Simultaneous Heat and Mass Transfer in DU Hydriding

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1. Introduction

The energy crisis is more aggravating in the present age than in past times, and many countries are developing next-generation energy sources. Among the next-generation energy sources, nuclear fusion energy is a concern for many countries, and common international research has been conducted. The sources of nuclear fusion reaction are deuterium (D) and tritium (T). Generally, D is fused into T, which generates helium atoms and neutrons. At this time, a tremendous amount of energy is generated [7].

$$D + T \rightarrow {}^{4}He + n \ (E = 17.6\ MeV) \qquad (1)$$

Hydrogen is a gas, and cannot be stored in large amounts. In addition, it can be explosive. Therefore, one of the storing methods for hydrogen is metal hydride. In this research, several kinds of metal hydrides [1-8] including U, Zr, ZrCo, ZrNi, and $LaNi_5$ have been simulated through modeling work of hydrogen absorption, desorption, and pressure effect in a bed using DU. For the exact modeling of the hydriding process, it is necessary to calculate simultaneous heat and mass transfer because, in the hydriding process, not only is hydrogen gas transported by mass transport and chemisorption but heat transfer also occurs through absorption. Therefore, in this paper, we tried to calculate the simultaneous heat and mass transfer using numerical analysis methods.

2. Methods and Results

1. Model assumptions.

For a simplified analysis, several hypotheses were stated for modeling.

- Hydrogen gas is an ideal gas.
- Physical properties of hydrogen follow the ideal gas law.
- The specific heat, thermal conductivity, and density of DU are constants.
- The pressure of the bed entrance is the same as the tank pressure, i.e., the pressure drop in a tube is negligible.
- Hydrogen gas flow Poiseuille flow (i.e., laminar flow proportional pressure difference).

2. The governing equation and generation terms.

The following equations are generally used to express the mass transfer phenomena [4]

- The mass balance for the gas phase.

$$\frac{\partial \rho_g}{\partial t} + \nabla\left(\overrightarrow{V_g} \cdot \rho_g\right) = -\dot{m} \qquad (2)$$

The mass balance for the atomic ratio.

$$\frac{\partial \xi}{\partial t} = \dot{m} \qquad (3)$$

where the value of $\overrightarrow{V_g}$ is obtained from the following Kozeny-Carman equation [6].

$$V_g = -\frac{R^2}{4\mu} \cdot \frac{\Delta P}{L} \qquad (4)$$

where R is the radius of a tube between the tank and bed, L is the length of the tube, μ is the viscosity, and ΔP is the pressure difference between the tank and bed.

In equations (2) and (3), $\dot{m}$ can be expressed through the following equations [5].

$$\dot{m} = -A_1\left(\frac{\xi - \xi_f}{\xi_o - \xi_f}\right)\exp\left(-\frac{E_a}{RT}\right)\ln\left(\frac{P_g}{P_e}\right) \qquad (5)$$

where E_a is the activation energy of the hydriding, and C_a is the rate constant of the hydriding. In addition, R is the universal gas constant, T is the absolute temperature, P_g is the present gas pressure, P_e is the equilibrium gas pressure, and ξ is the atomic ratio of DU.

2.3 Euler method.

In this paper, the method of numerical analysis is applied to Euler's method. let us see following initial-value problem on interval [a,b].

$$\frac{dy}{dt} = f(t, y) \quad y(a) = y_o \qquad (6)$$

Then, interval [a,b] is divided into N equal subintervals, and thus the mesh points are defined as

$$t_i = a + ih \qquad (7)$$

where h=(b-a)/N is the step size. Numerically solving for the initial-value problem, it starts the initial condition y_o and then generates values y_1, y_2,.....,y_N, which approximate the exact values y(t) at t_1, t_2,......,t_N.

To derive Euler's method, it applies to the Taylor series of y about t_i, for each i = 0, 1, 2,....., N-1. If y(t) is twice continuously differentiable on [a,b],

$$y(t_{i+1}) = y(t_i + h)$$
$$= y(t_i) + h\,y'(t_i) + \frac{h^2}{2}y''(\zeta) \qquad (8)$$

for some ζ between t_i and t_i +h.

