Design Optimization of Metal Hydride-Based Hydrogen Storage Reactor Using Fin Efficiency Concept

K Venkata Krishna, Praveen Kumar Kanti, M P Maiya

***Abstract*— The hydrogenation of metal hydrides (MHs) is a heat-driven mass transfer process. Hence, its rate is determined by the heat transfer rate from the MH reactor. A heat transfer system (HTS) with fins and a cooling tube is one such method to enhance heat transfer. The fin efficiency (FE), hitherto not researched for unsteady processes like the present one, is required for the optimization of the reactor. The present numerical study proposes a new technique to estimate the FE from the temporal temperature profiles in the MH reactor. The effects of fin thickness (FT) and shape are studied. The former is varied from 1 to 7 mm, and the latter is changed to 3 different tapered cross-sections. The FE increases with FT but has a minimal effect after 4 mm, while the fin tapering is found to have no significant influence. A performance evaluation parameter (PEP) is presented to optimize the fin thickness and shape.**

***Keywords*— Fin efficiency, Heat transfer, Hydrogen storage, Metal hydride**

I. INTRODUCTION

Hydrogen is one of the potential fuels that could meet the global energy need without producing any pollutants. However, its low density makes storage and utilization inefficient. Conventional storage methods, such as gaseous and liquid storage technologies, pose safety and cost considerations. Solid-state storage using MHs is an effective alternative with higher volumetric density than conventional methods at moderate temperatures and pressures. However, the poor thermal conductivity of MH limits heat transfer during the exothermic hydrogen absorption process. Heat transfer from the MH must be enhanced to reduce hydrogen absorption time.

Heat transfer from the MH can be improved by increasing the thermal conductivity or adding a heat transfer system (HTS). The thermal conductivity of the MH bed increases by adding copper wire structures [1], metal foam [2,3], metal compacts [4], etc. Employing an HTS to MH is much easier and requires less maintenance than thermal conductivity enhancements. HTSs generally consist of only simple tubes (straight or spiral) or a combination of fin and tubes. Adding fins to tubes greatly enhances heat transfer by improving the surface area [5]. So far, various shapes of fins, such as rectangular [6], circular [7], conical [8], corrugated [9], multilayer [10], tree-shaped [11], and leaf vein [12], etc., are used with tubes for heat transfer enhancement. Some studies proposed novel HTS designs for better performance [13–15]. However, most studies optimized the HTS by considering only hydrogen absorption/desorption time. In addition to time, few studies considered weight ratio (weight alloy to the container) [16], energy efficiency [17], and gravimetric exergy output rate [18,19] as the parameters to optimize the design conditions. However, these are unrelated to heat transfer between MH and HTS. A parameter based on heat transfer between MH and HTS needs to be evaluated to optimize the MH reactor design.

While research studies on optimizing the fin configurations in MH reactors are available in the literature but are based mostly on the time-based indirect method, the present study proposes a direct method based on the fin efficiency (FE) technique. 2D numerical simulations are conducted using COMSOL Multiphysics 5.6 on a rectangular element from a circular finned tube MH reactor. The FE is computed using the temporal temperature profiles of the simulation data. A performance evaluation index (PEP) is proposed by considering the FE, H_2 absorption quantity, and system weight to optimize fin thickness and shape.

II. MODEL DESCRIPTION

A cylindrical reactor with radial circular fins (Fig.1 a and b) is used to enhance the heat transfer from the $LaNi_5$-based MH reactor. A 2D single unit of fin surrounded by MH (Fig. 1c) is considered the computational domain by assuming there is no temperature variation along the length of the reactor. Fig. 2 represents the boundary conditions used for the simulations. The current study aims to optimize fin structural parameters such as fin thickness and shape using the FE. Due to internal heat generation in the MH bed, the temperature varies along the reactor length with time. As a result, calculating FE in the current situation is challenging. Hence, the complexity of the model is simplified using the following assumptions.

- Heat transfer occurs only from the fin base; all other boundaries are adiabatic.
- Fin base temperature (T_b) is constant with time.
- Convection and radiation heat transfer are negligible.
- The thermal contact resistance between the fin and MH bed is neglected.

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- The heat transfer between the fin and MH bed is directly proportional to their temperature difference.

