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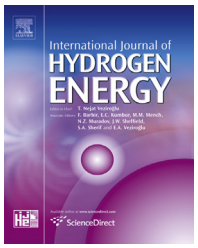

Predictive calculation of the effective thermal conductivity in a metal hydride packed bed

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ABSTRACT

The effective thermal conductivity of a metal hydride packed bed was calculated by considering the influence of expansion during hydrogen absorption and contraction during hydrogen desorption. The porosity was calculated using an experimental formula developed by direct observation, which was used in combination with other referenced methods. However, none of the methods could express the reported experimental value response to pressure change using only the experimental porosity formula. The area contact model was modified so that the porosity and the contact area changed with expansion and contraction. The contact area change was calculated by assuming a simple geometrical deformation caused the difference between the particle expansion and the packed bed expansion. The calculation results of the improved area contact model with the deformed factor and the shape factor were in good agreement with the reported experimental data. This calculation method of the effective thermal conductivity with the influence of expansion and contraction is expected to be useful for designing of heat transfer enhancement of a hydrogen storage tank.

Introduction

Metal hydrides are promising materials for safety-conscious methods of hydrogen storage because they do not easily explode. Metal hydrides can absorb hydrogen at moderate temperatures and relatively low pressures [1]. Before practical hydrogen storage applications are developed, the basic properties of metal hydrides should be studied more closely [2]. In particular, because the hydrogen absorption and desorption of a metal hydride are, respectively, exothermic and endothermic reactions, the effective thermal conductivity of packed bed of powdery metal hydride is an important property, which has not been previously studied in detail.

Various computational methods have been proposed for calculation the effective thermal conductivity for other simple powders [3–16]. However, these methods are too simple to describe the expansion and contraction of the metal hydride during hydrogen absorption and desorption, respectively. The packing structure (porosity, coordination number, and contact angle) has a large effect on the effective thermal conductivity of a packed bed [17]. Therefore, the effective thermal conductivity calculation method must be corrected with a porosity formula that describes the expansion by absorption and contraction by desorption.

Asakuma et al. [18,19] analyzed the effective thermal conductivity of a metal hydride bed using a homogenization

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method. Smith et al. [20] presented a multiphysics modeling approach for heat conduction in metal hydride powders, which contained the particle shape distribution, size distribution, granular packing structure, and effective thermal conductivity. Unfortunately, these studies did not focus on the porosity in detail. Therefore, we have developed an experimental porosity formula using direct observation of the volume change of a metal hydride packed bed [21–25].

In this work, we show the calculation method and results for the effective thermal conductivity of metal hydrides using our experimental porosity formula. First, the experimental porosity formula is used in combination with other referenced methods. Then, the area contact model was modified so that the porosity and the contact area change with expansion and contraction. The contact area was calculated by assuming a simple geometrical deformation was caused from the difference between the particle expansion and the packed bed expansion. The calculation results are evaluated using the experimental data reported by Yoshida et al. [26].

Calculation methods of the effective thermal conductivity for powders

Calculation methods of references

The effective thermal conductivity for powders is calculated using three primary parameters: fluid thermal conductivity, solid thermal conductivity, and porosity. The porosity is a rate of the space to the whole packed bed. Almost all of the methods use only three parameters.

Deissler and Boegli [3] determined the maximum and minimum limits for the thermal conductivity of a two-phase system. The maximum thermal conductivity corresponds to a weighted arithmetic mean, while the minimum thermal conductivity corresponds to a weighted harmonic mean. The maximum limit is given by

$$\lambda_e = \varepsilon\lambda_f + (1-\varepsilon)\lambda_s \tag{1}$$

The minimum limit is given by

$$\lambda_e = \frac{1}{\frac{\varepsilon}{\lambda_f} + \frac{1-\varepsilon}{\lambda_s}} \tag{2}$$

For both equations, λ_e is the effective thermal conductivity, λ_f and λ_s are the thermal conductivity of fluid and solid, respectively, and ε is porosity.

