ARTICLE IN PRESS

INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2016) 1–7

Available online at www.sciencedirect.com

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journal homepage: www.elsevier.com/locate/he

Thermal effect and flow-through cooling of an adsorptive hydrogen delivery tank

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ARTICLE INFO

Article history:
Received 23 January 2016
Received in revised form
24 March 2016
Accepted 29 April 2016
Available online xxx

Keywords:
Hydrogen delivery
Thermal effect
Flow-through cooling
Adsorption
Simulation

ABSTRACT

The effective hydrogen storage technology is one of the most difficult challenges for the application of hydrogen energy, and activated carbon adsorption hydrogen storage has been considered as one of the promising storage methods. The thermal effect during adsorption process has a great influence on the hydrogen storage capacity. In this paper, based on a large-scale hydrogen delivery tank whose volume is 51.4 m^3, we establish a two-dimensional axisymmetric model in Comsol. Then we research and simulate the thermal effect during the adsorption process under different charging conditions, and the effects of charging flow rate, pre-cooling and flow-through cooling on filling process are discussed respectively. The rates of feeding hydrogen and the effect of pre-cooling during the flow-through cooling process have been taken into consideration in order to improve the efficiency of hydrogen delivery tank packed with adsorbent material. The results show that the flow-through cooling combined with pre-cooling is an effective way to transfer the heat generated during adsorption process and increase the hydrogen storage capacity of the system.

Introduction

The effective hydrogen storage technology is one of the most difficult challenges for the application of hydrogen energy. There are four hydrogen storage methods, including compressed hydrogen storage, liquid hydrogen storage, chemical hydrogen storage and physisorption hydrogen storage. It is a common mode to bring a large amount of hydrogen from production site to final user by large-scale delivery tank for short distance transportation. And the methods of compressed hydrogen storage and liquefied hydrogen storage are frequently used in delivery tank. Zheng and co-works described a number of significant points of high pressure hydrogen safety, which included hydrogen embrittlement of metals, temperature rise during fast filling process, and some potential risks [1]. There are many factors affecting the temperature variation in hydrogen tank during fast filling. A series of experiments and numerical models have been

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http://dx.doi.org/10.1016/j.ijhydene.2016.04.242
0360-3199/

Please cite this article in press as: Tong L, et al., Thermal effect and flow-through cooling of an adsorptive hydrogen delivery tank, International Journal of Hydrogen Energy (2016), http://dx.doi.org/10.1016/j.ijhydene.2016.04.242

Nomenclature

ΔH	isosteric heat of adsorption, J/mol
c_{pg}	specific heat capacity of gaseous hydrogen, J/kg/K
c_{ps}	specific heat capacity of adsorbent, J/kg/K
c_{pa}	specific heat capacity of adsorbed hydrogen, J/kg/K
k_{eff}	effective thermal conductivity of activated carbon bed, W/m/K
k_s	thermal conductivity of adsorbent, W/m/K
k_g	thermal conductivity of gaseous hydrogen, W/m/K
M_{H_2}	molecular mass of hydrogen, kg/mol
n_a	absolute adsorption amount per unit adsorbent, mol/kg
n_{max}	limiting adsorption amount per unit adsorbent, mol/kg
Q	heat source term, W/m^3
Q_a	adsorption heat term, W/m^3
Q_p	pressure work term, W/m^3
R	universal gas constant, J/mol/K
T	temperature, K
$\vec{v}$	Darcy velocity vector, m/s
μ	dynamic viscosity of hydrogen, Pa s

Greek symbols

α	enthalpic factor, J/mol
β	entropic factor, J/mol/K
γ	volume expansion coefficient, 1/κ
ε_b	activated carbon bed porosity
κ	permeability, m^2
ρ_g	density of hydrogen gas, kg/m^3
ρ_b	density of activated carbon bed, kg/m^3
ρ_p	density of activated carbon particle, kg/m^3

performed for investigating such factors in recent years [2–6]. Compared with high pressure gaseous hydrogen delivery, liquid hydrogen delivery consumes more energy used for liquefying hydrogen, and the hydrogen delivery tank should be well insulated in order to maintain it under low temperatures. It is an effective way to decrease the pressure in hydrogen delivery tank with the help of chemical or physical adsorptive materials. A hydrogen delivery system based on liquid organic hydrides is taken into account, and the economic analysis of progress is carried out in detail [7].

