

## ABSTRACT

The aim of this doctoral dissertation was to develop and validate a simplified method for numerical modeling of thermochemical processes occurring in large-scale sorption heat storage systems. The proposed approach uses a modeling analogy of a porous heat storage bed, similar to that used for phase change materials. Consequently, instead of analyzing individual grains within the porous medium, it is modeled as a single, uniform element. This allows for bypassing the modeling of the chemical reaction, and the heat of adsorption is determined using the Interpolated Effective Heat Capacity method. A key assumption of this method is to adjust the material's heat capacity ( $C_p$ ) as a function of temperature ( $T$ ) to reproduce data obtained from Differential Scanning Calorimetry (DSC) measurements. The proposed method allows to simulate the temperature and pressure distribution within the analyzed heat storage volume. In the case of a sorption storage system, also considering mass transfer, it is possible to determine the adsorbate concentration in the sorption material.

To verify the accuracy of the calculations performed using the developed method in a model describing the adsorption process in a small zeolite bed section, a comparison of the investigated parameters resulting from the simplified and detailed models was conducted. The analysis was performed for two different bed volumes. The accuracy of calculations for full-scale heat storage models—phase change and sorption—was also verified. The verification was based on results obtained from laboratory measurement conducted on phase change and sorption heat storage units.

The obtained results confirm the hypothesis that the analogy between the thermophysical properties of a sorption material and the thermophysical properties of a phase change material can be effectively used to model the heat capacity of the heat storage material. Moreover, calculations performed using the developed method allowed to obtain temperature distribution, heat transfer fluid flow rate, and adsorbate mass distribution consistent with results obtained using the detailed method. In contrast to the detailed method, the new method enables modeling of full-scale heat storage operation. The deviation of the temperature distribution in the heat storage, obtained from simulations using the developed method, compared to measurements in the laboratory heat storage, was less than 15%. The simplified method proposed in this work exhibits significant research and application potential.

*Bożena Pyklat*