direction and thus the system represents two-dimensional. The fluid properties are also defined to be constant. The gravitational acceleration works in the negative y-direction.

4. Results and Discussion

4.1. Thermal properties and Boundary conditions

In the computation, the time step and time duration are set to 1E-3 and 30sec, respectively. The physical properties of aqueous solutions are given in Table 3.

Table 3. Physical properties of aqueous solution

	HCl	NaOH	NaCl	H_20
Density [kg/m^3]	1170	1742	1539	997.1
Specific heat [J/kg-k]	2640	2140	1150	4179
Thermal Conductivity [w/m-k]	0.518	0.599	0.590	0.6
Viscosity [kg/m-s]	1.73E-3	2.8E-3	1.49E-3	8.91E-4
Molecular weight [kg/m-s]	36.461	39.997	58.443	18.015
Enthalpy [J/mol]	-167.2	-469.4	-407.1	-285.8
Entropy [J/mol]	56.5	48.1	115.5	69.95

Table 4. Boundary condition for numerical simulation

Boundary condition	Velocity Inlet	Wall	Wall	Pressure Outlet
Velocity [m/s]	4.4E-3			
Pressure [Pa]	103125			103125
Mass Fraction of HCl[wt]	0.35	Mirror condition	Mirror condition	0
Mass Fraction of NaOH[wt]	0	Mirror condition	Mirror condition	0.12
Mass Fraction of H_20 [wt]	0.65	Mirror condition	Mirror condition	0.88

Inlet velocity has been determined to satisfy the Reynolds number and the data of injection leak rate by using equation (8)

$$v_{inlet} = \frac{\mu Re}{\rho D_H} \quad (8)$$

where ρ is density, Re is Reynolds number, D_H is hydraulic diameter and μ is viscosity. For hydraulic diameter for rectangular channel, is determined by equation (9)

$$D_H = \frac{2LW}{L+W} \quad (9)$$

where L is length and W is width of the cross section.

The characteristics of the nozzle also have been decided to meet up the data from the SWAT4 experiment. Initial temperature of the *HCl* and *NaOH* solution is 300K.

4.2. Time step and Simulation time

Considering the volume of reactor, simulation time depends on injection rate of *HCl* aqueous solution. For 3Mol *NaOH* and 10Mol *HCl* aqueous solution, the volume of the *NaOH* is 4.0E-5m^3(40ml) and the injection rate of 10 Mol *HCl* is 5.0E-8 m^3(5.0E-2ml). The neutralization reaction is second-order reaction, thus in order for the solution to be reacted fully, the simulation time couldn't exceed 160sec. Time step (ΔT) determined 1E-03 and scheme for the time is first-order Euler implicit.

4.3. Results of the simulation

4.3.1 Temperature distribution near the reaction zone

10Mol *HCl* solution has been injected to 3Mol *NaOH* through the nozzle for 30sec. Injection rate is 1.78E-8 m^3 (1.78E-2 ml).The result is given in figure 4. The temperature has increased to 326.5K in the reaction zone. The temperature distribution at the wax wall surface (at Y=1.0E-2m) is given in figure 5. This shows that near the nozzle wall that the highest temperature reached about 324K. This temperature exceeds the melting point of the paraffin which is (Paraffin wax-115) 47.2 degrees Celsius (320.5K).

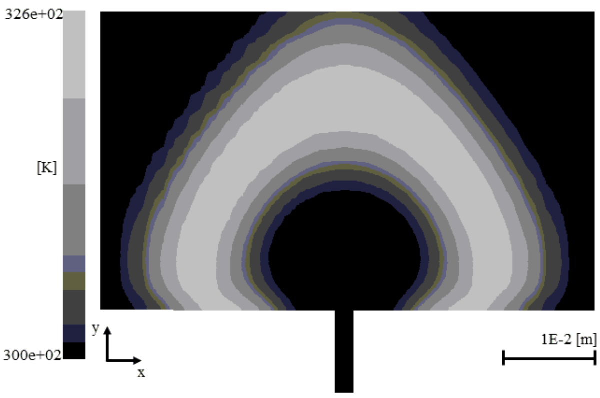

Figure 4. Temperature near the nozzle

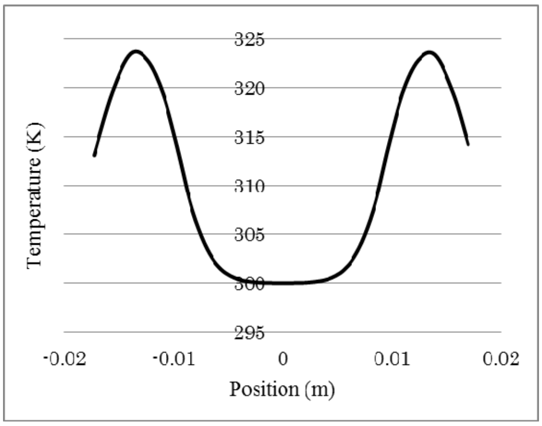

Figure 5. Temperature distribution at the nozzle surface (at Y=1.0E-2 [m])

It is indicated that the reaction heat is able to melt the surface of the wax. Then the reacting zone would move along to the surface of the wax. Then reaction heat would effect on the new surface as result, the leak hole would be enlarged as a cone shape.

5. Conclusion

From the numerical investigation of the experiment using simulant materials, the validation of the experiment has been proved. When 10Mol *HCl* aqueous solution is injected to 3Mol of *NaOH* with 0.01m/s through the paraffin wax nozzle, the neutralization reaction takes place near the nozzle and the temperature at the surface of nozzle increased to 326.5K which is enough to melt the paraffin wax. The effect of the self-wastage on the leak hole is able to be evaluated by considering the maximum diameter and the shape of the enlarged leak hole.

References

Fluent 2006 *Fluent 6.3 User's Guide*, Fluent Inc., Lebanon, New Hampshire, USA..

Kuroha, M. & Shinomiya, K. 1986 Micro-leak behavior on FBR Monju steam generator tube material – studies of micro-leak sodium-water reaction (3), PNC ZN9410 86-027, pp. 19-20.

Nippon Seiro Co.,Ltd. *Products guide.* (Http://seiro.co.jp/e/product.html#t01)

Takata, T. & Yamaguchi, A. 2003 Numerical approach to the safety evaluation of sodium-water reaction. *J. Nucl. Sci. Technol.*, Vol. 40, pp.708-718.

The Japanese Society of Mechanical Enegineering, *JSME Data book 2008 Thermophysical Properties of Fluids,* Maruzen, Tokyo, Japan. (In Japanese)