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Analysis for Convective Mass Transfer of Nitrogen toward H_2O in a nuclear system

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1. Introduction

Mass transfer can occur due to a concentration difference of nitrogen inside H_2O when nitrogen and H_2O are filled in any geometry of a nuclear system. Several studies for a mass transfer have not been sufficient to properly understand the key phenomena involved in a high temperature and pressure condition [1], [2]. In addition, there has been no existing correlation or model which can accurately predict a convective mass for a wide range of nuclear systems [3], [4], [5].

For understanding the characteristic of a convective mass transfer, the commercially available CFD computer model, FLUENT, was employed. H_2O filled a cylinder with a diameter of 1.06m, and a length of 1.18m. Nitrogen was supplied constantly at the interface between H_2O and nitrogen. The initial system pressure was maintained about 14.7MPa.

First, the concentration rate was compared with an analytic analysis and the results of FLUENT when only a diffusion was considered without a convection. By verifying the application of FLUENT for a mass transfer, the conditions in which the H_2O side has an effect of a natural convection by a heat transfer from a boundary of a medium was computed with FLUENT. Finally, sensitivity tests were conducted for several conditions.

2. Mass transfer by diffusion

To describe a diffusive mass transfer of nitrogen in the H_2O side, UDS (User Defined Scalar) in FLUENT was used with the diffusion coefficient (0.27×10^{-6} m^2/s) of nitrogen in H_2O at 100°C and 14.7MPa. In addition, the maximum solubility ($1.86 g_{N2}/kg_{H2O}$) was used to estimate the boundary condition of UDS at the interface between nitrogen and H_2O.

Diffusion equation, which was described as PDE (Partial Differential Equation) with non-homogeneous boundary conditions,

$$\frac{\partial C_A}{\partial t} = D_{AB}\frac{\partial^2 C_A}{\partial x^2} \qquad 0 \le x \le L, \quad 0 < t < \infty \tag{1}$$

$$C_A(x,0) = 0 \qquad 0 \le x \le L \tag{2}$$

$$C_A(0,t) = C_{A,s} \qquad 0 < t < \infty \tag{3}$$

$$\left.\frac{\partial C_A}{\partial x}\right|_{x=L} = 0 \qquad 0 < t < \infty \tag{4}$$

was solved analytically, where D_{AB} was the diffusion coefficient. The PDE was divided into a steady state and a transient equation. The PDE in the steady state was changed to the Laplace's equation type and a new initial condition was employed in the transient state. The PDEs and conditions are solved by SOV (Separation of Variables).

$$C_A(x,t) = 0.064 - \sum_{0}^{\infty}\frac{2\times0.064}{\left(n+\frac{1}{2}\right)\pi}e^{-\left[\left(\frac{1}{2}+n\right)\frac{\pi}{1.18}\right]^2\left(0.27\times10^{-6}\right)t}\sin\left[\left(\frac{1}{2}+n\right)\frac{\pi}{1.18}x\right] \tag{5}$$

The analytic results are compared with the result of FLUENT in the same condition. 2nd order implicit scheme was used for the unsteady condition. The cylinder was simplified to a 2-D axisymmetric geometry (Figure 1). All boundaries except for the top region of the nitrogen interface were insulated and impermeable. UDS model was employed to evaluate the behavior of nitrogen in the H_2O side. The scalar equation in FLUENT was

$$\frac{\partial \rho\phi_k}{\partial t} + \frac{\partial}{\partial x_i}\left(-\rho D_{AB}\frac{\partial \phi_k}{\partial x_i}\right) = 0 \tag{6}$$

The mole fraction rates of nitrogen in the H_2O side were computed and compared with the analytic solution as shown Figure 2. The analytic results showed a good agreement with those of FLUENT and that nitrogen was diffused in order from the top interface to the bottom wall as time past on. In the surface of 0.5m, it took about 250 hr that the concentration of nitrogen in the H_2O side was a half value of the maximum mole fraction.

