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Modeling Structural Changes in a Fixed Bed Reactor for Thermochemical Heat Storage During Continuous Cycling

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As countries around the world are trying to transition away from fossil fuels to renewable energy sources, short- and long-term storage of an increasing, yet unsteady, renewable energy supply becomes a major challenge. Further, as provision of heat is a major part of industrialized countries'energy needs, storing heat energy, in applications such as the capturing of excess heat from industrial processes or concentrated solar power plants, has the potential for great increase in energy efficiency.
Among the available heat storage technologies, thermochemical heat storage provides a large energy capacity for short- and long-term storage. To further develop the technology, DLR is developing models and simulations as well as experimental characterization methods for thermochemical heat storage. More specifically, storage in the CaO/Ca(OH)2-System is investigated because of the low price and environmental friendliness of the reactants.
However, a major challenge to modelling such systems, is the restructuring of the powder bed during repeated cycling, i.e., repeated charging and discharging of the reactor. This happens through mechanical and chemical alteration of the powder bed. The three dominant effects are, the compaction of the bed from the gas flow, the expansion/shrinkage of the powder particles through water uptake/release and the agglomeration of powder particles, where bonds between the particles form, solidifying the bed.
To model the compaction and solidification of the powder bed during cycling, we present an elasto-plastic mechanical model based on the Drucker-Prager-Cap yield surface, which has been used previously for powder compaction, see e.g. [1]. 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. While the exact mechanism of the agglomeration is yet unknown, it can be characterized by mechanical measurements.
Then, the plastic model is coupled to a reactor 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.
In this contribution, we will present a parameterization of the model based on experimental data, that was obtained from a test reactor, and the parameterization of the mechanical model, i.e. the plastic yield surface, is done via flow tester experiments.
Then, we will show simulation results with an emphasis on investigating the irreversible effects of continuous cycling on the powder bed. This includes the compaction of the powder bed during the pressurization of the reactor, the possible emergence of hysteresis effects in the deformation of the powder bed under repeated cycling, as well as degradation through irreversible structural changes, such as powder agglomeration.

Participation

In-Person

References

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