If $\frac{h^2}{2}y''(\zeta)$ drops the error term, we obtain the following equation,

$$y(t_i + h) = y(t_i) + h\,f(t_i, y_i) \qquad (9)$$

If we denote $y_i \simeq y(t_i)$, then

$$y_{i+1} = y_i + h\,f(t_i, y_i) \qquad (10)$$

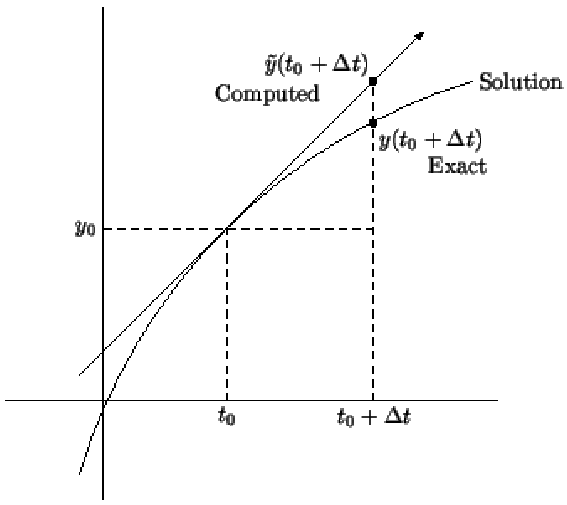

Fig. 1 Mathematical principle of Euler's method [8].

Eq. (10) is Euler's method. An algorithm of Euler's method is as follows.

$$\mathrm{h} \leftarrow \frac{b-a}{N}$$
$$\mathrm{y(a)} = y_o$$
$$\text{for} \qquad \mathrm{i} = 0,1,\ldots\ldots,\mathrm{N}-1$$
$$\llcorner \qquad y_{i+1} \leftarrow y_i + hf(t_i, y_i) \qquad (11)$$

The total energy balance of the DU bed applied to the FDM equation is as follows,

$$\mathrm{T}^{i+1} = \mathrm{T}^{i} + \frac{\dot{m}}{\rho \mathrm{C_p}}\left[\frac{\Delta \mathrm{H}}{\mathrm{M_g}} \pm \mathrm{T}\left(\mathrm{C_{p,g}} - \mathrm{C_{p,m}}\right)\right] \qquad (12)$$

In addition, the total mass balance of the DU bed is expressed as eq. (13).

$$\xi^{i+1} = \xi^{i} + \mathrm{A_1}\left(\frac{\xi^i - \xi_f}{\xi_o - \xi_f}\right)\exp\left(-\frac{\mathrm{E_a}}{\mathrm{RT}}\right)\ln\left(\frac{\mathrm{P_g}}{\mathrm{P_e}}\right) \qquad (13)$$

The total modeling procedure is expressed in fig. 2. The numerical analysis method uses Euler's method, and the computation engine uses Wolfram Mathematica.

3. Conclusions

Simultaneous heat and mass transfer in DU hydriding is well fitted compared to the experimental data, and is more reasonable considering only one variable. The hydriding process changes the temperature and atomic ratio simultaneously, and thus it is necessary to consider in company with two transport phenomena.

The numerical analysis method applied Euler's method; however, the Runge-Kutta method is a more widely used numerical solution of a differential equation. Therefore, when analyzing the hydriding process, Runge-Kutta or another method will henceforth be applied .

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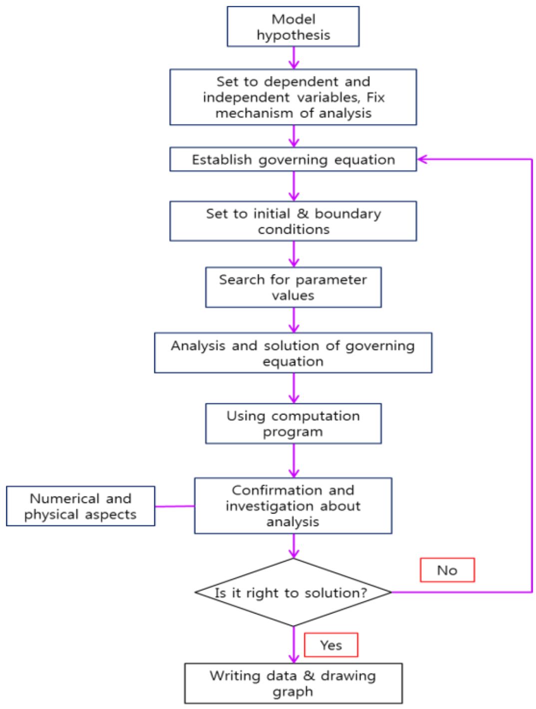

Fig. 2. Procedure of DU bed hydriding/dehydriding simulation to heat and mass transfer.

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