# CFD Modeling of a Laboratory-Scale Setup for Thermochemical Materials Performance Analysis

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## Abstract

The search for energy saving is nowadays mandatory because of the constant growth of CO2 emissions caused by an inefficient energy management. Thermal Energy Storage (TES) has an important role in designing of energy efficient systems, including solar energy storage (daily or seasonal) and waste heat from industrial batch processes. Different solutions are possible for thermal storage, based on sensible heat (e.g. water tanks), latent heat (phase change materials) or reaction enthalpy (thermochemical systems). In Thermochemical TES, a material is chosen so that it shows a high-enthalpy reversible chemical reaction at a desired temperature. In particular, water sorption in some inorganic salt hydrates is pointed out as one of the most suitable reactions for low temperature energy storage (60-120 °C). The reaction products, water and salt in a less hydrated form, are kept separated and consequently the heat is stored. Energy release is obtained with salt hydration. The main advantages are an energy storage capacity higher than other TES technologies and the possibility to control the energy release. On the other hand, one of the main issues is the difficulty to test materials performance, because standard characterization techniques use small amount of samples and their properties change dramatically when the system is scaled up to large reactors.

The aim of this work is to realize a laboratory scale setup to test the performance of salt hydrate composites. A scheme of the system is reported in the attached figure (above). The active material is kept in an evaporator at a temperature sufficient to generate the dehydration reaction. Extracted water mass is measured in time in a condenser at 0°C. Air flow, temperature and humidity are measured with sensors in the system.

The system was simulated using COMSOL Multiphysics® software. In particular the simulation was inspired by two models from the Application Library, Degradation of DNA in Plasma and Protein Adsorption. At first, a zero dimensional component was created with the Reaction Engineering interface with two reactions to evaluate both the dehydration and condensation steps:

H2Ocry->H2Ovap H2Ovap->H2Oliq

Where H2Ocry is the crystallization water in the salt hydrate, H2Ovap is the air humidity

and H2Oliq is the condensed water. Using a Parameter Estimation node, experimental data about dehydration were imported in the software and used to estimate the reactions kinetics constants. After that, using a Generate Space Dependent Model functionality we obtained a 3D component with a realistic system geometry (see attached figure below) including the interfaces Chemistry, Transport of Diluted Species, Surface Reactions, Heat Transfer in Fluids and Laminar Flow. Rate constants calculated in the zero-dimension model were used as first guess for the 3D model reactions. We verified that the model is able to evaluate temperature, flow and water concentration as well as the evolution of the two reactions in time.
We expect that this model will allow us to classify different Thermochemical TES materials about their efficiency in heat and mass exchange, as well as to refine the design of the thermal storage system.

## Figures used in the abstract

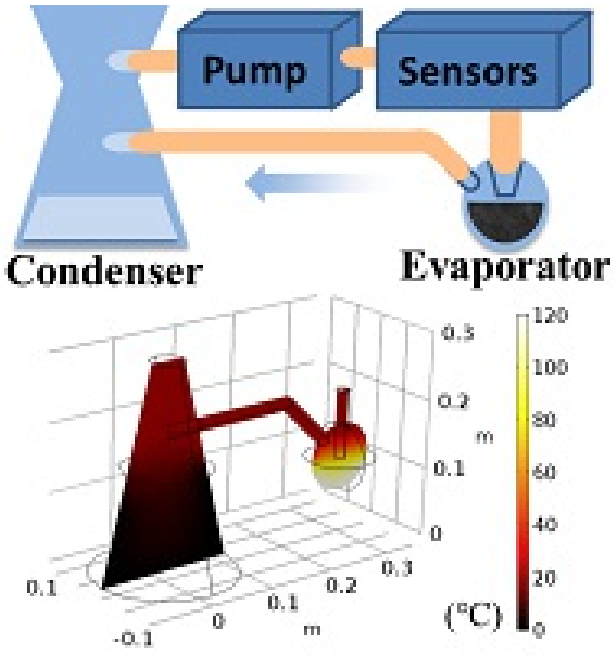


**Figure 1**: A general scheme of the system (above). Temperature profile of the simulation obtained with COMSOL Multiphysics® software (below).