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Simulation of Thermochemical Heat Storage in the CaO/Ca(OH)2-System on the Micro-Scale

Tuesday, 1 June 2021 11:45 (15 minutes)

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 for thermochemical heat storage in the CaO/Ca(OH)2-System on the microscopic level. In this talk, we shall give an overview over the project and the materials involved.

The geometrical micro-scale characterization of the material is done using a combination of micro computed tomography (µCT) and scanning electron microscopy (SEM). Both methods are complementary in the sense that SEM can be used to resolve fine scale details, up to crystallites, while µCT can resolve powder particles as well as agglomerates of numerous single particles. This is complemented by kinetics measured by thermogravimetric analysis (TGA).

The first goal in the project is to explain the measured kinetics using a spatially resolved model, which takes the three-dimensional morphology of the storage material into account. In general, this involves, thermal, hydrodynamic, mechanical, and chemical modeling. However, the first investigations involve a single crystallite model, where the thermal and hydrodynamic effects can be neglected, and which is solved using finite element simulations. Further models are developed to investigate the heat and mass transport in the powder bed inside the reactor. Heat transport being the limiting factor, modeling the thermal conductivity of the powder bed on the microscale, is given special attention. This is done, the using simulations based on µCT-Data. Finally, it is investigated how the cycling of the material influences the heat and mass transport in the powder bed inside the reactor. This happens through agglomeration of powder particles the cause of which, and the modeling of which, are under investigation and under development, respectively.

We will show results from experiments and from kinetic and micro-scale transport simulations. Finally, an outlook will be given on the upscaling of the micro scale model to the reactor-scale and computational optimization methods for reactor design.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

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