GEOMETRIC OPTIMIZATION OF THERMOCHEMICAL REACTOR FOR HEAT AND POWER APPLICATIONS

Summary

This work presents the design and evaluation of a thermochemical heat upgrade reactor using numerical simulations. The model was used to optimize reactor geometry and predict charging and discharging behavior. Key parameters included inlet-outlet port design, porous bed aspect ratio, empty zone aspect ratio, and discharge inclination angle. Performance indicators considered were conversion, reaction time, temperature profile, peak output temperature duration, pressure drop. The finding suggest Design-3 as the best inlet-outlet configuration for both modes. For dehydration, optimal values were a porous bed D/H of 1.16, empty zone D/H of 2.42, and 45° inclination. For hydration, a porous bed D/H of 0.48 for maximized peak temperature duration, while 1.16 reduced pressure drop. The empty zone aspect ratio of 8.89, and 15° inclination was found optimal. The optimized reactor will be fabricated by TMEC and tested at pilot scale by DLR.

Keywords: Calcium hydroxide, Thermochemical energy storage, Numerical simulation, Heat transfer

Field of application for the findings: Heat and Power Industry

Addressed audience: Academic Researcher and Industry Peoples working on Thermochemical Energy Storage

1. Introduction

Global energy consumption is steadily increasing and remains essential for national development. However, rising energy demand has intensified global warming, mainly due to the extensive use of fossil fuels, natural gas, and crude oil, which release harmful emissions [1]. These emissions raise global temperatures and lead to severe environmental impacts such as irregular rainfall, flooding, land subsidence, and other natural disasters. Although renewable energy sources such as solar, wind, biomass, geothermal, and nuclear have expanded significantly, complete dependence on them is still challenging because of intermittency, demand-supply mismatches, and seasonal variations. As a result, reliance on conventional fuels continues to remain high [2]. A viable solution to these challenges is energy storage. Among the available storage technologies, thermochemical energy storage (TCES) stands out as one of the most promising options. TCES offers several advantages, including high energy storage density, low cost, non-toxic operation, theoretical zero energy loss during storage, and excellent reusability over multiple cycles [3]. A thermochemical energy storage reactor system using the $Ca(OH)_2$/CaO thermochemical material (TCM) is illustrated in Figure 1. During the charging process, waste heat from industrial sources (shown by the blue line) and renewable energy from wind, concentrated solar power, or low-cost renewable electricity (shown by the green line) are supplied to a reactor filled with $Ca(OH)_2$. The material absorbs thermal energy and decomposes into CaO, releasing water vapor. The resulting CaO can then be stored for long durations with minimal energy loss. When energy is required, the system operates in the discharging mode. The heat transfer fluid (HTF) and CaO are preheated using low-grade industrial heat. Subsequently, a controlled amount of steam and HTF is supplied to the reactor filled with CaO. This initiates an exothermic hydration reaction, releasing heat and increasing the HTF temperature to a higher temperature (400-600°C) due to elevated steam pressure indicating upgradation The high-temperature HTF can then be utilized for various applications, such as district heating (after dilution and temperature reduction), power generation, and industrial process heat, as indicated by the red line in Figure 1. The reversible chemical reaction governing the storage and release of energy is given by [3]:

$$\mathrm{Ca(OH)_2} + \Delta H \rightleftharpoons \mathrm{CaO} + \mathrm{H_2O} \tag{1}$$

This study focuses on the $Ca(OH)_2$/CaO system. This TCM is selected due to its environmentally friendly nature, as steam is produced as a by-product, its suitable high-temperature operating range (400-600°C), low material cost (approximately 100 $/tonne), good cyclability, and its applicability for both heat and power generation systems [3–5]. Numerical modeling plays a crucial role in understanding the behaviour of such thermochemical systems, particularly in terms of fluid flow, heat transfer, chemical reactions, and mass transport phenomena. While experimental investigations are essential, combining them with numerical modeling provides the most effective approach for system development [6–8].

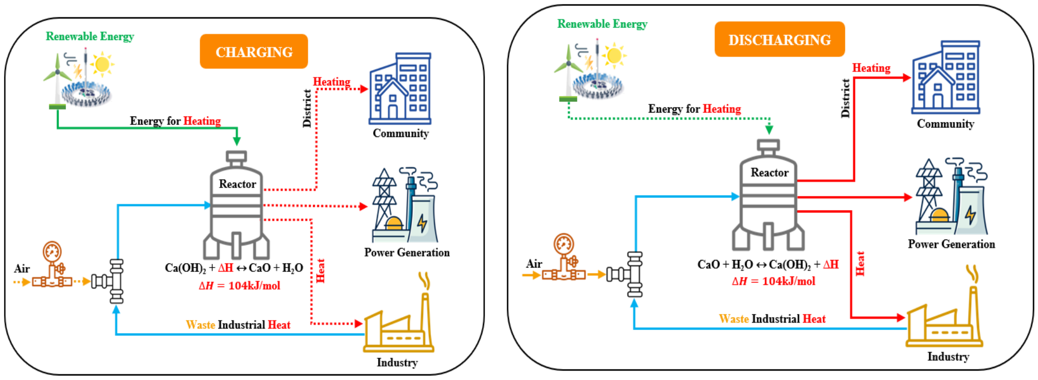

Fig. 1: Illustration of charging and discharging process in reactor for thermochemical energy storage with potential energy source and applications

