Numerical modelling of Thermochemical heat storage: modelling, model validation and simulations

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The global increase in demand for raw materials and energy is currently 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 the defense sector 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 thermal applications in isolated sites, for energy transport and in mobile equipment. Thermochemical heat storage using water adsorption/desorption in materials is particularly suitable for these needs [1]. Indeed, it allows thermal energy to be stored at room temperature by separating water from the adsorbent material. To restore heat, the material need to be re-moisten and this can be done with air humidity, which can be used as an energy-carrier. Several studies aim to develop new storage materials with specific performances adapted to the targeted applications. To do this, new generations of materials (zeolites, hydrated salts impregnated on porous materials, etc.) are developed, shaped and texturally, structurally and thermally characterized.

But the major challenges are to improve heat storage capacity (enthalpy of sorption), the heat and mass transfers within the material and more generally in a material bed while guaranteeing structural stability for better cyclability. Indeed, a good mass transfer allows the material rehydration to be control and consequently the heat power supplied. Moreover, a significant effective thermal conductivity (good heat transfer) reduces the risk of hot spots and the material stability while enabling to work over a wider range of temperatures.

The major problem is to reconcile these four targeted properties to obtain the best compromise for the chosen application. One solution is to develop a numerical tool, which can simulate a large number of configurations.

For this, a numerical tool was developed. It solves 2-Dimensional and unsteady continuity, momentum, mass (water and air) and energy balance differential equations taking into account the heat released by the material during hydration step. The program was written in Fortran 90. The reactor is cylindrical with an internal coaxial exchanger (water flow), which can be operate in co or counter current. This technology provides both hot air and water for different applications [2]. This calculation program was validated by comparison of simulated results with experiments conducted on a lab-scale facility presented in figure 1.

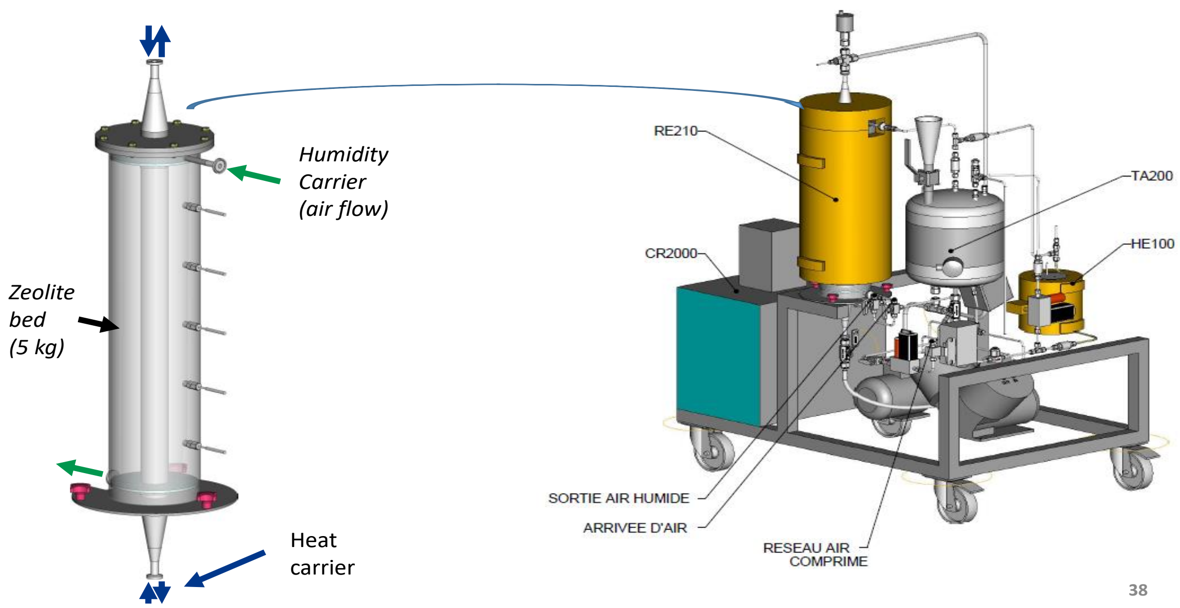

Figure 1: lab-scale facility and experimental reactor

After model validation, the program can be used to simulate different operating configurations. Especially, for each application or configuration, the thermal and transport properties of the material can be adjusted to obtain the best performances and consequently compromise between properties. For example, the figure 2 shows temperature profiles in the reactor several minutes after humid air injection. In this simulated case, the preference was given to a good mass transfer and an important enthalpy of sorption (case of zeolite for example). Consequently, the maximal temperature in the material do not exceed 150°C and provides hot air (> 100°C) during about 2 hours and 30 minutes. Against, the low thermal conductivity means that heat cannot be transferred efficiently to the central flow.

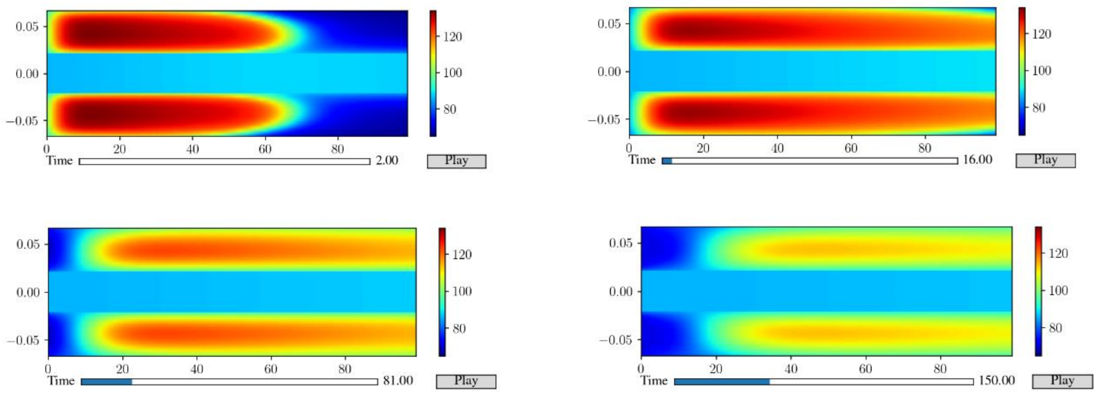

Figure 2: temperature profiles after 2, 16, 81 and 150 minutes in the reactor. Simulations of material hydration in the lab-scale reactor.

[1] S. Bennici et al., Heat storage: Hydration investigation of $MgSO_4$/active carbon composites, from material development to domestic applications scenarios, Renewable and Sustainable Energy Reviews, 2022

[2] E. Sciuller et al., Towards industrial-scale adsorptive heat storage systems: From state-of-the-art selected examples to preliminary conception guidelines, Journal of Energy Storage, 2022