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Numerical Analysis and Validation of a Novel Thermochemical Heat Transformer System

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Extended Abstract

The transition toward renewable energy necessitates cost-effective and scalable solutions capable of overcoming the inherent limitations of intermittent sources like solar thermal energy. Low-concentrated solar collectors are attractive options; however, their low output temperature restricts their widespread applicability. To address this challenge, this work proposes and evaluates a novel packed-bed thermochemical heat transformer (TCHT), operating in a closed-loop configuration with $SrBr_2/SrBr_2 \cdot H_2O$ as the reactive material. The system is designed to boost low-grade thermal energy to industrially relevant higher temperature levels without relying on electricity input, while simultaneously offering thermal energy storage.

In this study an innovative reactor was designed, fabricated and tested. Also a numerical simulation-based performance assessment was applied on the proposed reactor. In this regard, a 3D transient simulation framework replicates the actual geometry and operational conditions of the lab-scale prototype. The numerical model, incorporates detailed transport phenomena along with reaction kinetics, predicts the behaviour of discharging (hydration) and charging (dehydration) cycles. The main objective is to introduce a novel scalable TCHT to upgrade low-grade heat. The model is validated through comparison with data obtained in experimental analysis. The modular configuration allows for easy upscaling, and the configuration eliminates the need for external vapor compression, improving both efficiency and sustainability.

The main components of the system consists of a thermochemical reactor, an evaporator/condenser unit, a pump, and valves. The core process occurs within the thermochemical reactor, which is designed as an indirect heat exchanger. The system utilize the reversible hydration and dehydration of strontium bromide ($SrBr_2$) which is selected due to its favourable characteristics, like non-toxicity, reversibility, cyclability, and good reaction kinetics [1]. The reactive gas which proceed the reaction between monohydrate and anhydrous salt is water vapor. At the heart of the reactor lies the thermochemical material which either releases heat during the hydration phase (when water vapor is absorbed) or absorbs heat during dehydration (when the vapor is removed), depending on the operation mode. During periods of heat demand, pressurized water vapor is generated via the evaporator and injected into the reactor bed, initiating an exothermic hydration reaction that delivers high-temperature heat to the working fluid. Conversely, when solar thermal input exceeds demand, the system switches to charging mode; thus, heat from the solar collectors drives the endothermic dehydration reaction, causing the reactive material to release water vapor. The vapor is then condensed in a low-pressure condenser and the system stores the input thermal energy for later use.

The extent to which the salt temperature can be increased depends on the partial pressure of water vapor, theoretically described by the Van't Hoff equation and updated for $SrBr_2$ by recent experimental findings [2]. The modelling results indicate that despite factors such as non-uniform hydration levels, agglomeration over cycles, and potential thermal contact resistance between reactive material and adjacent heat exchanger surfaces, the numerical model demonstrates good fits with experimental data. The salt hydrate nearly fully converts and the predicted salt temperatures remain closely aligned with the theoretical thermodynamic limits. The model also proves the system's potential to achieve a temperature upgrade of up to 100 °C between charging and discharging operations, highlighting areas for future refinement and optimization.

References

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