International Journal of Hydrogen Energy
Volume 43, Issue 29, 19 July 2018, Pages 13356-13372

Design of a large-scale metal hydride based hydrogen storage reactor: Simulation and heat transfer optimization

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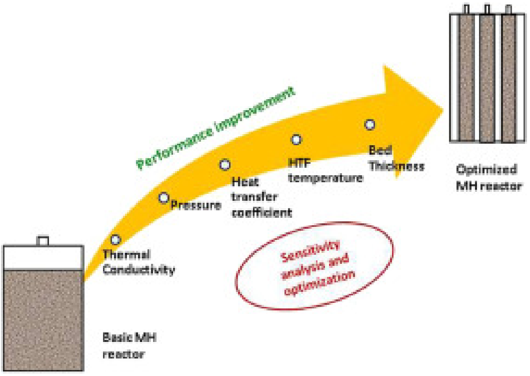
Received 1 February 2018, Revised 12 May 2018, Accepted 14 May 2018, Available online 5 June 2018, Version of Record 4 July 2018.

https://doi.org/10.1016/j.ijhydene.2018.05.084

Abstract

An optimized design for a 210 kg alloy, Ti—Mn alloy based hydrogen storage system for stationary application is presented. A majority of the studies on metal hydride hydrogen systems reported in literature are based on system scale less than 10 kg, leaving questions on the design and performance of large-scale systems unanswered. On the basis of sensitivity to various design and operating parameters such as thermal conductivity, porosity, heat transfer coefficient etc., a comprehensive design methodology is suggested. Following a series of performance analyses, a multi-tubular shell and tube type storage system is selected for the present application which completes the absorption process in 900 s and the desorption process in 2000 s at a system gravimetric capacity of 0.7% which is a vast improvement over similar studies. Th[illegible] also indicates that after fifty percent reaction completion, heat transfer ceases to be the major contr[illegible] factor in the reaction. This could help prevent over-designing systems on the basis of heat transfer, a[illegible] ensure optimum system weight.

Graphical abstract



Introduction

Metal hydrides are a favorable hydrogen storage alternative offering safe and efficient storage. Hydrogen reacting with a metal or metal alloy, forms a metal hydride, and thus gets stored in solid state. Of the various metal hydrides, AB_2 type Ti-based metal hydrides have a promising potential because of their comparatively high hydrogen storage capacity, fuel cell friendly operating temperatures and pressures, and good reversibility [1]. However, the storage of hydrogen in metal hydrides is primarily limited by heat transfer associated with the reaction. While the absorption reaction is accompanied by release of heat which needs to be removed from the system; for desorption to occur heat needs to be supplied to the system. This reaction heat has a great bearing upon the system performance as it controls the MH bed temperature which in turn controls the equilibrium pressure. The rate of absorption/desorption of hydrogen is a function of the equilibrium pressure. If the equilibrium pressure is higher than the supply pressure of hydrogen the absorption reaction will cease. Similarly if the equilibrium pressure is lower than the discharge pressure of hydrogen desorption reaction will be stalled. Therefore, heat transfer to/from the MH bed is an important factor for ensuring efficient hydrogen storage.

Multiple studies have addressed the issue of heat transfer in metal hydride based hydrogen storage. Studies have suggested various designs for hydrogen storage systems to facilitate effective heat transfer. These designs are as diverse as the heat transfer enhancements themselves and include addition of fins, cooling tubes, cooling coils etc. Attempts have been made to improve thermal conductivity of the MH bed by addition of foam and ENG (expanded natural graphite) [2], [3], [4], [5], [6], [7], [8], [9], [10], improve heat transfer area by addition of fins and cooling tubes [11], [12], [13], [14], [15], [16], [17], [18], [19]. More recently, combinations of these techniques have been employed, yielding favorable results. Garrison et al. studied the effect of a concentric cooling tubes equipped with a) transverse fins b) longitudinal fins on a sodium alanate system [20]. The results pointed to a configuration involving multiple cooling tubes at small distances as the most viable. Ferekh et al. compared the performance of metal fins versus metal foam and found that metal foam based design was superior to the fin based design [10]. Helical coil based hea exchangers have also been shown to improve system performances by reducing charging/dischargin significantly [21], [22], [23], [24]. A comparative study involving finned cooling tube reactor, helical coil reactor and shell-tube type reactor was performed by Raju et al. Working with sodium alanate, for a filling time of 10.5 min they found that the helical coiled heat exchanger gave better volumetric and gravimetric densities over the other designs [25]. Mazzucco et al. studied three different heat exchanger configurations:

a) metal hydrides with embedded cooling tubes b) metal hydrides tubes surrounded by heat transfer fluid in annular space and c) metal hydride tubes in a heat transfer fluid shell [26]. Their results indicated that the last configuration was of most significant interest for storage applications.