Russell [4] showed the effective thermal conductivity of a structure where the pores are cubes of the same size with solid walls of uniform thickness:

$$\lambda_e = \frac{\lambda_s\left\{\varepsilon^{2/3} + \frac{\lambda_s}{\lambda_f}\left(1-\varepsilon^{2/3}\right)\right\}}{\varepsilon^{2/3} - \varepsilon + \frac{\lambda_s}{\lambda_f}\left\{1+\varepsilon-\varepsilon^{2/3}\right\}} \tag{3}$$

Moreover, Russell showed the effective thermal conductivity of the reverse structure by replacing ε with 1-ε and interchanging λ_f and λ_s:

$$\lambda_e = \frac{\lambda_f\left\{(1-\varepsilon)^{2/3} + \frac{\lambda_f}{\lambda_s}\left(1-(1-\varepsilon)^{2/3}\right)\right\}}{\varepsilon + (1-\varepsilon)^{2/3} - 1 + \frac{\lambda_f}{\lambda_s}\left\{2-\varepsilon-(1-\varepsilon)^{2/3}\right\}} \tag{4}$$

Woodside and Messmer [8] showed the effective thermal conductivity using a weighted arithmetic mean of the individual conductivity logarithms:

$$\lambda_e = \lambda_f^{\varepsilon}\lambda_s^{1-\varepsilon} \tag{5}$$

Chaudhary and Bhandari [9,10] showed the effective thermal conductivity using a combination of the weighted arithmetic mean and the weighted harmonic mean:

$$\lambda_e = (\varepsilon\lambda_f + (1-\varepsilon)\lambda_s)^n \left(\frac{1}{\frac{\varepsilon}{\lambda_f} + \frac{1-\varepsilon}{\lambda_s}}\right)^{1-n} \tag{6}$$

$$n = \frac{1-\log\varepsilon}{\log\left(\varepsilon(1-\varepsilon)\frac{\lambda_s}{\lambda_f}\right)}$$

Dul'nev and Zarichnyak [11] showed the effective thermal conductivity using a different combination of the weighted arithmetic mean and the weighted harmonic mean.

$$\lambda_e = A(\varepsilon\lambda_f + (1-\varepsilon)\lambda_s) + B\left(\frac{1}{\frac{\varepsilon}{\lambda_f} + \frac{1-\varepsilon}{\lambda_s}}\right) \tag{7}$$

$$A + B = 1$$

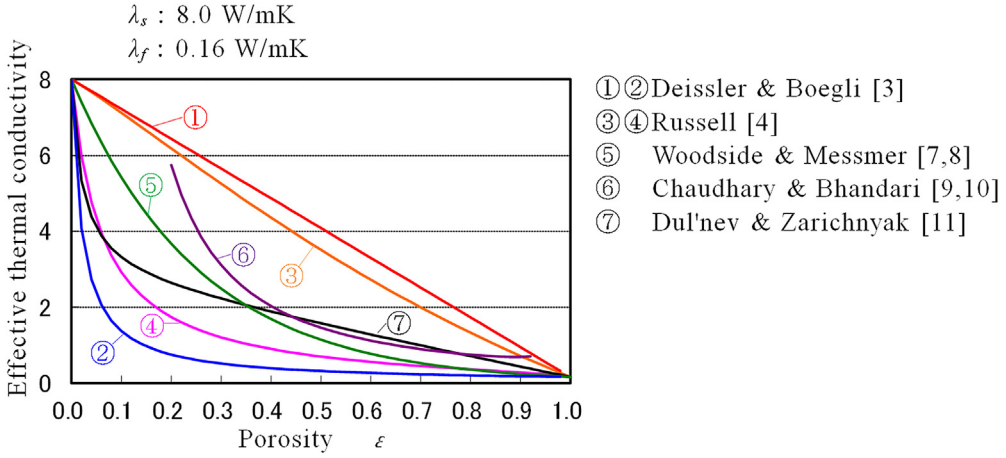

Fig. 1 – Relationship between the effective thermal conductivity and porosity for the referenced methods.