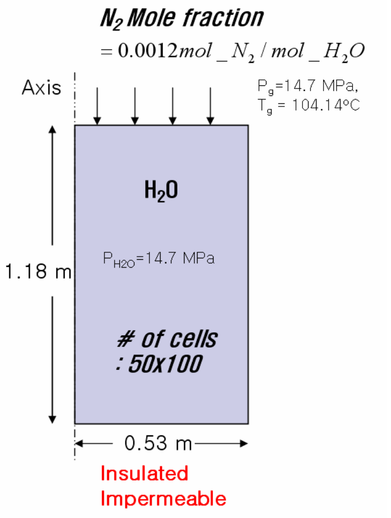

Figure 1. The computed boundary conditions

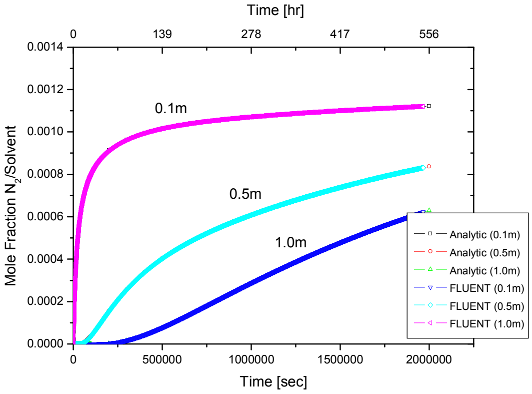

Figure 2. The comparison of the mole fractions (Diffusion)

3. Convective mass transfer

The scalar equation in FLUENT including convection was

$$\frac{\partial \rho\phi_k}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho u_i\phi_k-\rho D_{AB}\frac{\partial \phi_k}{\partial x_i}\right)=0 \tag{7}$$

The number of cells was 12,000, the bottom wall temperature was 110°C, the vertical wall heat transfer coefficient was 496 W/m^{2}K, and the vertical ambient temperature was 94°C to assess the convective mass transfer using the models in FLUENT. By a natural convection, H_2O showed an upward bulk motion near the central region and a downward one near the vertical wall. According to the flow of H_2O, the nitrogen also had a convection effect. As seen in Figure 3, convective mass transfer rate was faster than those of a diffusion. In addition, it was shown that the mole fraction in the surface of 1.0m was slightly higher than those in the surface of 0.5m in the early stages due to a bulk flow motion by a natural convection.

The sensitivity tests of the number of cells and the bottom wall conditions, the case 1 of 135°C and case 2 of 120°C (Figure 4), were performed. As shown Figure 4, the trends of the mole fraction rates were similar for each test.

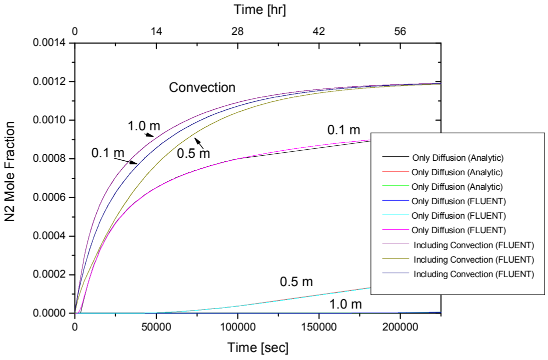

Figure 3. The comparison of the mole fractions (Convection and Diffusion)

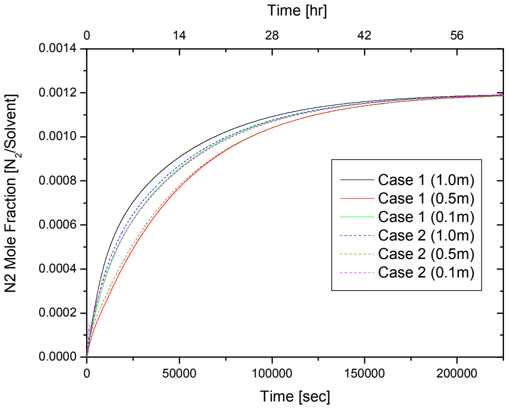

Figure 4. Sensitivity tests of the bottom wall condition

4. Conclusion

Our research work seeks to analyze and understand the mass transfer phenomena of nitrogen toward H_2O using FLUENT, when H_2O side has an effect of a natural convection by a heat transfer from a boundary of a medium.

In the condition of a diffusive mass transfer without a convection, the analytic results to solve the PDE with non-homogeneous boundary conditions showed an excellent agreement with those of FLUENT in the same condition.

The convective mass transfer phenomena were analyzed with FLUENT in which the usage of UDS for a mass transfer was verified. The result of FLUENT showed that nitrogen was transferred simultaneously in the entire region by the H_2O convection effect and it took about 5~10 hr that the concentration of nitrogen in the H_2O side was a half of the maximum value.

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