Clearly, there is no dearth of studies on design of metal hydride hydrogen storage systems but the studies on large scale systems are far less than those on small-scale systems [27]. Further investigation of large-scale practical systems is important keeping in view the issues that are unique to these systems such as creation of hot spots (pockets of extremely high temperature where heat transfer enhancements may not be able to reach), parasitic system weight, volumetric efficiency etc. More importantly, the design methodology for large-scale systems is also unclear. While every heat transfer enhancement results in improved system performance, it also leads to reduced gravimetric and volumetric capacities. Therefore, the question of which heat transfer enhancements should be preferred is very significant. In this study an attempt is made to present a unified design policy which can serve as a road-map for the design of such systems. Using a 100 kWh Ti—Mn based (Hydralloy C5) hydrogen storage system as an example, the most important parameters that affect the system performance are studied and a procedure outlined to serve as a tool for the design of future systems. The gravimetric capacities of the final designs are compared to ensure that there is a healthy trade-off between system performance and weight.

Section snippets

Design objective

The objective of this exercise is to design an optimized Ti based, 100 kWh metal hydride hydrogen storage system for stationary applications and to outline a design methodology for the same. The considerations governing the design process have been outlined in Table 1. To begin with, the volume required to store the metal alloy powder was evaluated on the basis of the mass of alloy required to store the hydrogen and the density of the alloy ($5500 kg/m^3$) [1], [28]. Assuming a porosity of 0.5,…

Mathematical modeling

The reactor of the said dimensions was first simulated under free convection conditions and its performance was analyzed. The system was modeled as a 2-d axisymmetric domain. To model the MH hydrogen storage system, mass, momentum and energy conservation equations are used.

The following assumptions have been used for modeling the system:

1) The solid and gas are at the same temperature (local thermal equilibrium).…

2) Gas phase: hydrogen behaves as an ideal gas.…

3) Solid phase: MH is isotropic and has…

…

Results and discussions

The baseline mathematical model discussed in section Conservation of momentum is based upon the above governing equations and developed in COMSOL 5.2. The basic cylindrical reactor of radius 15.24cm and height 1.256m was simulated operating at a pressure of 25bar and a temperature of 298K under free convection, exposed to air at 298K. Ordinarily, in the design of any heat exchanger, if the heat load is known, starting with an initial value of heat transfer coefficient, the area of the...

Conclusions

On the basis of sensitivity to different design and operating parameters such as porosity, thermal conductivity, pressure etc., the performance of a large-scale 210kg Ti—Mn based MH hydrogen storage system was analyzed. It was noted that the performance was most sensitive to changes in thermal conductivity and pressure. With this as starting point an improvised design was suggested. As a result of the series of studies involving different heat exchange configurations, a design procedure was...

Acknowledgement

The authors are thankful to Prof. Suneet Singh, Department of Energy Science and Engineering, IIT Bombay for providing us the computational facility and Indian Space Research Organisation for financially supporting the research vide project code 16ISROC001. The authors would also like to thank Prof. P. Muthukumar for helpful discussions....

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Citation Excerpt :

…In the hot fluid temperature range of 60–80 °C, discharge rates of 12–75 SLPM were demonstrated. Afzal and Sharma [20] proposed an industrial-scale hydrogen storage reactor (210 kg Ti–Mn alloy) with a tube bundle layout based on simulation outcomes. The proposed multi-tubular storage unit was predicted to attain 80% storage capacity within 900 s. Jana and Muthukumar [21] proposed a tube bundle reactor configuration comprising 19 MH tubes for macro-scale hydrogen storage.…

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