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## Performance simulation and experimental confirmation of a mini-channel metal hydrides reactor



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#### ABSTRACT

A theoretical and experimental study about a proposed mini-channel reactor was carried out to enhance heat transfer performance for metal hydrides applications, such as hydrogen storage, hydrogen compression and chemical heat pumps. The configuration of the reactor and working principles are described in detail. The predicted hydride bed temperature profiles in the reactor are compared with the experimental data from the performance test system, and a reasonable agreement is observed. The simulation of the hydrogen adsorption and desorption processes in a mini-channel reactor packed with LaNi<sub>5</sub> is conducted, and the influences of some important parameters, e.g. the bed thickness, the number of the mini-channels, hydrogen supply and discharge pressure are analyzed. Comparing with the traditional reactors, such as tubular reactor and disc reactor, the mini-channel reactor has some obvious advantages, therefore can be recommended for applications.

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#### 1. Introduction

Metal hydrides can be applied in many industrial applications, such as hydrogen storage [1–3], thermal sorption compressors and chemical heat pumps. The main features of metal hydrides include the generation of a large amount of heat during adsorption or desorption, high volumetric density for hydrogen storage and the reversibility of the reactive process. Conventional metal hydrides are commercially available and are much safer than compressed hydrogen for hydrogen storage [4], as evidenced by their application in fuel-cell-

powered mining locomotives [5]. Although metal hydrides have many merits, they also have several shortcomings. A serious drawback is associated with low hydriding and dehydriding rates, which are limited in great extent by the thermal properties of metal hydrides materials. Hydriding processes of the metal and hydrogen release large amounts of heat, which is usually expressed as the heat of reaction. If the heat is not removed efficiently, the resulting temperature rise can be so large that the processes will stall. Furthermore, metal hydrides may sinter at high temperatures and lose hydrogen storage capacity. The dehydriding process requires

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heating at a specific temperature to proceed. Without sufficient heat supply, the release of hydrogen will cease because of the reduced temperature in the hydride bed. Therefore, enhanced internal heat transfer is essential to improve system performance and to maintain system reliability [6]. Many researchers have carried out numerous studies on this theme. Muthukumar et al. [7,8] studied the influences of the operating and configuration parameters on the hydrogen compressor system performance. As a result of studying the compression efficiency of the Ti<sub>0.98</sub>Zr<sub>0.02</sub>V<sub>0.43</sub>Fe<sub>0.09</sub>Cr<sub>0.05</sub>Mn<sub>1.5</sub> based thermal compressor, a relationship between the cooling and heating temperatures for the optimal operation was recommended [7]. In addition, they also pointed out that the reactor's hydrogen adsorption limitation depends on the cooling temperature [8]. Furthermore, they proposed several types of hydrogen storage units, which were used to evaluate the system performance. These hydrogen storage units were different both in the type of hydride materials employed (with materials tailored either for low temperature applications, or for room temperature use), and in the design of the container [9]. The latter is known to be the crucial factor for the capacity of adding or removing heat from the hydride bed, a feature ultimately determines the charging/discharging rates. Unless the heat released during hydriding (or absorbed during dehydriding) is rapidly transferred to or from the environment, there is a significant increase of temperature during charging or a decrease during discharging. This may result in slowing down of the process, and limit the usable storage capacity of the container. These considerations clearly show the importance of heat management features in manufacturing the storage container. A common solution to this problem is to add conductive powders (Mg or Cu) to the low conducting hydride materials [10], or to use Al foam and/or metallic conductive matrices to accelerate the internal heat flow [11]. Other solutions include packing MH materials in a multilayer waved sheet structure, microencapsulated metal hydride compact [12], compacting metal hydride powder with expanded graphite [12,13], using thermostat water jackets, or introducing an internal coaxial inner U-shaped tube, through which cooling water or heating agent can be circulated during charging or discharging [14]. Mohan et al. [15] investigated a novel device, which consists of many filters to distribute hydrogen gas and heat exchanger tubes to cool or heat the hydride bed. The results showed that the device has a faster reaction rate than other traditional reactors. However, the enhancement of heat transfer by the above techniques is still limited. Consequently, developing a reactor to remove heat from the hydride bed efficiently is still a very interesting topic for researchers.

Mini-channel heat sinks are beneficial in thermal and chemical process engineering applications, especially when large heat transfer rates and small sizes of the devices are needed. Since the early work of Tuckerman et al. [16], the mini-channel heat sink has been studied and tested as an efficient and compact cooling scheme in microelectronics cooling applications. It was shown that a thermal resistance was controllable for mini-channel heat sinks, which was substantially lower than the conventional heat sinks. There are many experimental studies in the literatures, such as those by Tuckerman et al. [16], Missaggia et al. [17], Kleiner et al. [18], and also some numerical studies by Samalam [19] and Weisberg et al. [20]. Design factors that have been studied include coolant selection (air [18] and liquid coolant [20]), inclusion of phase change (one phase or two phases by Visaria and Mudawar [21]), Khan et al. [22], Revellin and Thome [23] and structural optimization by Knight et al. [24]. From the above investigations, we know that the mini-channel heat sink possesses many unique attributes that are ideally suited for intensive heat transfer, and local hot spots in the device surface can be effectively avoided.

The work introduced in this article is an extension of the recent efforts by the authors [25–27] to realize efficient heat and mass transfer in the metal hydride reactor. The configuration and working principles of the new prototype of minichannel reactor, which is proposed by us to this end, are described in detail. The experimental test system of the reactor performance was set up, and the temperatures at different positions of the reactive bed were measured. Numerical simulation was performed for hydrogen sorption and desorption processes using commercial software COMSOL MULTIPHYSICS 3.5a. The simulation results were confirmed by the experimental data, and optimization issues for design parameters were addressed as well. The results indicated that this mini-channel reactor shows higher rates of hydrogen sorption and desorption than conventional metal hydride reactors. Also discussed in this paper were various unique features about the reactor's temperature and reactive fraction distribution during the reactive process. Some factors were discussed about their influences on the reactor performance, and the trend of the reactor development was also pointed out.

## 2. Configuration and working principles of the reactor

#### 2.1. Description of the reactor's configuration

The proposed mini-channel metal hydride reactor is shown in Fig. 1. The device contains many mini-channels spaced uniformly inside a rectangular shell. Metal hydrides material



Fig. 1 – Internal configuration of the reactor.

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