THERMOCHEMICAL ENERGY STORAGE FOR PROCESS WASTE HEAT: SIMULATION AND MODEL VALIDATION

M. Molenda, M. Bouché, H. Jockenhöfer, M. Linder, A. Wörner

Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR)
German Aerospace Center
Institute of Technical Thermodynamics | Pfaffenwaldring 38-40 | 70569 Stuttgart | Germany
Telephone +49 711 6862-713 | margarethe.molenda@dlr.de

Thermochemical energy storage is based on the application of reversible chemical reactions for storage of thermal energy. Gas-solid reactions are well suited due to easily separable products and high reaction enthalpies resulting in high storage densities. In addition, heat transformation processes can be realized with this energy storage technology. The reaction temperature can be adjusted by variation of the partial pressure of the gaseous component resulting in discharging temperatures being higher than charging temperatures of the storage. Therefore this technology is interesting especially for the utilization of process waste heat. To realize technical application simulation tools for development of reactor concepts have to be evolved and validated by experimental results.
Since various gas-solid reactions are known, the reaction system can in principle be adapted to the respective industrial process. However, reaction kinetics as well as cycling stability of the system can hinder technical application. In the range of 80 to 200°C, which is relevant for process waste heat, full conversion and full reversibility with reasonable kinetics has been demonstrated [1] for the reaction:

$$CaCl_2 \cdot 2\ H_2O_{\ (s)} \rightleftharpoons CaCl_{2\ (s)} + 2\ H_2O_{\ (g)}$$

The endothermic dehydration of calcium chloride dihydrate is used for charging the thermal storage leading to separation of the products water vapour and calcium chloride. During discharge of the storage heat is released by recombining these products. Both reactions (hydration and dehydration) take place with intermediate products.
The reaction system $CaCl_2/H_2O$ has been tested in a reaction bed in laboratory scale using a closed system with indirect heat transfer (Fig. 1). A tube bundle heat exchanger has been used as reactor. The reaction bed was located inside the tubes (Fig. 2). The temperature in the reaction bed was measured at different positions. A 2D reaction model of a reaction tube was set up and solved by the Finite Element Method in COMSOL Multiphysics® (Fig. 3). Thermodynamic equilibrium and reaction kinetics of products, educts and all intermediate steps were measured by means of simultaneous thermal analysis and implemented in the model. Material properties such as thermal conductivity and permeability of the bed were determined experimentally and included in the mass and heat balances.

The presentation will outline the results of the simulation and their validation with the experiments. Special attention will be given to possible heat and mass transfer limitations depending on the reactor geometry. For dehydration in a reaction bed with small particles mass transport limitations dominate whereas hydration seems to be limited by heat transfer processes.

Intended form of presentation: oral presentation

[1] Molenda, Bouché, Linder, Wärmespeicherung und -transformation mittels Gas-Feststoffreaktionen, Jahrestreffen der Fachgruppen Energieverfahrenstechnik & Hochtemperaturtechnik, DECHEMA, Frankfurt, March 2012

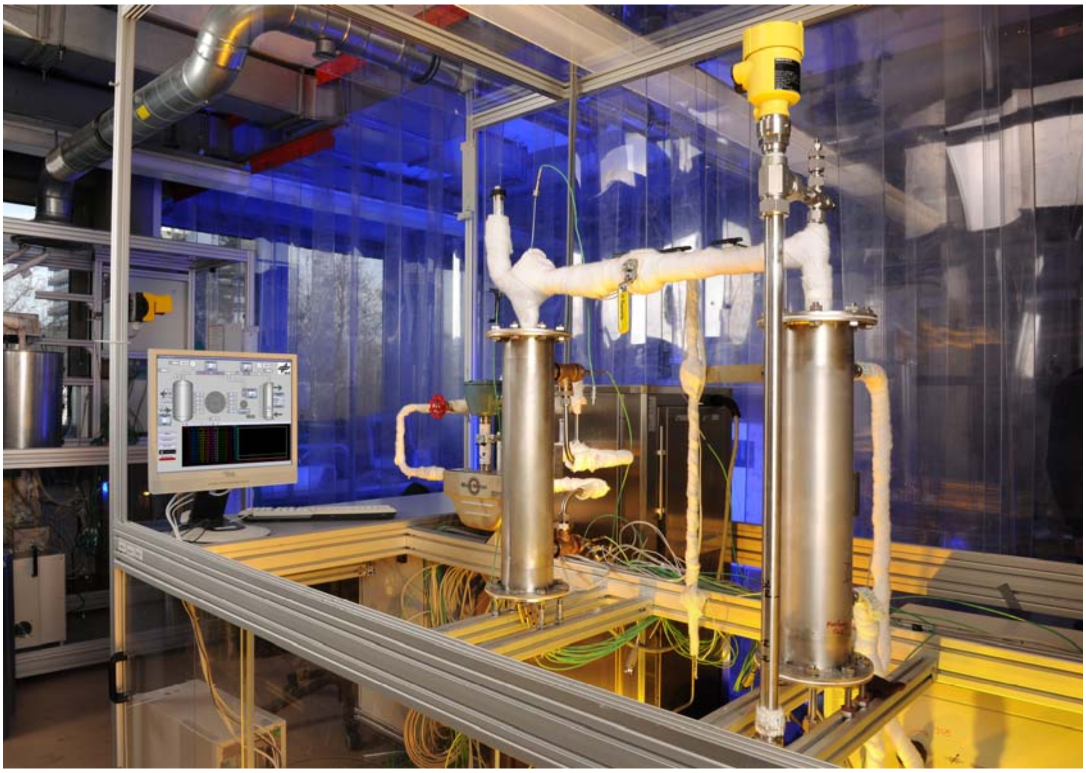

Fig. 1: Experimental setup:
Left heat exchanger: reactor; Right heat exchanger: condenser/evaporator

Fig. 2: Reactor:
Reaction bed inside the tubes

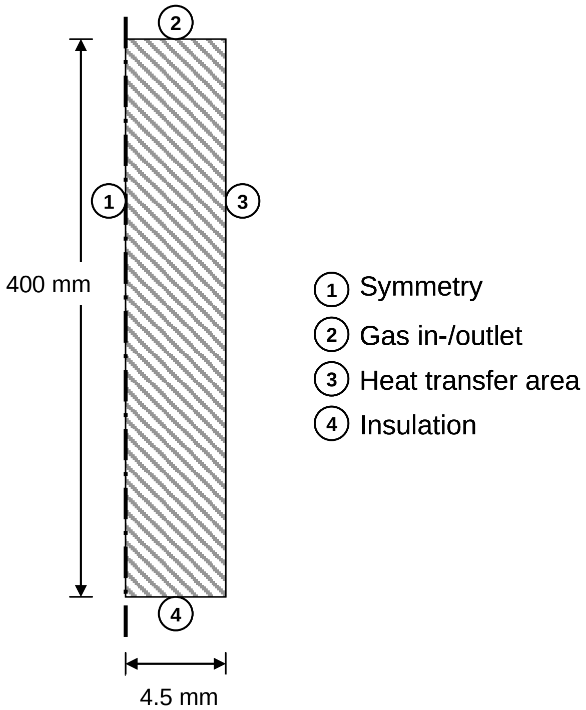

Fig. 3: Model geometry (rotationally symmetric)
of one reactor tube