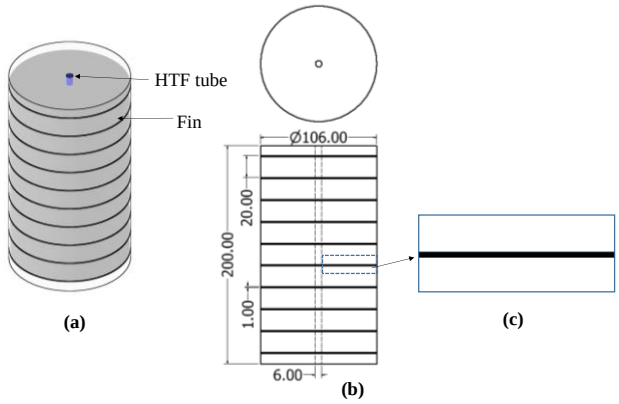

Fig. 1 Schematic of mh reactor (a) isometric view of the design (b) top and side views (c) extended view of a single unit of fin and mh bed

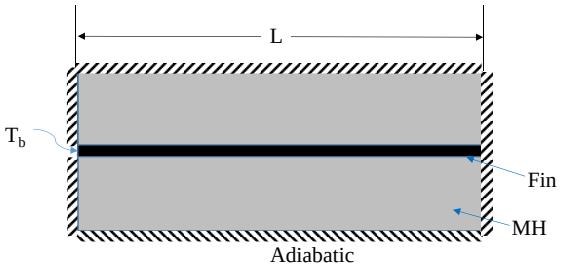

Fig. 2 Simulation model with adiabatic boundary

III. NUMERICAL METHODOLOGY

A finite element method-based package COMSOL 5.6 is used for conducting simulations in the $LaNi_5$ MH bed. The simulation methodology used in the present work to analyze the behavior of hydrogen absorption is the same as that described in the author's previous article [12].

A. Methodology for calculating FE

The present problem involves only conduction heat transfer from MH to fin and fin to fin base. In contrast to the typical fin problem, there is no convection heat transfer, and the MH temperature varies along its length. In the present problem, the actual and maximum heat transfer for calculating FE is determined from the temporal temperature profiles of simulation data. Assuming the heat transfer between the fin and MH is directly proportional to the temperature difference between the fin and MH due to pure conduction. The FE is defined as the ratio of the actual mean temperature difference (MTD) between the MH and fin to the maximum mean temperature difference between MH and fin, i.e., when the fin is at base temperature.

$$FE = \frac{(MTD)_{act}}{(MTD)_{\max}} \tag{1}$$

The MH domain is divided into several elements to obtain a temperature profile. The MTD for an actual case between the fin and MH is calculated using the log mean temperature difference (LMTD) technique as

$$(MTD)_{act} = \frac{\Delta T1 - \Delta T2}{\log\left(\frac{\Delta T1}{\Delta T2}\right)} \tag{2}$$

The calculation of ΔT1 and ΔT2 are represented schematically in Fig. 3.

Similarly, the maximum heat transfer between the fin and MH would exist when the fin is at base temperature. Considering this assumption, the maximum MTD is calculated as

$$(MTD)_{\max} = \frac{\Delta T1_{\max} - \Delta T2_{\max}}{\log\left(\frac{\Delta T1_{\max}}{\Delta T2_{\max}}\right)} \tag{3}$$

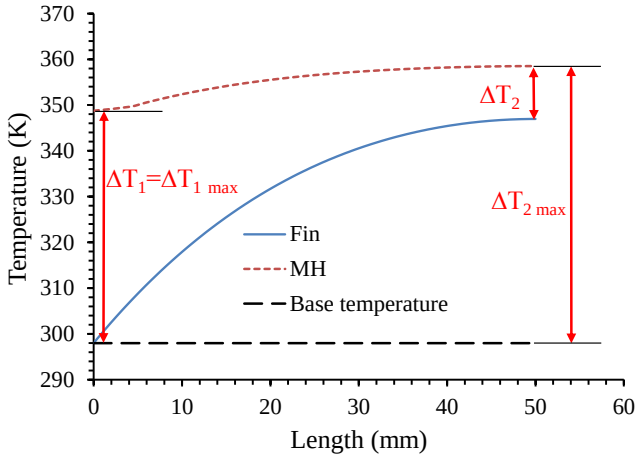

Fig. 3 Schematic of the MH and fin temperature profiles for calculating MTD

IV. RESULTS AND DISCUSSION

A. Validation

The numerical model's accuracy is confirmed by comparing it with the experimental findings of Singh et al. [20] conducted under comparable design and operating conditions. In Fig. 4, the experimental and numerical results are compared. The MH bed's hydrogen absorption behavior and temperature profiles align closely with the experimental data, with a maximum deviation of less than 2%. This affirmation establishes the validity of the numerical model for conducting subsequent simulations.

B. Fin thickness (FT) optimization

Fig. 5 depicts the changes in the time required to achieve 90% saturation and the quantity of H_2 absorption with different fin thicknesses (FTs). The FT is adjusted between 1 to 7 mm while keeping a consistent pitch between fins. It is observed that both the time for H_2 absorption and the absorption quantity decrease as the FT increases. This can be ascribed to the heightened heat transfer associated with larger FT, which takes

up more space, reducing the amount of MH in the reactor and lowering the H_2 absorption quantity.