The method of physical adsorption is attractive for hydrogen storage, and activated carbon adsorption hydrogen storage has been considered as one of the promising storage methods. In order to find an effective and economical way of storing hydrogen, an ideal material with high hydrogen storage capacity should be given higher priority [8]. Previous research has shown that the hydrogen adsorption capacity can increase by Ni-modified materials [9]. The effect of each parameter during the feeding process should be taken into consideration and understood carefully in order to maintain safety and to improve the efficiency of hydrogen storage. Petitpas et al. have described the cryo-compression and cryo-adsorption hydrogen storage methods respectively, and performed a comparative analysis of them [10]. The authors of this paper established a variety of models based on different software, simulated the hydrogen storage based on activated carbon, and compared the simulation results with experiment data. The results shown the models were valid under different experiment environment since the simulation agreed well with the experiments [11–14]. In order to achieve the DOE2017 targets, Corgnale et al. adopted a new approach based on cooling concept to decrease the temperature of feeding hydrogen, so as to provide a proper environment for the adsorbent bed [15]. Based on validated model of 2.5 L hydrogen storage tank, Ubaid et al. built flow-through model and predicted the hydrogen storage process of a large bulk reservoir filled with MOF-5 [16]. Utz et al. fabricated a lab-scale hydrogen storage tank packed with sodium alanate, and their results showed that there was a significant influence on temperature near the inlet area with flow-through mode [17].

The heat generated during filling process can induce temperature rise in the delivery tank, which is not good for hydrogen storage. It is important to research the challenge and take effective measures to solve the thermal effects and improve hydrogen storage capacity. In our previous works, a similar two-dimensional axisymmetric model was implemented in Comsol, and was validated by experiments [12,14]. Considering the direct experiment using a volume of 51.4 m^3 tank is unreasonable, the validated model of lab-scale hydrogen storage tank can be extended and enlarged to research thermal effect of large-scale delivery tank. And then, based on mass, momentum and energy conservation equations of the large-scale hydrogen delivery tank, a receivable model is established in the same way. The rates of hydrogen filling, the pre-cooling and the flow-through cooling have been taken into consideration in order to improve the efficiency of hydrogen delivery tank packed with adsorbent material.

Governing equations for hydrogen storage system

The mass, momentum, energy conservation equations and the modified Dubinin-Astakov isotherm are performed in this model by Comsol. The simulation results of a similar finite element model are in agreement with experiments in small hydrogen storage tank, and the introduction of governing equations are detailed in previous work [12,14].

Mass and momentum conservation equation

The mass and momentum conservation equation in porous media can be expressed as [12,14]:

$$\frac{\partial}{\partial t}\left(\varepsilon_b \rho_g\right) + \nabla\cdot\left(\rho_g\left(-\frac{\kappa}{\mu}\nabla p\right)\right) = -(1-\varepsilon_b)\rho_p M_{H_2}\frac{\partial n_a}{\partial t} \tag{1}$$

where ε_b is the bed porosity, ρ_g(kg/m^3) is the gaseous hydrogen density, κ (m^2) is the permeability, μ(Pa s) is the dynamic viscosity of hydrogen, and ∇p(Pa/m) is the pressure gradient. The right hand side of equation is the mass source term. ρ_p is the particle density of adsorbent, M_{H_2} is the molecular mass of hydrogen, and n_a is the absolute adsorption amount per unit adsorbent.

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