Filtration and Hydrogen Reaction Modeling in a Depleted Uranium Bed

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1. Introduction

The storage and delivery system (SDS) is a part of the ITER fuel cycle. The SDS stores the hydrogen isotopes and delivers them to the fuel injection system. Depleted uranium (DU) was chosen as a hydrogen isotope storage material. The hydrogen isotopes stored in the SDS are in the form of DU hydride confined in the primary and secondary containment within a glove box with an argon atmosphere (Refs. 1-3).

In this study, we performed a modeling study of the SDS. A modeling study is practically important because an experimental study requires comparatively more money and time. We estimated the hydrogen atomic ratio in DU hydride by two empirical equations we formulated. Two empirical equations are used to determine Pressure-Composition-Temperature (PCT) curves and the hydrogen atomic ratio in DU hydride. In addition, we present the effect of pressure and temperature in the hydriding and dehydriding.

2. Mathematical Model

Many researchers discovered that the kinetics of metal hydrides can be explained by the combination of complex mechanisms. Some researchers developed mathematical models for metal hydrides (Refs. 1, 4, 5).

In this study, we formulated two empirical equations (Eq. 1, 2). The empirical equations are modified from M. H. Chang's equations (Ref. 1) and D. W. Sun's equations (Ref. 5).

$$\frac{dX}{dt} = \lambda \left(\frac{X_F - X}{X_F - X_I} \right) \left(\frac{P_{ref} - P}{P_{ref}} \right) e^{\left(-\frac{\Delta H}{RT} \right)} \tag{1}$$

$$log(P_{ref}) = A + B/T + C \tan\left\{\frac{\pi}{3}\left(X - \frac{3}{2}\right)\right\}$$
(2)

X is the atomic ratio in DU hydride. X_I and X_F are the initial and final atomic ratio in DU hydride, respectively. *P* and P_{ref} are the bed pressure and reference pressure, respectively. ΔH is the standard enthalpy change. *R* and *T* are the universal gas constant and the bed temperature, respectively. *t* is time. The coefficients λ , *A*, *B*, and *C* can be derived from the experimental data. The coefficient λ includes the filter effect and affects the hydriding and dehydriding rates. The coefficients *A* and *B* are widely used to obtain the dissociation pressure of metal hydride (Refs. 1, 5-7). Coefficient *C* is used to consider the pressure difference according to the atomic ratio in the DU hydride in the PCT curves.

3. Numerical Results

3.1 PCT Curve for Reference Pressure

The PCT curve was obtained by solving Eq. 2 and is shown in Fig. 1. The coefficients A and B were derived from the experimental data. Coefficient C was adjusted adequately.



Fig. 1. PCT curve based on internal pressure in a DU bed $(T=400^{\circ}C)$.

3.2 Effects of pressure and temperature in hydriding and dehydriding

Hydriding and dehydriding performances were estimated by solving Eq. 1. The coefficient λ was derived by regressing from the experimental data. simulations for the hydriding Numerical and dehydriding are performed under different pressures and temperatures. In Fig. 2, the increase in pressure leads to a decrease in the atomic ratio at the final time and a decrease in the hydriding reaction. In Fig. 3, the increase in temperature leads to an increase in the atomic ratio at the final time and an increase in the hydriding reaction rate. The increase in the hydriding reaction rate (slope) occurs as the temperature increases. In Fig. 4, the increase in pressure leads to a decrease in the atomic ratio at the final time and a decrease in the dehydriding reaction. In Fig. 5, the increase in temperature leads to an increase in atomic ratio at the final time and an increase in the dehydriding reaction rate. The increase in the dehydriding reaction rate (slope) occurs as the temperature increases.



Fig. 2. Hydriding simulation results under pressures (P=15 and 95 Pa) and constant temperature (T=35 $^\circ$ C).



Fig. 3. Hydriding simulation results under constant pressure (P=25 Pa) and temperatures (T=0 and 225°C).



Fig. 4. Dehydriding simulation results under pressures (P=15 and 15000 Pa) and constant temperature (T= 400° C).



Fig. 5. Dehydriding simulation results under constant pressure (P=15 Pa) and temperatures (T=200 and 400° C).

4. Conclusions

A modeling study of the SDS was performed in this study. It is practically important to save more money and time. The hydrogen atomic ratio in the DU hydride was estimated using two empirical equations. The two empirical equations are modified and reformulated to determine PCT curves and the hydrogen atomic ratio in DU hydride. All parameters that are required to solve two empirical equations are obtained from the experimental data. The derived parameters are utilized for the numerical simulations. In the numerical simulations, the effects of pressure and temperature on both the hydriding and dehydriding reaction rates are confirmed. In both the hydriding and dehydriding simulations, better performances are observed at a lower pressure and higher temperature. The hydriding performance deceased significantly with a slight increase in pressure.

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