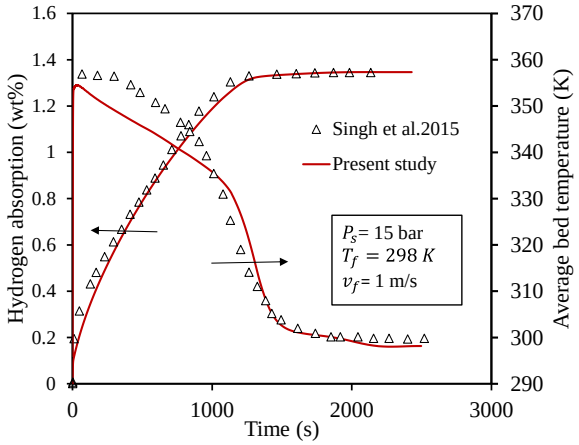

Fig. 4 Comparison of numerical results with experimental results

In the present situation, selecting the FT based solely on absorption time is not feasible because a higher FT may result in a shorter absorption time and reduced hydrogen absorption. For optimal design, it is crucial to balance these two factors. The Fin Efficiency (FE) is initially determined to evaluate heat transfer, and subsequently, a performance parameter is introduced to achieve optimal hydrogen absorption time and quantity.

FE is calculated at each moment using Eq. 1. Fig. 6 illustrates the variation of FE over time for different FTs. It is observed that FE increases over time for each FT, reaching a maximum value and then stabilizing. This phenomenon is attributed to the exothermic heat generation within the MH bed, enabling the fin to transfer more heat and consequently improving FE. Once the exothermic reaction is complete, the availability of heat to the fin no longer impacts FE.

Increasing FT beyond 4 mm has a less significant effect on FE. The maximum FE for each thickness is plotted in Fig. 7. FE is significantly enhanced when the FT is increased from 1 to 4 mm. However, this enhancement is minimal after 3 mm thickness. Increasing FT adds weight and decreases the amount of MH, leading to a decrease in H_2 absorption quantity. To have a balance between FE, H_2 absorption quantity, and total system weight (MH+fin), a parameter known as the performance evaluation parameter (PEP) is defined as

$$PEP = \frac{FE(\%) \times H_2 absorption}{Weight of the system} \quad (4)$$

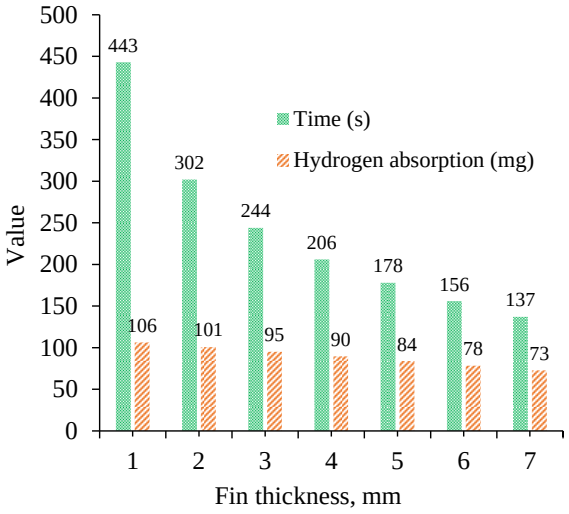

Fig. 5 Time to reach 90% saturation and H_2 absorption quantity with fin thickness

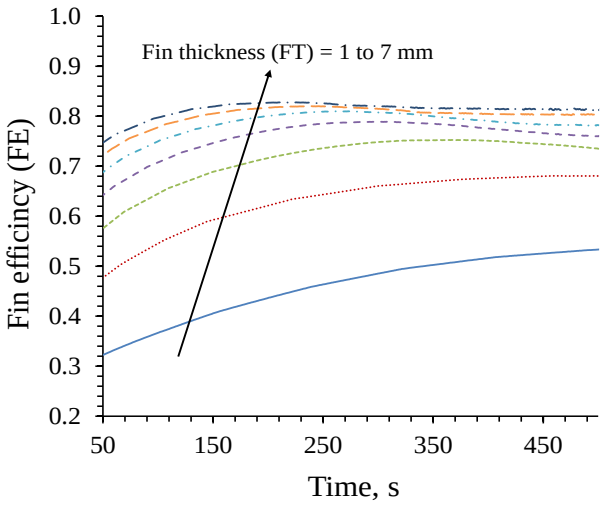

Fig. 6 Variation of fin efficiency (FE) with timefor different fin thicknesses (FT)

