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Efficient hydrogen storage in up-scale metal hydride tanks as possible metal hydride compression agents equipped with aluminium extended surfaces

Evangelos I. Gkanas [a,b,*], *David M. Grant* [a], *Martin Khzouz* [a,b], *Alastair D. Stuart* [a], *Kandavel Manickam* [a], *Gavin S. Walker* [a]

[a] *Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, Nottingham, NG7 2RD, UK*
[b] *School of Mechanical, Aerospace and Automotive Engineering, Faculty of Engineering, Environment and Computing, Coventry University, Gulson Road, Coventry, CV1 2JH, UK*

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ABSTRACT

In the current work, a three-dimensional computational study regarding coupled heat and mass transfer during both the hydrogenation and dehydrogenation process in up-scale cylindrical metal hydride reactors is presented, analysed and optimized. Three different heat management scenarios were examined at the degree to which they provide improved system performance. The three scenarios were: 1) plain embedded cooling/heating tubes, 2) transverse finned tubes and 3) longitudinal finned tubes. A detailed optimization study was presented leading to the selection of the optimized geometries. In addition, two different types of hydrides, $LaNi_5$ and an AB_2-type intermetallic were studied as possible candidate materials for using as the first stage alloys in a two-stage metal hydride hydrogen compression system. As extracted from the above results, it is clear that the case of using a vessel equipped with 16 longitudinal finned tubes is the most efficient way to enhance the hydrogenation kinetics when using both $LaNi_5$ and the AB_2-alloy as the hydride agents. When using $LaNi_5$ as the operating hydride the case of the vessel equipped with 60 embedded cooling tubes presents the same kinetic behaviour with the case of the vessel equipped with 12 longitudinal finned tubes, so in that way, by using extended surfaces to enhance the heat exchange can reduce the total number of tubes from 60 to 12. For the case of using the AB_2-type material as the operating hydride the performance of the extended surfaces is more dominant and effective compared to the case of using the embedded tubes, especially for the case of the longitudinal extended surfaces.

* *Corresponding author.*
E-mail address: ac1029@coventry.ac.uk (E.I. Gkanas).
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Introduction

Hydrogen is a promising alternative energy carrier that could potentially facilitate the transition from fossil fuels to sources of green energy due to its high energy density (141 MJ/kg), variety of potential sources and low environmental impact [1]. Hydrogen can be stored as a high pressure gas or low temperature liquid or alternately, it can, by undergoing a chemical reaction, be stored in solid form metal hydrides or cryo-adsorbents [2,3]. Issues associated with hydrogen storage materials are the storage capacity, the thermal stability of the hydride, the kinetics of hydrogenation and dehydrogenation, thermophysical properties and crystal structures. Specifically fast reaction kinetics and high hydrogen storage capacity are the most important properties of the alloys used in thermal devices [4], compression systems [5–12] and heat pumps [13,14]. Generally the limiting factor controlling the hydrogen charging/discharging in a metal hydride reactor is the rate at which heat can be transferred between the hydride and the reactor. Due to the exothermic nature of the hydrogenation process, large amounts of heat are produced inside the reactor, forcing the equilibrium pressure to increase and subsequently lowering the driving force for the hydrogen storage. On the other hand, providing heat and consequently lowering the internal pressure is necessary for the dehydrogenation process to take place. The thermal management of a metal hydride reactor must take into account both the cooling during the hydrogenation process heating during the dehydrogenation process. Two active heat management techniques can be employed to accomplish this, internal heat management and external heat transfer [15,16]. Heat exchangers are used in many industrial applications the most widely used being those intended to exchange heat between two fluids. Less attention has been given to the design of heat exchangers involving the heat flow between a stationary reacting metal hydride powder and a cooling/heating fluid as required in the field of solid state hydrogen storage.

Despite many efforts dedicated to enhancing the rate of the external heat transfer, the performance of the metal hydride systems is still limited [17]. Therefore, internal heat transfer enhancements have become more attractive and can roughly divided in two ways: 1) Enhancement of the thermal conductivity of the metal hydride powder by insertion of aluminium foam [18–20], copper wire net structure [21] or by creating metal hydride compacts [22–25], 2) Integration of heat exchangers inside the bed such as embedded heat exchanger tubes [26–28], finned tube heat exchangers [29–33], spiral heat exchangers [34,35] or heat pipes [36].

In a previous work [37], the authors described the simulation study of the operation of a two-stage metal hydride hydrogen compression system and studied the combination of different materials. The heat management process of the reactors for that study did not go any further than the fact that external heating/cooling jackets used for all the reactors, as the main focus of the study was the understanding the operation of the coupled compressor stages. In the current work, three different heat management scenarios are studied numerically using Finite Element Analysis software COMSOL Multiphysics 4.4 in order to decide which scenario, if incorporated into an up-scale metal hydride tank, will result in the most efficient operation of the compression system. The first scenario involves the use of a differing number of plain cooling/heating tubes embedded in the reactor. The second scenario includes transverse Al surfaces extending from the cooling/heating tubes and the third scenario deals with longitudinal Al extended surfaces. For each scenario, a two dimensional study was conducted to optimise the number of cooling/heating tubes, diameter of the tubes (scenario 1), number of heating/cooling tubes, number of Al fins and fin thickness (scenarios 2 and 3). The optimised geometry was then modelled in 3D. In this study a novel AB_2-based intermetallic is introduced, validated and simulated under three different heat management scenarios for both the hydrogenation and dehydrogenation process. Furthermore, the results are compared with the performance of $LaNi_5$ in order to suggest a potential candidate material for the first stage of a multistage metal hydride hydrogen compression system. The results showed that the presence of the Al fins can reduce both the hydrogenation and dehydrogenation time and in terms of charging time, 60 cooling tubes may be replaced with only 12 or 16 finned tubes with faster kinetics. The effect on reactor performance was also compared using two different first stage storage materials. The first material was $LaNi_5$ and the second material was a Laves-phase AB_2 Ti–Zr based intermetallic.

Methodology

In the current numerical work the reactor performance was modelled by the simultaneous use of COMSOL Multiphysics chemical reactions, to implement the reaction of hydrogen with the metal hydride, and heat transfer in solids, for the heat transfer through the hydride bed and heat exchange components. Prior to conducting these simulations the performance of the model was validated using experimental results extracted from a lab-scale Sievert's type apparatus. After the validation process, the optimization study of the three scenarios was performed. For scenario 1, the impact of the number of cooling/heating tubes was explored by modelling the reactor performance using 18, 24, 30, 36, 48 and 60 heat exchange tubes. For scenarios 2 and 3, three different parameters were optimised i.e., the radius, number and thickness of the fins. For all three scenarios, the radius of the heating/cooling tubes was selected at 3.2 mm corresponding to a commercial available ¼ inch stainless steel tube. The expansion of packed beds during the hydrogenation process can produce additional stress on the vessel wall, therefore for the purpose of the model, the reactors are assumed to be filled to 50% at the beginning of the hydrogenation process. Table 1 presents all the details about the optimization parameters studied in the current model.

Model assumptions

A number of assumptions were made which serve to simplify the modelling process. These were:

a) Initially the temperature and pressure profiles are uniform.