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Thermochemical Heat Storage: heat and mass transfer modelling in the reactor

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Abstract The global increase in demand for raw materials and energy is a source of geopolitical concerns and tensions, and this is leading governments and industries to secure their resources and supplies. This observation leads companies and also countries to secure operational supply by improving system performances and reducing needs. In this context, heat storage is solution for energy management improvement since it makes it possible to use waste heat or solar sources for different thermal applications. Thermochemical heat storage (THS) using water adsorption/desorption in porous materials is particularly suitable. Indeed, it allows heat to be stored at room temperature by separating water from the adsorbent material. To restore heat, the material needs to be re-moisten and this can be done with air humidity (energy-carrier). These materials are shaped and thermally characterized. Especially, an improvement in storage capacity and the heat and mass transfers in the reactor are required and while guaranteeing structural stability for better cyclability. They are tested under different operational conditions in a laboratory reactor. The reactor performances were simulated by using numerical modelling of heat and mass transfer in the experimental device. After experimental validation, the numerical model can be used to simulate different operational scenarios.

Keywords: Thermochemical heat storage, numerical modelling, experimental validation, heat and mass transfer

1. Introduction

The thermochemical heat storage is an attractive solution for heat management and for improving system performances. Especially, water adsorption / desorption in an adsorbent is interesting because it is non-toxic and environmental-friendly. It allows to store heat at room temperature without loss and restores heat after rehydration of the material. For this, indoor air coming from controlled mechanical ventilation (warm humid air) can be used as water carrier for domestic heat purpose. The mass flow of water allows to drive the heat flow restored, the duration of the operation and the temperature level.

A numerical modelling was developed to simulate the reactor behaviour. It solves heat and mass balances, continuity and momentum differential equations in the material and air. The thermal properties of the material (heat of sorption, material density, specific heat capacity, effective thermal conductivity) are included in the calculation as a function of water uptake and temperature.

2. Materials and methods

2.1. Materials

The materials used in this study are porous and highly hygroscopic (zeolites, hydrated salts, etc.). They are shaped and thermally characterized. Especially, an improvement in storage capacity (enthalpy of adsorption) and the heat and mass transfers within the material are required and more generally in a material bed while guaranteeing structural stability for better cyclability.

2.2. Thermo-physical properties

These properties estimations are technically challenging due to the specific nature of the material (hygroscopic and reactive) [E. Sciuller (2022)]. This makes it very difficult to obtain the specific heat capacity and the thermal conductivity owing to the estimation techniques that still requires a temperature rise or gradient in the material. These changes of temperature modify the equilibrium between water in material and the outside environment. Consequently, the material exchanges heat with the outside environment. In this context, a new methodology [E. Sciuller (2023)] (figure 1) for investigating the specific heat capacity of reactive and hygroscopic material was developed based on corrective calculations of calorimetry results. First, the reaction heat is obtained from TG-DSC experiments performed at different temperature. This enthalpy is used to adjust the Cp estimations by correcting heat balance due to the mass variation of the sample.

3. Results

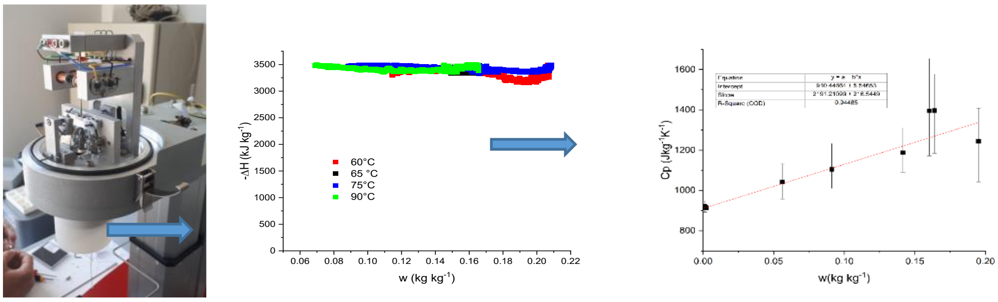

Figure 1. a) TG-DSC apparatus b) heat of sorption c) specific heat capacity of hydrated material

The simulated reactor is cylindrical requiring a 2D-unsteady modelling. A water pipe is in the centre of the reactor and it aims to exchange heat (co and counter-current flow operating). Figure 2 (left) shows a scheme of the reactor used.

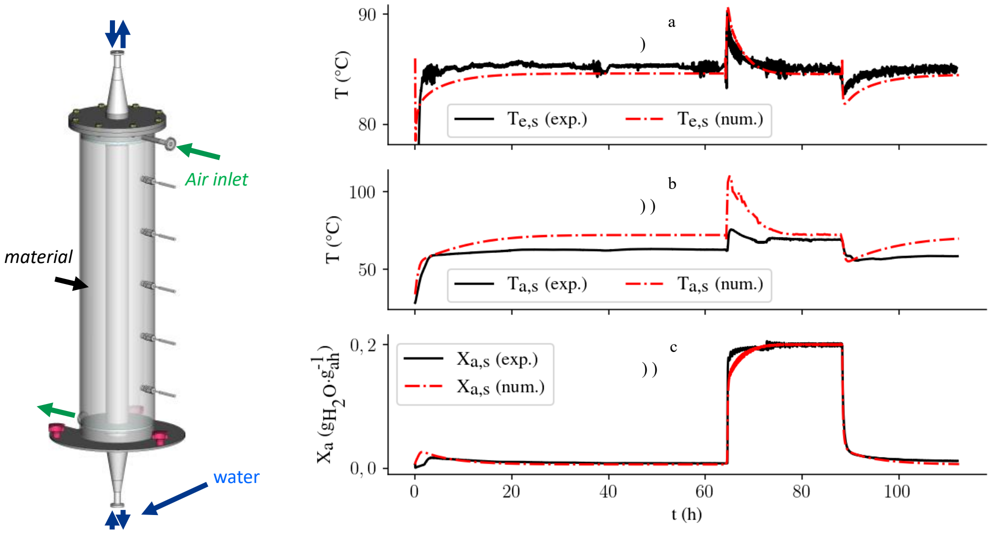

Figure 2. Experimental set-up (left) and Model validation: Experimental and simulated outlet temperatures in water (a), air (b) and outlet air moisture (c) as a function of time.

Figure 2 (right) shows outlet air and water temperatures during the test. These results show a good agreement between experimental and simulated results. The reactor performances were simulated by using numerical modelling of heat and mass transfer in the experimental device. After experimental validation, the numerical model can be used to simulate different operational scenarios (use of different heat sources, for different applications, temperature up-grade, …).

4. Conclusion

Thermo-physical properties of THS materials were investigated using new methodology specifically dedicated to obtain properties of hygroscopic and reactive materials. The numerical modelling included these properties and is validated by experimental results. This numerical tool can be used for simulating different operations. Especially, it can be used to search the best possible compromise between material properties and operating conditions for the application intended.

References

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