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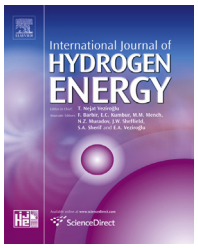

Numerical study of heat and mass transfer processes in a metal hydride reactor for hydrogen purification

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ABSTRACT

The present paper describes a numerical study of heat and mass transfer processes in a metal hydride reactor for hydrogen purification with aluminium foam. A numerical simulation was done with the help of the mathematical model, which had been used previously for a numerical simulation of heat and mass transfer processes in different types of metal hydride reactors during sorption/desorption processes. The results illustrate that the major factors that reduce the rate of sorption, and consequently the efficiency of the system, are increasing the temperature of the reactor and the pressure drop, which is due to filtering the mixture through a metal hydride bed with low permeability. It is shown that the use of aluminium foam allows us to realise a more effective system for hydrogen purification from impurities, compared to a case without aluminium foam, while the volumetric capacity of the system is reduced slightly (9%). Increasing pressure at the reactor inlet also increases the efficiency of the system.

Introduction

Hydrogen is used in many industries: chemical, metallurgical, food, electronics, etc. For many years, it was regarded as the primary energy carrier in the concept of hydrogen energy [1,2]. In order to efficiently use energy from hydrogen, it needs to be separated from the mixed gases, especially for supplying fuel cells. One of the applications of metal hydride is hydrogen purification [3–5]. The metal hydride method has the advantages of a simple device layout, low energy consumption, and simple and safe operation. However, the hydrogen recovery ratio of the present process is only 75%–95%, and impurities have a negative influence on the performance of metal hydride devices (they have poisonous effects, and they slow down the reaction of hydrogen sorption). These problems define the subject of ongoing studies: the development of the poisoning-tolerant metal hydride materials (see, e.g., [6]), optimising reactors, and the purification process [7]. Although there are a lot of works (see, e. g. Refs. [8–12]) that focus on the optimisation of the thermal behaviour of metal hydride reactors for hydrogen storage, compression, etc, there are a small number of works devoted to the same problems for the hydrogen purification systems. The present paper focuses on

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the optimisation of the design of a metal hydride reactor for hydrogen purification from a gas mixture containing inert impurities using a method based on filtering the mixture through a metal hydride bed. In this case, one can focus on the analysis of the main factors that reduce the effectiveness of such a type of hydrogen purification: the reduction of the effective thermal conductivity and decreasing the hydrogen partial pressure in the system by increasing the mole fraction of impurities, the pressure drop due to filtering the gas mixture through a metal hydride bed, and increasing the temperature of the metal hydride bed due to the thermal effect of reaction. Similar issues were investigated in Refs. [13,14], numerically, but [13,14] focused on the pre-set configuration of metal hydride reactors, which corresponds to the design of reactors investigated experimentally in Refs. [15,16].

In Refs. [13], a verification of a complex mathematical model on experimenal data of hydrogen purification in the cylyndrical flow-through type metal hydride reactor was performed. Results show that the sorption of hydrogen from a gas mixture within the reactor occurs quite nonuniformly. In the reactor, it is possible to identify three characteristic areas. The first area lies near the cooled wall, where hydrogen sorption occurs in a rather thin layer in flow direction (in the front) in which the partial pressure of hydrogen changes from a value close to the partial pressure at the entrance (pressure drop due to the flow of the gas mixture should be considered) to the equilibrium pressure at some temperature at the front. This layer moves downward during the process of saturating the bed with hydrogen. The second area lies on the reactor axis. Hydrogen sorption in this area also occurs in a rather thin layer and is of the same type as the sorption at the front. The velocity of this front is lower than its value near a wall because removing heat from the centre of the bed is difficult. This part of the bed has a higher temperature, which leads to a reduction in the sorption intensity and an increase of the hydrogen concentration in the gas phase behind the front. The direction of the additional hydrogen flow in the intermediate area is from the area behind the first front to the area before the second front. The rather complicated map of the hydrogen concentration is formed. As a result, only part of the metal hydride alloy in the reactor is used effectively, and specific characteristics of the system under consideration (per unit mass or per unit volume) are reduced. It should also be noted that a decrease in the concentration of hydrogen in the gas phase leads to an abrupt decrease in the effective heat conductivity of the bed and a decrease in the intensity of the heat transfer. The strong dependence of equilibrium pressure on temperature makes the optimisation of the heat transfer in reactors a critical point in their design.