2. Numerical Methodology

The proposed reactor is a silo-type, cylindrical, batch-wise moving bed, as illustrated in Figure 2 through isometric and sectional views. The thermochemical material is fed from the top through a removable loose and blind flange arrangement. This is used to make reactor sealed tight during the course of reaction, also it is used for maintenance and to feed the material. The bottom section is equipped with a rotary valve, which remains closed during the reaction and is opened only during material discharge. The HTF and steam are introduced from the bottom through two separate inlets. Numerical modeling of the complete three-dimensional reactor would be computationally expensive and time-consuming. Since the reactor is geometrically symmetric, a two-dimensional (2D) simulation is therefore performed. The computational geometry used in the study is shown in Figure 2, along with the corresponding dimensions and boundary conditions. The outer boundary is treated as a no-slip wall for fluid flow and is assumed to be thermally insulated. The green region represents the porous bed, while the blue region denotes the fluid (gas) zone. The interface between the fluid and porous zones is modeled as a wall everywhere except at the porous interface (open boundary), through which the fluid enters the porous bed.

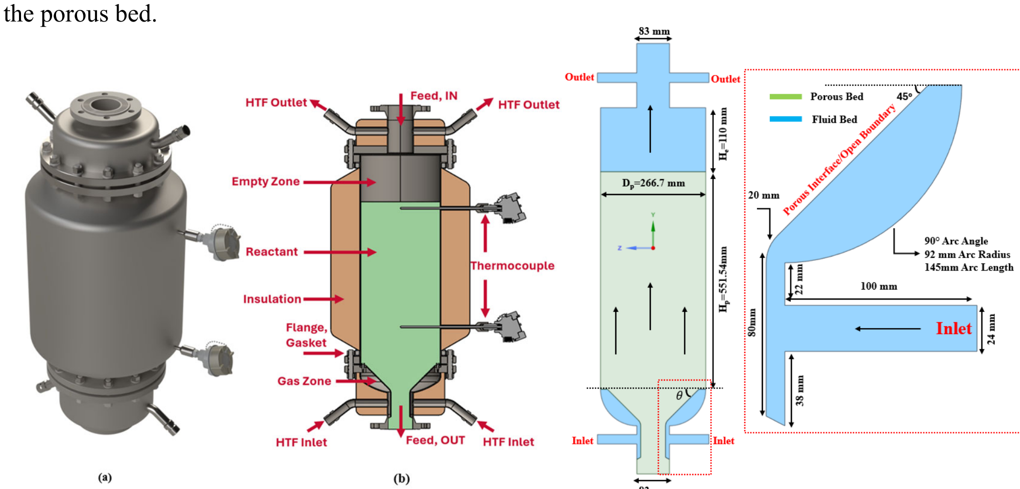

Fig. 2: Left (a) Isometric view of the proposed reactor; (b) Sectional view of the reactor with nomenclature; Right: Computational geometry used in the simulation with dimensions and boundary condition

3. Results and Discussions

The model was employed to optimize the reactor geometry and evaluate its performance during both charging (dehydration) and discharging (hydration) modes. The key geometric parameters studied included the inlet-outlet port configuration, the porous bed aspect ratio, the empty zone aspect ratio, and the inclination angle for material discharge. Performance metrics considered during the optimization included the extent of conversion, reaction time, temperature distribution, peak output temperature and its duration, and pressure drop. The results indicate that Design-3 provides the most effective inlet outlet configuration for both dehydration and hydration operations. For dehydration, the optimal parameters were a porous bed aspect ratio (D/H) of 1.16, an empty zone aspect ratio of 2.42, and a discharge inclination angle of 45°, which collectively ensured high conversion and efficient heat transfer. During hydration, a porous bed aspect ratio of 0.48 maximized the duration of the peak output temperature, while a ratio of 1.16 minimized pressure drop. The empty zone aspect ratio of 8.89 and a 15° inclination were found to provide optimal thermal performance. The optimized reactor design will be fabricated by TMEC considering manufacturing constraints and delivered to DLR for pilot-scale testing. Post-experimental validation will further refine the design and confirm the simulation predictions, providing a robust framework for efficient thermochemical heat storage applications.

4. References

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