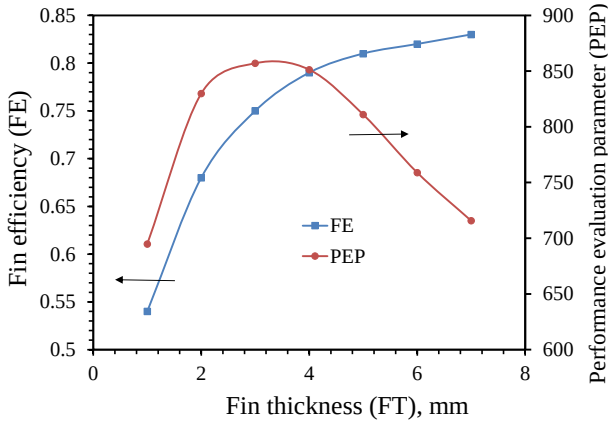

Fig. 7 Variation of FE and pep with FT

The higher value of PEP confirms the design optimality in heat transfer and H_2 quantity. The PEP value increases to 3 mm and decreases later (Fig. 7). Increasing FT reduces the H_2 absorption quantity and increases system weight, but the FE has a minimum effect after 3 mm. The optimum fin thickness of 3 mm is selected for further investigation.

C. *Fin shape optimization*

The fin shape changed from rectangular to three different (4 to 2, 5 to 1, and 6 to 0 mm) tapered cross-sections, maintaining its weight constant. The fin tapering enhances the heat transfer near the fin base due to the larger thickness. But more MH with smaller FT decreases heat transfer towards the fin tip. As a result, high-temperature regions exist surrounding the fin, as shown in Fig.8. Fin tapering has minimal effect on both FE and PEP, as noticed in Fig. 9. FE increased from 0.75 to 0.77 when the FT changed from a constant thickness to a tapering thickness of 4 to 2 and 5 to 1 mm. Similarly, PEP also improved from 0.86 to 0.88. The fin tapering from 6 to 0 mm has the same FE and PEP as the fin with no tapering. For long-term usage, small improvement gives a greater advantage in terms of cost and energy savings. So, the optimal fin configuration can be chosen as 4 to 2 mm or 5 to 1 mm, depending on the manufacturing flexibility.

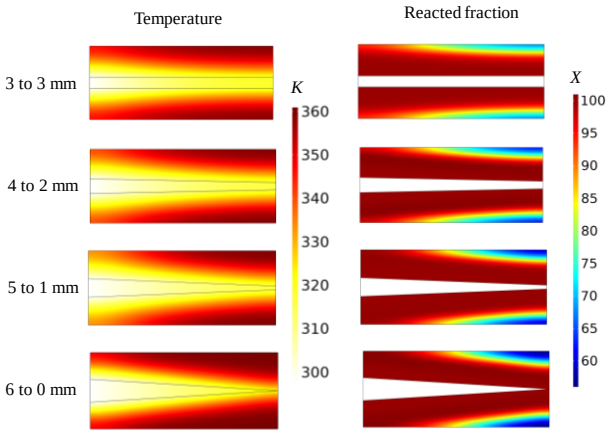

Fig. 8 Temperature and reacted fraction profile of different fin configurations at 300 s

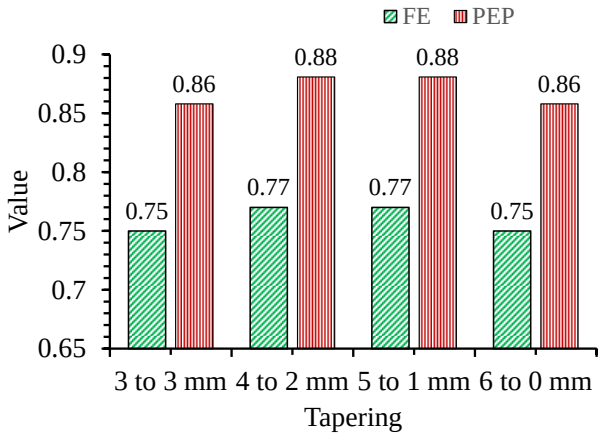

Fig. 9 Effect of fin configuration on FE and PEP

V. CONCLUSIONS

The present study proposes an FE technique to optimize the fin thickness and shape in an MH-based hydrogen storage reactor. The temporal temperature profiles of fin and MH obtained from simulation data are used for calculating FE. The following outcomes are drawn from the study.

- Increasing FT increases FE, but it has minimal effectafter a thickness of 3 mm.
- The FT of 3 mm is selected as optimum based on the PEP.
- Tapering of the fin has minimal effect on FE and PEP.

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