In the work by Fujisawa, Miura, Mitsutake, and Monde [14], a numerical model of hydrogen purification in a flow-type metal hydride reactor was developed. In Refs. [14], a hydrogen purification experiment was carried out with two types of metal hydride containers differing in size. The experimental results were compared with the calculation results obtained with the proposed numerical analysis model. A good agreement was obtained. However, the authors only compared integral characteristics of the purification system (hydrogen concentration in/off gas and differential pressure in a metal hydride packed bed) and did not describe the processes inside the reactor or their influence on the integral characteristics of the purification system.

The main goal of the present paper is a systematic study of the thermal behaviour of the reactor during the purification process and the determination of the main factors determining its effectiveness.

Mathematical model

In this work, a mathematical model, which was previously developed to analyse the processes in metal hydride systems for hydrogen storage and purification [17,18], was used. The model is similar to models used by other authors (see, e. g. Refs. [19,20]), but unlike those models, it takes into account the presence of unabsorbed gas in the gaseous phase. This is important because effective thermal conductivity strongly depends on the composition of the gas mixture. To account for the presence of a metal foam in a metal hydride bed, in Ref. [18] the mathematical model was modified by analogy with [9,10]. In these papers, one [9] and two-dimensional [10] models were used to study the effect of the impact of different characteristics of aluminium foam and reactors on the performance of hydrogen storage systems.

The mathematical model includes a set of three-dimensional nonsteady-state equations for the conservation of mass and energy for the solid phase, an energy conservation equation for the gas phase, mass conservation equations for the components, and a momentum equation for the gas phase. In these equations, it was assumed: the gas phase is a homogeneous mixture of N components, one of which is hydrogen; the solid phase is motionless; the change in volume of the solid phase over the course of sorption was not considered; the thermodynamic properties of the gas phase correspond to the equation of state for an ideal gas; the isobaric heat capacities of the gas mixture components are constant values; the work of compression and viscous dissipation in the gas phase are negligible. The differential equations for the mathematical model in the Cartesian coordinate system are written as follows:

For the solid phase:

Mass conservation equation

$$(1-\varepsilon_{MH})\varepsilon_{Al}\rho^0_{s,MH}\frac{d\overline{X}}{dt}=\frac{M_{MH}}{M_H}\dot{m}. \tag{1}$$

Energy conservation equation

$$\left(\rho^0_{s,MH}c_{p,s,MH}\cdot(1-\varepsilon_{MH})\cdot\varepsilon_{Al}+\rho^0_{s,Al}c_{p,s,Al}\cdot(1-\varepsilon_{Al})\right)\frac{\partial T_s}{\partial t}= \\ =\nabla\left[(1-\varepsilon_{MH}\cdot\varepsilon_{Al})\lambda^*_s\nabla T_s\right]+\alpha_{sg}A_{sg}\left(T_g-T_s\right)+\dot{m}\Delta H_{sg}. \tag{2}$$

For the gas phase:

Mass conservation equation for the jth component

$$\frac{\partial}{\partial t}\left(\varepsilon_{MH}\varepsilon_{Al}\rho^0_g x_j\right)+\nabla\cdot\left(\varepsilon_{MH}\varepsilon_{Al}\rho^0_g\overrightarrow{w}_g x_j-\varepsilon_{MH}\varepsilon_{Al}\rho^0_g D^*_j\nabla x_j\right)=-\dot{m}_j x_j, j=1\ldots N \\ \dot{m}_1=\dot{m}(\text{hydrogen}),\dot{m}_j=0, j\neq 1(\text{impurity gases}); \tag{3}$$

Projection of the momentum conservation equation onto the i-axis