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Modeling of Powder Bed Dynamics in Thermochemical Heat Storage

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Storing energy in the form of heat has been under long-standing investigation for prospective applications, such as the capturing of excess heat from industrial processes as well as storing energy in concentrated solar power plants. Investigated mechanisms for the heat storage include the adsorption in porous media, materials undergoing phase changes and thermochemical reactions. Among these, thermochemical heat storage provides a large energy capacity and next to perfect reversibility. More specifically, storage in the CaO/Ca(OH)2-System is investigated because of the low price and environmental friendliness of the reactants.
In the project THEMSE, DLR is developing models and simulations as well as experimental characterization methods for thermochemical heat storage in the CaO/Ca(OH)2-System. In this talk, we shall give an overview over the project with a focus on the modeling activities.
Special attention is given to the investigation of how the cycling of the material influences the heat and mass transport in the powder bed inside the reactor. This happens through mechanical and physical alteration of the powder bed, mainly through three mechanisms. First, the gas flow through the reactor exerts a force on the powder particles, compacting the powder bed. The resulting densification of the bed increases its flow resistance, while improving the heat transport. Second, the agglomeration of powder particles, where bonds between the particles form, turning the bed into a solid. The exact mechanism of the agglomeration is yet unknown, but it can be characterized by mechanical measurements. Third, the expansion of the powder particles through water uptake during the hydration stage, and the corresponding contraction during dehydration.
To model the compaction and solidification of the powder bed during cycling, we present a mechanical model based on Drucker-Prager-Cap plasticity, which has been used previously for powder compaction, see e.g. [1]. The parameterization of the model, i.e., the plastic yield surface, is done via flow tester experiments. The changes in the powder bed during cycling are modeled by hardening mechanisms, i.e., a changing yield surface, corresponding to powder compaction and agglomeration, respectively.
Then, the plastic model is coupled to a reactor scale model, simulating the heat and mass transport, as well as the thermochemical reaction using a model, similar to [2]. This enables the study of the powder bed dynamics under different boundary conditions during cycling, such as pressure drop, water vapor fraction and reactor geometry.
Finally, an outlook will be given on the multi-scale modeling of the reactor. The geometrical micro-scale characterization of the material is done using micro computed tomography (µCT). From the µCT-Images, effective transport parameters, such as diffusivity and permeability are computed for different stages of agglomeration. These are then used in the reactor-scale model to produce predictions, which can be verified on the reactor-scale.

References

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[2] Nagel, Thomas & Shao, Haibing & Singh, Ashok & Watanabe, Norihiro & Roßkopf, Christian & Linder, Marc & Wörner, A & Kolditz, Olaf. (2013). Non-equilibrium thermochemical heat storage in porous media:

Part 1 – Conceptual model. Energy. -. 10.1016/j.energy.2013.06.025.

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